Modeling Electromagnetic Wave Propagation in Electrically Large Structures

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MODELING ELECTROMAGNETIC WAVE PROPAGATION IN
ELECTRICALLY LARGE STRUCTURES

by

Jon W. Wallace

A dissertation submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

Department of Electrical and Computer Engineering
Brigham Young University
April 2002
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ABSTRACT

MODELING ELECTROMAGNETIC WAVE PROPAGATION IN ELECTRICALLY LARGE STRUCTURES

Jon W. Wallace
Electrical and Computer Engineering
Doctor of Philosophy

Existing unified numerical electromagnetic methods are often unable to analyze electrically large structures due to the amount of memory and processing power required, necessitating approximate analyses with limited applicability. In this research a hybrid modeling methodology is adopted to solve these complex problems more efficiently than unified numerical methods and more accurately than analytical methods. Electromagnetic modeling problems are divided into two or more levels of scale. Each level analyzes a specific level of detail and only promotes the required information to the next level. The method is demonstrated by successful application to three important problems: (1) remote sensing of snow, (2) modeling an optical Bragg resonator, and (3) modeling the MIMO wireless channel. First, complex snow media is analyzed with a hybrid FDTD/radiative transfer model. FDTD is used to compute phase matrices and extinction coefficients required for radiative transfer. Comparison with exact analytical methods proves the validity of the FDTD method for modest domain sizes ($[5\lambda]^3$) and number of Monte Carlo realizations (32). The method is used to illustrate a penetrating sphere model, which is not possible with
existing analysis techniques. Backscatter from the resulting model is about 3 times higher than that of existing dense-medium theories, underlying the importance of exact characterization of the media. Second, a hybrid FD/FDTD/S-parameter analysis is developed to model a large ($10^4$ section) optical Bragg resonator: a simple FD method computes propagation constants and field profiles, FDTD analysis provides reflection and transmission coefficients for the single section, and S-parameter analysis combines the sections to obtain the complete device response. A detailed study on error suggests that the method provides better than 2% accuracy in reflection and transmission response. Third, a hybrid electromagnetic/SVA model is developed to study the indoor MIMO wireless channel. A MIMO measurement platform is discussed for simultaneous probing of up to 16 transmit and receive antennas, which was required to assess the validity of later modeling. FDTD or MOM antenna analysis coupled with the SVA model gives capacity predictions which match measured data. The model is used to explore the impact of antenna spacing, directivity, and polarization on channel capacity. Closely spaced antennas lead to an approximate halving of receive power. Directivity effectively doubles receive power for aligned transmit and receive. Dual polarization increases system capacity anywhere from 10% to 70%, depending on the spacing of elements and the amount of multipath richness. This analysis of MIMO systems underlines the need for models that describe both multipath richness and average receive power.
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Chapter 1

Introduction

Electromagnetic modeling is an active area of research that pursues the development of accurate mathematical descriptions of electromagnetic fields in physical structures. Such models must be sufficiently detailed for high accuracy, but not so detailed as to preclude a numerical solution on real-world computers. Today, electromagnetic modeling finds broad application in many fields of science and engineering as depicted in Figure 1.1.

![Figure 1.1: The broad application of electromagnetic modeling](image)

Microwave remote sensing (see Figure 1.2) requires models that link microwave instrument data to geophysical quantities, such as snow accumulation, vegetation type, and sea ice concentration. Empirical models are possible if sufficient
Figure 1.2: In remote sensing, electromagnetic models are required to estimate geophysical parameters from active and passive microwave data.

Figure 1.3: Schematic representation of microwave/optical device development cycle. Time-to-market may be reduced significantly by accurate electromagnetic modeling tools.

microwave data and corresponding ground truth exist. However, as the number of physical scenarios and parameters grow, the required volume of data becomes prohibitive. On the other hand, if the basic structure of the snow, vegetation, or ice is understood, electromagnetic modeling may find a precise relationship between the microwave data and model parameters.

Figure 1.3 depicts the application of electromagnetic modeling to microwave and optical device fabrication. Initially, microwave and optical devices were developed with minimal electromagnetic modeling, requiring many design, prototype, and
Figure 1.4: Accurate electromagnetic channel models can assess the realistic capacity limits of wireless channels as well as the performance of existing coding algorithms.

test phases. In today’s highly competitive markets, shorter and shorter product development cycles are required. Accurate electromagnetic modeling of devices reduces the number of prototype stages and may eliminate faulty designs at the outset. Also, tradeoffs of various designs may be gauged in the design stage, rather than after costly prototyping and testing.

Today’s world is highly saturated with wireless devices such as cell phones, pagers, and broadband networking hardware, as depicted in Figure 1.4. In the development of wireless systems, not only is device characterization important, but also an understanding of the environment through which information-carrying electromagnetic signals propagate. Electromagnetic modeling of indoor and outdoor environments allows the system-level designer to assess the impact of temporal and spatial coding algorithms and antenna design on system performance, without the need of costly prototype development and deployment.

1.1 Problem: Limitations of Conventional Modeling

Electromagnetic modeling techniques fall into two basic categories: analytical and numerical. Analytical methods begin with the appropriate governing equations, such as Maxwell’s equations, and employ mathematical manipulations to
obtain quantities of interest. Some very simple structures may be analyzed this way in closed form, yielding concise and exact mathematical models. For more complicated structures, analytical methods require simplifying assumptions that limit the accuracy of the resulting models. Numerical methods, on the other hand, begin with the same governing equations, but cast them in a discrete form which may be solved on a computer. Although numerical methods are also approximate, the tuning of modeling detail and simulation time usually reduces error to acceptably low levels. Numerical methods usually solve broad classes of problems, obviating time-consuming analyses of multiple structures. The advent of inexpensive memory and processing power also renders numerical methods very attractive.

General numerical methods \([1]\), such as the finite element method (FEM), the method of moments (MOM), and finite-difference (FD) methods, give acceptable accuracy when (1) the size of the structure is not much larger than the excitation wavelength and (2) the number of numerical unknowns is sufficiently small for present-day computers. Unfortunately, these two requirements are often violated in real-world applications. Parallelization of numerical algorithms has achieved some success in extending modeling scale. However, the required processing hardware is often not within easy reach of typical scientists and engineers.

1.2 Solution: The Hybrid Method

This dissertation develops powerful hybrid methods to overcome the difficulty of large simulation scale. These hybrid methods can capture accuracy of exact numerical solvers on scales that far exceed their native capability.

Figure 1.5 depicts the application of the hybrid method to a general large-scale electromagnetic modeling problem. The method must analyze the given structure and produce the required output quantities. The structure is analyzed by dividing the problem into a number of levels of scale. At each level, an analysis combines key information from previous levels with knowledge about the physical structure to produce inputs to higher levels. Simulation efficiency is obtained by only promoting
Figure 1.5: Flow diagram of the general hybrid method (left) and a possible application of the method (right). A modeling problem is divided into several analysis layers. A specific level of detail is modeled at each layer, and required information is promoted from one level to the next.

the most significant information from one level to the next and only simulating the required detail at each layer.

At the lowest layer, simulation extent and the number of unknowns are small, and exact electromagnetic methods based on Maxwell’s equations compute microscopic quantities, such as time-harmonic electromagnetic fields. Processing of the microscopic quantities yields macroscopic information such as energy propagation and dissipation. At the highest level, analysis of the macroscopic quantities yields the desired solution outputs: reflection and transmission coefficients, radar cross section, emissivity, etc.

This dissertation demonstrates the hybrid modeling technique through successful application to three large-scale modeling problems: (1) modeling of snow for remote sensing, (2) modeling an optical Bragg resonator, and (3) statistical modeling
of the indoor multiple-input multiple-output (MIMO) wireless channel. The problems are quite diverse, and show the wide applicability of the general method. Many other problems will fall conveniently within the framework of one of these problems, requiring little or no alteration to the basic schemes.

1.3 Problem 1: Modeling of Snow for Remote Sensing

Scientists argue that change in large snow and ice masses such as the Greenland Ice Sheet indicates long-term environmental change. In order to assess this change, scientists must relate snow parameters to archived scatterometer and radiometer data, which space-borne microwave instruments have collected over the past few decades. Lack of detailed empirical data on snow necessitates accurate electromagnetic modeling, which is difficult since the satellite footprints may easily cover thousands of wavelengths. Additionally, snow media has a very complex structure consisting of randomly ordered and densely packed particles. Therefore, this problem requires a method which can accurately model electromagnetic wave interaction with complex snow media. Also, the model must accommodate scales on the order of thousands of wavelengths.

Radiative transfer has demonstrated the ability to model wave propagation in very large structures consisting of random media \[2,3\]. This method requires knowledge of statistical quantities such as phase matrices and extinction coefficients, which are constant over large layers of media. Traditionally, these quantities have been solved with analytical methods, resulting in expressions which are applicable to simple media only. Recent work has demonstrated the use T-matrix methods combined with Monte Carlo analysis to obtain the statistical quantities for densely packed spheres \[4\]. However, T-matrix methods are difficult to apply to non-spherical geometries. Also, the existing work does not provide a comprehensive method for determining key simulation parameters, such as the required number of Monte Carlo realizations and simulation volume sizes.
In this work, the problem of remote sensing of snow is divided into two basic levels: (1) the finite-difference time-domain method (FDTD) to compute phase matrices and extinction coefficients, and (2) radiative transfer (RT) to compute backscattering coefficients and brightness temperatures. The first level follows a methodology similar to [4], where the Monte Carlo method is used to compute the inputs to the radiative transfer equations. However, accurate use of the method requires an understanding of the error induced by finite simulation volumes and number of Monte Carlo realizations, neither of which has been previously addressed. Also, the use of FDTD (as opposed to T-matrix methods) extends the method to more complex media, such as refrozen snow.

1.4 Problem 2: Modeling an Optical Bragg Resonator

The ability to design complex optical devices is greatly enhanced by simulation tools that characterize wave propagation in arbitrary guiding structures. For example, distributed-feedback (DFB) lasers consist of a Bragg grating which is cleaved to obtain desired reflection and transmission properties at the ends of the lasing cavity. Error in the cleaving process may lead to unacceptable yield in the manufactured devices. Electromagnetic modeling could be used to predict yield when the accuracy of the cleaving process is known.

Prior work in optical waveguide modeling has focused on two-dimensional (2D) planar waveguide approximations [5, 6], the approximate beam-propagation method [7, 8], and finite-difference solutions for propagation constants and mode profiles [9, 10]. None of these methods provide a comprehensive analysis tool for full-wave analysis of arbitrary guiding structures.

Simulation of the Bragg resonator encompasses three basic layers: (1) an FD 2D mode solver for finding exact mode propagation constants and field profiles, (2) a three-dimensional (3D) FDTD solver for obtaining mode propagation in the presence of waveguide discontinuities and transitions, and (3) S-parameter analysis to combine the various 3D sections. The FD mode solver employs a straightforward discretization of Maxwell’s equations, similar to the FDTD method. Either sparse
eigenvalue/eigenvector methods or iterative sparse linear methods provide solutions for the resulting equations.

The simulated Bragg resonator is a buried heterostructure device that is very large ($\approx 5000\lambda_g$) compared to the mode wavelength ($\lambda_g$). The numerical sensitivity of this problem requires an understanding of error induced by truncation boundaries and the finite-difference approximations, which are both addressed in this research.

1.5 Problem 3: Indoor MIMO Channel Modeling

An understanding of the radio propagation channel is important when designing wireless communication systems. Electromagnetic wave propagation in these channels is subject to multipath interference, resulting in random fluctuation of the received signal power. Accurate radio propagation models predict important system parameters such as required transmit power, maximum transmit/receive separation, and outage statistics. Recent work demonstrates that MIMO wireless systems may exploit multipath fading to realize increased data throughput [11]. The assessment of performance of MIMO systems requires accurate statistical models that capture the true spatial behavior of the channel.

Initial work in this area has relied heavily on modeling the channel with the multivariate i.i.d. (independent and identically distributed) complex normal distribution. Such simple models ignore important system and channel parameters such as antenna directivity, polarization, mutual coupling, and multipath richness. Statistical models based on basic principles of wave propagation in a scattering environment hold more promise for modeling true MIMO channels.

The problem of simulating the indoor MIMO wireless channel falls neatly into two basic layers: (1) FDTD or MOM for obtaining antenna array radiation patterns and network characteristics and (2) use of the Saleh-Valenzuela model with angle-of-arrival (AOA) and angle-of-departure (AOD) (referred to as the SVA model) to generate random channels. Simple extension of the SVA model accommodates dual-polarized antennas. The resulting model demonstrates the tradeoffs associated
with various antenna design strategies: dual-polarization, directivity, and mutual
coupling.

Design, fabrication, and deployment of a MIMO measurement system
demonstrates the ability of the model to match measured capacity PDFs for realistic
model parameters. The system employs two basic antenna configurations: 10-element
monopole arrays and 4-element dual-polarized patch arrays.

1.6 Limitations of the Hybrid Method

Though useful for many problems, the hybrid method has two basic draw-
backs which require mention: information loss and problem division. Information
loss means that higher levels often discard information available at the lower levels
to gain efficiency. Thus, the method works well for problems with redundancy (such
as the Bragg resonator analyzed in Chapter 5). In this case, modeling the entire
structure results in wasted effort by obtaining redundant information. The method
also works well for problems where not all of the electromagnetic behavior requires
promotion from one level to the next. The channel modeling in Chapter 8, for ex-
ample, only requires information on far-field patterns and network behavior of the
antenna arrays, and not all of the near-field effects. On the other hand, problems
which contain no redundancy or where all information is equally significant will not
benefit from multiple levels of scale. Problem division involves finding natural places
to divide the problem into levels of scale, which is not always obvious. Also, time
and care is often required to store the results of one simulation and excite them in
another simulation.

1.7 New Contributions

The new contributions of this research fall into three basic categories: ap-
plication of the hybrid method, new theoretical results which aided each application,
and a deeper understanding of MIMO channels.

This hybrid method employs many tools which are not new to the electri-
cal engineering discipline: radiative transfer, finite-difference methods, FDTD, mode
extraction, network analysis, and path-based channel models. The main contribution of this dissertation is the innovative combination of these relatively simple modeling tools to analyze very complex structures.

At certain stages of the modeling effort, the underlying tools required extension or more rigorous analysis. Where appropriate, this dissertation highlights new theory resulting from these efforts.

The final significant contribution of this work is an extended understanding of MIMO wireless channels. Early effort in MIMO systems was limited to very simplistic closed-form models of the channel, which may grossly overpredict MIMO system capacity. Data collected in this effort combined with the hybrid modeling technique provides a much more realistic view of such channels.

1.8 Organization of the Dissertation

The material of this dissertation falls logically into four basic sections: (1) a treatment of modeling components required for the hybrid models, (2) remote sensing modeling of snow, (3) optical modeling of the Bragg resonator, and (4) indoor MIMO wireless channel modeling. Appendices contain detailed explanations and derivations which are necessary, but may detract from the primary subject matter. The following paragraphs provide a synopsis of each section.

The first two chapters contain a thorough treatment of two basic modeling tools employed in this research. Chapter 2 provides information on finite-difference methods for optical waveguide mode computation and the FDTD method which finds application throughout the work. Chapter 3 discusses radiative transfer theory and accompanying numerical solution techniques. Placement of these lengthy descriptions in separate chapters avoids breaking up later chapters concerned primarily with the hybrid modeling.

Chapter 4 outlines the hybrid FDTD/radiative transfer method for remote sensing modeling of snow. The chapter describes the Monte Carlo method for finding phase matrices and extinction coefficients, an important study assessing modeling
error due to simulation constraints, and a comparison of modeling results with existing methods.

Chapter 5 presents the hybrid FD/FDTD/S-parameter method for modeling the optical Bragg resonator. The material provides a description of the heterostructure under analysis, followed by 2D propagating mode solutions, and 3D response of a single Bragg section. S-parameter analysis yields the complete Bragg response of the resonator. Due to numerical sensitivity, this discussion provides a detailed analysis of error sources and their impact on the final solution.

Chapters 6, 7, and 8 provide information on the MIMO wireless channel probing hardware, data collection, and modeling, respectively. The author chose to place the information on the probing system and data collection in separate chapters to allow uninterested readers to safely skip the material. Chapter 6 discusses the complete microwave system design, antenna design, and data post-processing methods. Chapter 7 presents representative data that was collected with the platform. Chapter 8 describes the hybrid FDTD/SVA technique for channel modeling, compares model results with measured data, and provides simulations assessing the impact of mutual coupling, directive antennas, and dual-polarization on system capacity. The text also compares the SVA model to simpler multivariate complex normal models and highlights important differences.

Finally, Chapter 9 presents some concluding remarks and suggestions for future research.
Chapter 2

Finite-Difference Methods

This chapter explains the finite-difference methods applied in this research. Section 2.1 treats the two-dimensional (2D) finite-difference (FD) schemes for obtaining sinusoidal steady-state mode profiles and propagation constants for optical guided waves. Section 2.2 treats the three-dimensional (3D) finite-difference time-domain (FDTD) technique which finds use in both the snow modeling in Chapter 4 and the modeling of optical waveguide discontinuities in Chapter 5.

Nearly all of the material in this chapter represents new applications of the finite-difference concept or detailed analyses of existing methods that were unavailable at the time of writing. The principal new contributions in this chapter are as follows:

1. Section 2.1 presents a new method for computing mode solutions of waveguides with arbitrary cross-sectional geometry by applying a direct discretization of Maxwell’s equations and a simple iterative linear system technique.

2. Section 2.1.6 studies the influence of discrete time stepping and finite grid resolution on modal propagation constants. This information is crucial to ensure complete compatibility between the 2D finite-difference mode solver and FDTD.

3. Section 2.2.3 explains the use of the incident/scattered field formulation for waveguides, which previously has only found use in free-space scattering problems.
4. Section 2.2.5 provides a new analysis of modal propagation in the perfectly-matched layer (PML) \[12\] in FDTD, proving that modes in the PML are identical to those in standard Maxwellian space. This fact is critical for optical modeling where the PML must present a reflectionless surface.

5. Section 2.2.6 describes a simple volume-averaging method for modeling particles which are small compared to the illumination wavelength in FDTD. This method is useful for the snow modeling in Chapter 4.

6. Section 2.3 describes an efficient one-dimensional method for obtaining single-mode solutions to the FDTD update equations.

In addition to this new material, Section 2.2 presents some information on existing FDTD techniques for the sake of completeness.

2.1 Finite-Difference Mode Solutions

Finite-difference methods based on discretizations of the time-harmonic Helmholtz equation have been successfully applied for vectorial mode extraction \[9\]. However, such methods often require special treatment of material boundaries, and the mode solutions obtained often deviate slightly from modes supported by other discretizations (FDTD, for example). Full vectorial mode solutions have also been demonstrated by applying a Fourier transform to the FD-Vector Beam Propagation Method (FD-VBPM) \[10\].

This work employs a new mode solution method based on a straightforward discretization of the time-harmonic form of Maxwell’s equations, which is similar to Yee’s discretization scheme. One obvious advantage of this method is its natural compatibility with subsequent 3D FDTD simulations. The method is free of spurious modes since the FDTD gridding scheme automatically satisfies Maxwell’s divergence relations. Also, if material parameters are specified for each FD cell, the gridding arrangement ensures satisfaction of appropriate field continuity conditions across material boundaries.
The following subsections describe this new method in detail. Section 2.1.1 demonstrates how to discretize Maxwell’s time-harmonic equations into a form suitable for mode solutions. Section 2.1.2 treats the subject of domain truncation and presents a decay-type boundary condition appropriate for the simulation of dielectric waveguides. Sections 2.1.3 and 2.1.4 present two sparse solution methods for the 2D mode equations under analysis. Section 2.1.5 validates the method by analyzing a stepped-index optical fiber. Finally, Section 2.1.6 provides a detailed analysis of the compatibility between this new FD mode solution method and FDTD simulations, ensuring minimal modeling error in Chapter 5.

2.1.1 Discretization of Maxwell’s Equations

Assuming \( \exp(j\omega t) \) time-harmonic variation and a mode which propagates in the \( \hat{z} \) direction with \( \exp(-j\beta_z z) \) longitudinal spatial variation, we write Maxwell’s equations for a non-magnetic medium as

\[
\begin{align*}
H_x &= \frac{1}{k_0} \left( j \frac{\partial E_z}{\partial y} - \beta_z E_y \right) \\
H_y &= \frac{1}{k_0} \left( \beta_z E_x - j \frac{\partial E_z}{\partial x} \right) \\
H_z &= \frac{j}{k_0} \left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) \\
E_x &= \frac{1}{\epsilon_r k_0} \left( \beta_z H_y - j \frac{\partial H_z}{\partial y} \right) \\
E_y &= \frac{1}{\epsilon_r k_0} \left( j \frac{\partial H_z}{\partial x} - \beta_z H_x \right) \\
E_z &= \frac{j}{\epsilon_r k_0} \left( \frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} \right),
\end{align*}
\]

where \( E \) denotes electric field intensity, \( H \) represents magnetic field intensity multiplied by the free-space intrinsic impedance \( \eta_0 \), and the subscripts \( \{x, y, z\} \) denote field polarization. Also, \( k_0 = \omega \sqrt{\mu_0 \epsilon_0} \) is the free space wave number and \( \epsilon_r \) is the material relative permittivity. To discretize these equations, we use the standard Yee grid assignment \[13\] collapsed onto a two-dimensional surface as shown in Figure 2.1.

After applying first-order central differences we obtain

\[
\begin{align*}
H_{x,ij} &= \frac{1}{k_0} \left( j \frac{E_{z,ij} - E_{z,i,j-1}}{\Delta y} - \beta_z E_{y,ij} \right) \\
H_{y,ij} &= \frac{1}{k_0} \left( \beta_z E_{x,ij} - j \frac{E_{z,ij} - E_{z,i-1,j}}{\Delta x} \right) \\
jH_{z,ij} &= \frac{1}{k_0} \left( \frac{E_{x,ij} - E_{x,i,j-1}}{\Delta y} - \frac{E_{y,ij} - E_{y,i-1,j}}{\Delta x} \right)
\end{align*}
\]

15
Figure 2.1: Simulation domain for two-dimensional finite-difference mode solution.

\[
\begin{align*}
E_{x,ij} &= \frac{1}{\varepsilon_r k_0} \left( \beta_z H_{y,ij} - j \frac{H_{z,i,j+1} - H_{z,i,j}}{\Delta y} \right) \\
E_{y,ij} &= \frac{1}{\varepsilon_r k_0} \left( j \frac{H_{z,i+1,j} - H_{z,i,j}}{\Delta x} - \beta_z H_{x,ij} \right) \\
\frac{1}{\varepsilon_r k_0} j E_{z,ij} &= \left( \frac{H_{y,i+1,j} - H_{y,i,j}}{\Delta x} - \frac{H_{x,i,j+1} - H_{x,i,j}}{\Delta y} \right), \\
\end{align*}
\]

where \( \varepsilon_r \) now represents the relative permittivity averaged over one cell centered about the component on the left-hand side of each equation.

### 2.1.2 Boundary Truncation Conditions

The FD method requires a truncation condition which directly relates fields on the domain boundary to components inside of the simulation domain. The simplest truncation condition sets all field components on the domain boundary to zero, which is identical to placing a perfectly conducting sheet on the boundary. This will be referred to as the \textit{zero boundary condition}. More general Neumann or Dirichlet conditions may also be employed. However, such non-physical boundaries may induce unacceptable error when placed near the guiding structure. This section develops a new truncation boundary condition that provides a more accurate means of truncating the domain for dielectric waveguides.
In the dielectric waveguides analyzed in Chapter 5, the field profile for propagating modes will tend to decay as a function of radial distance from the center of the waveguide core. Approximating an arbitrary guiding structure as a cylindrical waveguide, fields for the HE_{11} mode vary as (see Appendix A)

\[ f(\rho) = f_0 H_1^{(1)}(j \sqrt{\beta_z^2 - \omega^2 \mu_1 \epsilon_1 \rho}), \]

where \( \rho \) is radial distance from the center of the core, \( f \) is any field component, \( f_0 \) is a constant related to the field strength, \( H_1^{(1)}(\cdot) \) is the first order Hankel function of the first kind, and \( \mu_1 \) and \( \epsilon_1 \) are the permeability and permittivity outside the cylindrical core. The asymptotic form of this equation may be written as

\[ f(\rho) \approx f_0 \frac{1}{\sqrt{\rho}} \exp(-\alpha \rho), \quad \alpha \rho > 2, \]

which provides an approximate functional relationship between fields that lie on the truncation boundary and those just inside the boundary. This condition will be referred to as the decay boundary condition. Since this condition is a non-linear function of \( \beta_z \), application is difficult in the case of the eigenvalue/eigenvector method, and a simple

\[ f(\rho) = \frac{f_0}{\sqrt{\rho}} \]

decay is assumed instead. As will be shown later, use of the decay boundary condition significantly reduces the required size of the computational grid for a given level of accuracy.

### 2.1.3 Eigenvalue/Eigenvector Method

The traditional approach to solving (2.2) involves forming the equations into a standard eigenvalue equation. Substituting \( jH_z \) and \( jE_z \) in (2.2) into the other four equations, and rearranging the equations results in

\[
\begin{align*}
\beta_z E_{x,ij} &= \frac{1}{k_0 \Delta x} \left[ \frac{H_{y,i+1,j}}{\epsilon_{r,ij}^z} \Delta x - \frac{H_{y,i,j+1} - H_{x,ij}}{\epsilon_{r,ij}^z} \Delta y + \frac{H_{y,i-1,j}}{\epsilon_{r,i-1,j}^z} \Delta x - \frac{H_{x,i-1,j+1} - H_{x,i-1,j}}{\epsilon_{r,i-1,j}^z} \Delta y \right] + k_0 \left( \frac{1}{\epsilon_{r,ij}^z} + \frac{1}{\epsilon_{r,i-1,j}^z} \right) \Delta \frac{1}{\Delta x} \frac{H_{y,ij}}{\Delta y} \\
&= \frac{1}{k_0 (\Delta x)^2} \left( \frac{1}{\epsilon_{r,ij}^z} + \frac{1}{\epsilon_{r,i-1,j}^z} \right) \frac{H_{y,ij}}{\Delta y}
\end{align*}
\]

17
\[
\beta_z E_{y,ij} = \frac{1}{k_0 \Delta y} \left[ \frac{H_{y,i+1,j} - H_{y,ij}}{\epsilon_{r,ij}^z \Delta x} - \frac{H_{x,i,j+1}}{\epsilon_{r,ij}^z \Delta y} \right] - \frac{H_{y,i,j+1} - H_{y,i,j-1}}{\epsilon_{r,i,j-1}^z \Delta x} - \frac{H_{x,i,j-1}}{\epsilon_{r,i,j-1}^z \Delta y} \\
+ \left[ \frac{1}{k_0 (\Delta y)^2} \left( \frac{1}{\epsilon_{r,ij}^z} + \frac{1}{\epsilon_{r,i,j-1}^z} \right) - k_0 \right] H_{x,ij}
\]

\[
\beta_z H_{x,ij} = \frac{1}{k_0 \Delta x} \left[ \frac{E_{x,i+1,j} - E_{x,i+1,j-1} - E_{x,i,j} + E_{x,i,j-1}}{\Delta y} \right] - \frac{E_{y,i+1,j} + E_{y,i+1,j-1} - E_{y,i,j-1} - E_{y,i,j-1}}{\Delta x} \\
+ \left[ \frac{2}{k_0 (\Delta x)^2} - \epsilon_{r,ij}^y k_0 \right] E_{x,ij}
\]

\[
\beta_z H_{y,ij} = \frac{1}{k_0 \Delta y} \left[ \frac{E_{x,i,j+1} + E_{x,i,j-1}}{\Delta y} \right] + \frac{E_{y,i,j+1} + E_{y,i,j-1} - E_{y,i,j-1} - E_{y,i,j-1}}{\Delta x} \\
+ \left[ \epsilon_{r,ij}^x k_0 - \frac{2}{k_0 (\Delta y)^2} \right] E_{x,ij},
\]

(2.6)

where \( \epsilon_{r,ij}^{x,y,z} \) represents the relative permittivity averaged about the \( E_{x,ij} \), \( E_{y,ij} \), or \( E_{z,ij} \) component, respectively. These equations represent the block matrix equation

\[
\begin{bmatrix}
E_x \\
E_y \\
H_x \\
H_y
\end{bmatrix}
= \begin{bmatrix}
\overline{A}_{11} & \overline{A}_{12} & \overline{A}_{13} & \overline{A}_{14} \\
\overline{A}_{21} & \overline{A}_{22} & \overline{A}_{23} & \overline{A}_{24} \\
\overline{A}_{31} & \overline{A}_{32} & \overline{A}_{33} & \overline{A}_{34} \\
\overline{A}_{41} & \overline{A}_{42} & \overline{A}_{43} & \overline{A}_{44}
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
H_x \\
H_y
\end{bmatrix},
\]

(2.7)

where \( \overline{E}_x \), \( \overline{E}_y \), \( \overline{H}_x \), and \( \overline{H}_y \) are stacked versions of \( \{E_{x,ij}\}, \{E_{y,ij}\}, \{H_{x,ij}\}, \) and \( \{H_{y,ij}\} \). Rearranging into the standard eigenvalue equation \((\overline{A} - \beta_z \overline{I})\overline{F} = 0\), this matrix equation is easily solved with a sparse eigenvalue solver (the ARPACK sparse eigenvalue/eigenvector solver was used in this research). Also, the \( E_z \) and \( H_z \) components may be found by substituting the solutions for the \( x \) and \( y \) components into (2.2).

In simulations run by the author involving small cell sizes, the \( \Delta^2 \) terms lead to coefficient matrices with poor numerical conditioning, and consequently sparse eigenvalue solvers like ARPACK have difficulty converging. For finer resolution, better success was obtained with the iterative sparse linear solution given in Section 2.1.4.
2.1.4 Iterative Linear Method

Mode solutions may also be obtained by retaining all 6 components in (2.2) giving

\[
\begin{bmatrix}
E_x \\
E_y \\
E_z \\
H_x \\
H_y \\
H_z
\end{bmatrix} = \begin{bmatrix}
\overline{A}_{11} & \overline{A}_{12} & \cdots & \overline{A}_{16} \\
\overline{A}_{21} & \overline{A}_{22} & \cdots & \overline{A}_{16} \\
\vdots & \vdots & \ddots & \vdots \\
\overline{A}_{61} & \overline{A}_{62} & \cdots & \overline{A}_{66}
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z \\
H_x \\
H_y \\
H_z
\end{bmatrix}.
\] (2.8)

If the \( k \)th element of \( \mathcal{F} \) is forced to a nonzero constant \( C_0 \), the matrix relationship 
\((\overline{\mathcal{A}}(\beta_z) - \mathcal{I})\mathcal{F} = \mathcal{C}\) is obtained, where

\[
C_i = \begin{cases} 
C_0, & i = k \\
0, & \text{otherwise}
\end{cases}
\] (2.9)

and

\[
\mathcal{A}'_{ij} = \begin{cases} 
1, & (i = k) \text{ and } (j = k) \\
0, & (i = k) \text{ and } (j \neq k) \\
A_{ij}, & \text{otherwise}
\end{cases}
\] (2.10)

When \( \beta_z \) is fixed, this equation may be solved with a sparse linear solver to obtain the mode profile. In order to obtain the correct value of \( \beta_z \), an optimization is performed that minimizes the vector norm \( \| \overline{\mathcal{A}}(\beta_z) \mathcal{F} \| \), which is identically zero for the correct value of \( \beta_z \). The initial guess for \( \beta_z \) may be obtained by the eigenvalue/eigenvector method of Section 2.1.3, an analytical approximation, or an exhaustive search. This research employed the SuperLU package and a subplex optimization loop, with initial guesses for \( \beta_z \) determined with the eigenvalue/eigenvector method.

2.1.5 Method Validation

This section establishes the validity of the new mode solution method by analyzing a stepped-index optical fiber depicted in Figure 2.2 whose field profiles and propagation constants can be obtained exactly in closed form (see Appendix A).
The exact propagation constant for the HE\textsubscript{11} mode for this geometry is
\[ \beta_z = 9.104405/\lambda_0 \] and corresponding field profiles were found using the method in Section A.3. Next, the eigenvalue formulation was solved on a 60×60 cell grid with dimensions 30\(\lambda_0\)×30\(\lambda_0\), yielding \[ \beta_z = 9.104498/\lambda_0 \] (1.0 \times 10^{-5} fractional error). Refining the solution with the linear solver on a more detailed grid (120×120 cells) with the same dimensions resulted in \[ \beta_z = 9.104400/\lambda_0 \] (5.5 \times 10^{-7} fractional error). Figure 2.3 depicts the absolute percent error in the field profile for the eigenvalue solution and the linear solution as compared to the exact solution. The large drop in absolute error is due to two factors: (1) the linear solution employed a more detailed grid, resulting in more accurate approximations of the spatial derivatives, and (2) the boundary condition is asymptotically exact in the linear solution (2.4) but very approximate in the eigenvalue case (2.5).

2.1.6 Compatibility of Modal Solutions and FDTD

Chapter 5 demonstrates the simulation of waveguide discontinuities by coupling the new mode solution method in this section with 3D FDTD simulations. However, mode solutions obtained with the new method are not strictly compatible with the finite-difference time-domain method, due to discrete stepping in time and in the propagation direction. Such incompatibility may cause deformation of the mode shape and artificial reflections in subsequent FDTD simulations. This incompatibility is eliminated by adjusting the equations given in (2.2) and (2.6) to account for discrete sampling in time and space.

Assuming time-harmonic fields of the form \(\exp(j\omega t)\), the temporal central finite difference (\(D_t\)) with a step size of \(\Delta t\) of any field quantity \((F)\) is

\[
D_t \left[ F(x, y, z)e^{j\omega \Delta t} \right] = j\omega \operatorname{sinc} \left( \frac{\omega \Delta t}{2} \right) F(x, y, z)e^{j\omega \Delta t},
\]

where \(\operatorname{sinc}(x) = \sin(x)/x\), and \(n\) is the time index. Since the \(k_0 = \omega/c_0\) appearing in (2.2) and (2.6) results from a continuous derivative, \(k_0\) must be replaced with \(k_0 \operatorname{sinc}(\omega \Delta t/2)\). Next, for fields with \(\exp(-j\beta_z z)\) spatial variation in the propagation direction, the spatial central finite difference (\(D_z\)) with a step size of \(\Delta z\) of any field
Figure 2.2: Cylindrical core fiber parameters for validating the 2D finite-difference mode solution methods

<table>
<thead>
<tr>
<th>Grid Sizes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eigenvalue Solver:</td>
</tr>
<tr>
<td>( N = 60 )</td>
</tr>
<tr>
<td>Linear Solver:</td>
</tr>
<tr>
<td>( N = 120 )</td>
</tr>
</tbody>
</table>

Figure 2.3: Percent error in the \( E_x \) field component of the finite-difference methods compared to the exact solution for a cylindrical core optical fiber
quantity \( F \) is
\[
D_z \left[ F(x, y, t)e^{-j\beta_z k\Delta z}\right] = -j\beta_z \text{sinc} \left( \frac{\beta \Delta z}{2} \right) F(x, y, t)e^{-j\beta_z k\Delta z},
\]
(2.12)
where \( k \) is the spatial index in the \( z \) direction. Thus, we must replace \( \beta_z \) in (2.2) and (2.6) with \( \beta_z \text{sinc}(\beta_z \Delta z/2) \). In this case, however, we can use the unaltered equations as before to obtain \( \beta_z \), and find the true propagation constant \( \beta'_z \) for the discrete case by solving
\[
\beta_z = \beta'_z \text{sinc}(\beta'_z \Delta z/2).
\]
(2.13)
Application of these two modifications ensures that the finite-difference mode solution methods and FDTD solve the exact same equations, and therefore support identical modes.

2.2 Finite-Difference Time-Domain

The finite-difference time-domain (FDTD) technique \cite{13,14} found extensive use in this research due to its ease of implementation, flexibility, and numerical efficiency. This section provides a treatment of the subject of FDTD as relating to this research. Sections 2.2.1 and 2.2.2 provide implementation details on the FDTD code developed in this research, and similar information is available in other sources \cite{1,13}. Section 2.2.3 applies the FDTD incident/scattered field formulation to waveguides, a new interpretation that improves the modeling accuracy of discontinuities in waveguides. Sections 2.2.4 and 2.2.5 provide implementation details of the PML and a new analysis of modal propagation in the PML, respectively. Finally, Section 2.2.6 presents a simple volume-averaging method appropriate for simulating electrically small structures.

2.2.1 Simulation Domain

The FDTD simulator used in this research is based on the standard staggered grid depicted in Figure 2.4. Nodes are numbered using whole integers 0, 1, 2, ..., rather than the usual half integer notation, since whole integers simplify translation from the equations to the actual computer implementation. The full grid of nodes is
represented internally using a multi-dimensional array of pointers. Then, each pointer may point to a different structure depending on the type of node.

2.2.2 Governing Equations

The time-domain differential forms of Maxwell’s equations may be written as

\[
\begin{align*}
\frac{\mu_r}{c_0} \frac{\partial H_x}{\partial t} &= \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} + \frac{\epsilon_r}{c_0} \frac{\partial E_x}{\partial z} + \sigma \eta_0 E_y = \eta_0 \left( \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right) \\
\frac{\mu_r}{c_0} \frac{\partial H_y}{\partial t} &= \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} + \frac{\epsilon_r}{c_0} \frac{\partial E_y}{\partial x} + \sigma \eta_0 E_z = \eta_0 \left( \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) \\
\frac{\mu_r}{c_0} \frac{\partial H_z}{\partial t} &= \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} + \frac{\epsilon_r}{c_0} \frac{\partial E_z}{\partial y} + \sigma \eta_0 E_x = \eta_0 \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_y}{\partial y} \right) \\
\end{align*}
\]

(2.14)

where \( \mu_r \) is the relative permeability, \( \epsilon_r \) is the relative permittivity, \( c_0 \) is the free-space wave speed, \( \sigma \) is the conductivity, and \( \eta_0 \) is the free-space wave impedance.

Application of central finite differences in time and space yields

\[
\eta_0 H_{x,ijk}^{n+1} = \frac{c_0 \Delta t}{\mu_r} \left[ \frac{E_{y,j,k+1}^{n+1} - E_{y,j,k}^{n+1}}{\Delta z} - \frac{E_{z,i,j+1,k}^{n+1} - E_{z,i,j-1,k}^{n+1}}{\Delta y} \right] + \eta_0 H_{x,ijk}^n
\]

Figure 2.4: Simulation domain of the FDTD simulator and gridding scheme
where $\epsilon$, $\mu$, and $\sigma$ are the physical quantities averaged about the field component on the left-hand side of each equation. The superscripts and subscripts on field quantities represent time and spatial indices, respectively. Also, field computation occurs in the order $E^0, H^0, E^1, H^1, \ldots$.

### 2.2.3 Scattered Field Formulation

For many free-space scattering and guided mode problems, the field scattered by the obstacle may be significantly weaker than the incident field or mode. In these situations, finite precision arithmetic may produce unacceptable levels of error.

To minimize the dynamic range requirements as well as remove the need to absorb the strong incident field at the domain boundaries, the scattered field formulation is utilized in the FDTD implementation \cite{15}. This approach, which has been extensively used to model electromagnetic scattering in free space, can also be applied to waveguide analysis. In this case, however, the incident field and corresponding geometry are the incident mode and unperturbed waveguide structure, respectively,
where the waveguide material parameters are represented by $\epsilon_i$, $\mu_i$, and $\sigma_i$. If the actual (perturbed) waveguide geometry is characterized by material parameters $\epsilon$, $\mu$, and $\sigma$, we may write Maxwell’s equations for the scattered fields ($\overline{E}_s$ and $\overline{H}_s$) as

$$\nabla \times \overline{E}_s = -\mu \frac{\partial \overline{H}_s}{\partial t} - (\mu - \mu_i) \frac{\partial \overline{H}_i}{\partial t}$$ (2.16)

$$\nabla \times \overline{H}_s = \epsilon \frac{\partial \overline{E}_s}{\partial t} + \sigma \overline{E}_s + (\epsilon - \epsilon_i) \frac{\partial \overline{E}_i}{\partial t} + (\sigma - \sigma_i) \overline{E}_i,$$ (2.17)

where $\overline{E}_i$ and $\overline{H}_i$ represent the incident modal fields. These equations are identical to Maxwell’s equations for total field with the addition of source terms. For a non-conductive, non-magnetic medium, we must include a source term only where $\epsilon \neq \epsilon_i$.

To illustrate the excitation of this source in the FDTD code, consider the FDTD update equation for $E_x$ given as

$$E_{x,ijk}^{n+1} = \frac{\Delta t}{\epsilon} \left[ \frac{H_{z,i,j+1,k}^n - H_{z,i,j-1,k}^n}{\Delta y} - \frac{H_{y,i,j,k+1}^n - H_{y,i,j,k-1}^n}{\Delta z} \right] + E_{x,ijk}^n$$

$$\equiv G.$$ (2.18)

The incident/scattered field formulation introduces an additional term such that

$$E_{x,ijk}^{n+1} = G + \frac{(\epsilon_i - \epsilon)}{\epsilon} \frac{\partial E_{x,ijk}^{inc}}{\partial t} \bigg|_{t=(n+1/2)\Delta t}$$

$$= G + \frac{(\epsilon_i - \epsilon)}{\epsilon} (E_{x,ijk}^{inc,n+1} - E_{x,ijk}^{inc,n}),$$ (2.19)

where $E^{inc}$ is the incident field specified by the known mode shape. The second equality employs a finite difference on the incident source to ensure compatibility of the mode in the discretized domain. After the FDTD simulation, scattered fields may be converted to physical total fields by adding the known incident mode shape at each simulation node. Similar modifications must be made to the other field components. For details on the precise equations used, see the *FDTD Simulator User’s Manual* [16].

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2.2.4 Perfectly Matched Layer

The FDTD simulator employs Berenger’s perfectly matched layer (PML) \[ \text{[12]} \] to absorb radiated waves and guided modes at domain boundaries. The continuous time-domain differential equations governing fields in the PML are

\[
\begin{align*}
\mu_r \frac{\partial H_{xz}}{\partial t} + \frac{\sigma_z^*}{\eta_0} H_{xz} &= \frac{\partial E_y}{\partial z} \\
\mu_r \frac{\partial H_{xy}}{\partial t} + \frac{\sigma_y^*}{\eta_0} H_{xy} &= -\frac{\partial E_z}{\partial y} \\
\mu_r \frac{\partial H_{yx}}{\partial t} + \frac{\sigma_x^*}{\eta_0} H_{yx} &= \frac{\partial E_z}{\partial x} \\
\mu_r \frac{\partial H_{yz}}{\partial t} + \frac{\sigma_y^*}{\eta_0} H_{yz} &= -\frac{\partial E_x}{\partial z} \\
\mu_r \frac{\partial H_{zy}}{\partial t} + \frac{\sigma_y^*}{\eta_0} H_{zy} &= \frac{\partial E_x}{\partial y} \\
\mu_r \frac{\partial H_{zz}}{\partial t} + \frac{\sigma_z^*}{\eta_0} H_{zz} &= -\frac{\partial E_y}{\partial x}
\end{align*}
\]

(2.20)

where \( \sigma_p \) and \( \sigma_p^* \) are electric and magnetic conductivities for fields polarized in the \( \hat{p} \) direction. The corresponding discretized update equations are

\[
\begin{align*}
\eta_0 H_{xz,i,j,k}^{n+1} &= \left[ \frac{E_{y,i,j,k+1}^{n+1} - E_{y,i,j,k-1}^{n+1}}{\Delta z} + \eta_0 H_{xz,i,j,k}^n \left( \frac{\mu_r}{c_0 \Delta t} - \frac{\sigma_z^* / \eta_0}{2} \right) \right] \left( \frac{\mu_r}{c_0 \Delta t} + \frac{\sigma_z^* / \eta_0}{2} \right)^{-1} \\
\eta_0 H_{xy,i,j,k}^{n+1} &= \left[ \frac{E_{z,i,j,k+1}^{n+1} - E_{z,i,j,k-1}^{n+1}}{\Delta y} + \eta_0 H_{xy,i,j,k}^n \left( \frac{\mu_r}{c_0 \Delta t} - \frac{\sigma_y^* / \eta_0}{2} \right) \right] \left( \frac{\mu_r}{c_0 \Delta t} + \frac{\sigma_y^* / \eta_0}{2} \right)^{-1} \\
\eta_0 H_{yx,i,j,k}^{n+1} &= \left[ \frac{E_{z,i,j,k+1}^{n+1} - E_{z,i,j,k-1}^{n+1}}{\Delta y} + \eta_0 H_{yx,i,j,k}^n \left( \frac{\mu_r}{c_0 \Delta t} - \frac{\sigma_x^* / \eta_0}{2} \right) \right] \left( \frac{\mu_r}{c_0 \Delta t} + \frac{\sigma_x^* / \eta_0}{2} \right)^{-1} \\
\eta_0 H_{yz,i,j,k}^{n+1} &= \left[ \frac{E_{z,i,j,k+1}^{n+1} - E_{z,i,j,k-1}^{n+1}}{\Delta z} + \eta_0 H_{yz,i,j,k}^n \left( \frac{\mu_r}{c_0 \Delta t} - \frac{\sigma_y^* / \eta_0}{2} \right) \right] \left( \frac{\mu_r}{c_0 \Delta t} + \frac{\sigma_y^* / \eta_0}{2} \right)^{-1} \\
\eta_0 H_{zy,i,j,k}^{n+1} &= \left[ \frac{E_{z,i,j,k+1}^{n+1} - E_{z,i,j,k-1}^{n+1}}{\Delta z} + \eta_0 H_{zy,i,j,k}^n \left( \frac{\mu_r}{c_0 \Delta t} - \frac{\sigma_x^* / \eta_0}{2} \right) \right] \left( \frac{\mu_r}{c_0 \Delta t} + \frac{\sigma_x^* / \eta_0}{2} \right)^{-1} \\
\eta_0 H_{zz,i,j,k}^{n+1} &= \left[ \frac{E_{y,i,j,k+1}^{n+1} - E_{y,i,j,k-1}^{n+1}}{\Delta x} + \eta_0 H_{zz,i,j,k}^n \left( \frac{\mu_r}{c_0 \Delta t} - \frac{\sigma_z^* / \eta_0}{2} \right) \right] \left( \frac{\mu_r}{c_0 \Delta t} + \frac{\sigma_z^* / \eta_0}{2} \right)^{-1}
\end{align*}
\]

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Figure 2.5 depicts the placement strategy of the PML. The code in this work used an \(n\)th order conductivity gradient for the electric and magnetic conductivities in the PML. The conductivity gradient in the PML is depicted in (b) with the associated parameters.
PML, or

\[ \sigma(z) = \sigma_{\text{max}} \left( \frac{z}{\Delta z} \right)^n, \]  

(2.22)

where \( \sigma_{\text{max}} \) is the maximum conductivity at the FDTD grid truncation boundary, \( \Delta z \) is the width of the PML, and \( z = 0 \) corresponds to the PML/normal field interface. The conductivity in each cell is set according to (2.22) with the \( z \) coordinate corresponding to the center of the cell. To ensure undisturbed propagation of normally incident modes, \( \varepsilon_r, \mu_r, \) and \( \sigma \) naturally extend into the PML in the direction normal to the PML/normal field interface. Generally, specifying the normal reflection coefficient for plane wave or modal incidence is more convenient, in which case

\[ \frac{\sigma_{\text{max}}}{\varepsilon_r} = -\frac{(n + 1) \ln(R)v_p}{2c_0\eta_0\Delta z}, \]  

(2.23)

where \( \varepsilon_r \) is the relative permittivity that extends from the normal/PML boundary to the domain edge, \( R \) is the normal reflection coefficient, \( v_p \) is the phase velocity of the propagating plane wave or mode, and \( \Delta z \) is the width of the PML.

### 2.2.5 The Perfectly Matched Layer and Modal Propagation

Several ABCs have been applied for waveguide termination: methods based on the one-way wave equation [17, 18], PML techniques [12, 19, 20], modal eigenfunction expansion approaches [21], absorption based on discrete time-domain Green’s functions for the waveguide [22, 23], and filter-bank methods [24]. The problems in this research require absorption of both guided modes and radiated fields, suggesting the use of robust PML-based methods. Berenger’s PML [12] is well-suited for free-space scattering problems, and special consideration is required for application to guided-mode problems. This section presents a new analysis of modal propagation in the PML which demonstrates the ability of the PML to absorb guided modes effectively.

Consider Figure 2.6, which depicts typical use of the PML in a guided-mode problem. The PML has two basic requirements. First, PMLs in the transverse directions should absorb radiated fields without overly disturbing the guided mode. The effect of the PML on the guided mode will be proportional to the strength of
the modal fields at the boundary. Thus, placing the PML sufficiently far from strong fields in the guiding structure avoids disturbance of the mode. In the optics research presented in Chapter 5, simulations demonstrate the very small disturbance caused by the PML. Second, we desire that the PML in the propagation direction provide a reflectionless surface, which is addressed in the remaining part of this section.

Past work has demonstrated that the PML may be applied to a dielectric waveguide by simply extending the waveguide into the PML and ensuring that \( \sigma_{1,z}(z)/\sigma_{2,z}(z) = \epsilon_1/\epsilon_2 \), where \( \sigma_{1,z}(z) \) and \( \sigma_{2,z}(z) \) are the \( z \)-directed conductivities in the PML for the core and cladding and \( \epsilon_1 \) and \( \epsilon_2 \) are the permittivities in core and cladding, respectively [25]. This condition ensures that the decay rate of the propagating mode in the core and cladding remains equal. Many other researchers have studied Maxwell’s equations in the PML [19, 20, 26].

The proof that follows demonstrates that if the guiding structure naturally extends into the PML, the modes are identical in the PML and normal regions, leading to a (theoretically) reflectionless interface. Note that matching of modes does not guarantee absorption. In the case of metallic waveguides, for example, we have the difficulty of evanescent modes, and other methods must be employed. Also, even
though the surface may be theoretically reflectionless, numerical reflection exists due to discretization.

Beginning with the governing equations for the fields in the PML (2.20), assuming \( \exp(j\omega t) \) time variation, and combining split components results in the equations

\[
\begin{align*}
H_x &= a_z \frac{\partial E_y}{\partial z} - a_y \frac{\partial E_z}{\partial y} \\
H_y &= a_x \frac{\partial E_z}{\partial x} - a_z \frac{\partial E_x}{\partial z} \\
H_z &= a_y \frac{\partial E_x}{\partial y} - a_x \frac{\partial E_y}{\partial x}
\end{align*}
\]

\[
\begin{align*}
E_x &= b_y \frac{\partial H_z}{\partial y} - b_z \frac{\partial H_y}{\partial z} \\
E_y &= b_z \frac{\partial H_x}{\partial z} - b_x \frac{\partial H_z}{\partial x} \\
E_z &= b_x \frac{\partial H_y}{\partial x} - b_y \frac{\partial H_x}{\partial y},
\end{align*}
\]

(2.24)

where

\[
a_i = \frac{1}{j\omega \mu_r / c_0 + \eta_0 \sigma_i^*}
\]

(2.25)

and

\[
b_i = \frac{1}{j\omega \epsilon_r / c_0 + \eta_0 \sigma_i}.
\]

(2.26)

Substitution of the equations in (2.24) with \( E \) on the left-hand side into those with \( H \) on the left-hand side yields the equations

\[
\begin{align*}
H_x &= a_z \left( b_z \frac{\partial^2 H_x}{\partial z^2} - b_x \frac{\partial^2 H_z}{\partial x \partial z} \right) - a_y \left( b_y \frac{\partial^2 H_y}{\partial y \partial z} - b_y \frac{\partial^2 H_x}{\partial y^2} \right) \\
H_y &= a_x \left( b_x \frac{\partial^2 H_y}{\partial x^2} - b_y \frac{\partial^2 H_x}{\partial x \partial y} \right) - a_z \left( b_y \frac{\partial^2 H_z}{\partial y \partial z} - b_z \frac{\partial^2 H_y}{\partial z^2} \right) \\
H_z &= a_y \left( b_y \frac{\partial^2 H_z}{\partial y^2} - b_z \frac{\partial^2 H_y}{\partial z \partial y} \right) - a_x \left( b_z \frac{\partial^2 H_x}{\partial z \partial x} - b_x \frac{\partial^2 H_z}{\partial x^2} \right).
\end{align*}
\]

(2.27)

Rearranging produces the wave equation

\[
\begin{bmatrix}
  a_x b_z \frac{\partial^2}{\partial x^2} + a_y b_y \frac{\partial^2}{\partial y^2} + a_z b_z \frac{\partial^2}{\partial z^2} - 1
\end{bmatrix}
\begin{bmatrix}
  H_x \\
  H_y \\
  H_z
\end{bmatrix}
= \begin{bmatrix}
  b_z \frac{\partial}{\partial x} \\
  b_y \frac{\partial}{\partial y} \\
  b_z \frac{\partial}{\partial z}
\end{bmatrix}
\begin{bmatrix}
  a_x \frac{\partial H_x}{\partial x} + a_y \frac{\partial H_y}{\partial y} + a_z \frac{\partial H_z}{\partial z}
\end{bmatrix}.
\]

(2.28)
Taking central finite differences of the equations in (2.24) and using Yee’s FDTD gridding scheme it can be shown that the central finite difference of $a_i(\partial H_i/\partial i)$ is identically zero. The wave equation becomes

$$\left[a_x b_x \frac{\partial^2}{\partial x^2} + a_y b_y \frac{\partial^2}{\partial y^2} + a_z b_z \frac{\partial^2}{\partial z^2} - 1\right] \begin{cases} H_x \\ H_y \\ H_z \end{cases} = 0. \quad (2.29)$$

If the equations in (2.24) with $H$ on the left-hand side are substituted into those with $E$ on the left-hand side, the same development results in

$$\left[a_x b_x \frac{\partial^2}{\partial x^2} + a_y b_y \frac{\partial^2}{\partial y^2} + a_z b_z \frac{\partial^2}{\partial z^2} - 1\right] \begin{cases} E_x \\ E_y \\ E_z \end{cases} = 0. \quad (2.30)$$

Having obtained the proper wave equation for a general PML medium, we now show that normal/PML interfaces and PML/PML interfaces cause no reflection of the incident mode. Assuming a normal field half-space in the $-\hat{z}$ direction and a PML medium in the $+\hat{z}$ direction, which corresponds to the direction of propagation, 

$$\frac{1}{\omega^2 \mu \epsilon} \left[\frac{\partial \psi^2}{\partial x^2} + \frac{\partial \psi^2}{\partial y^2} + \frac{1}{\mu_{zr} \epsilon_{zr}} \frac{\partial \psi^2}{\partial z^2}\right] + \psi = 0, \quad (2.31)$$

where $\mu_{zr} = [1 - j \sigma_{zr}^a/(\omega \mu)]$, $\epsilon_{zr} = [1 - j \sigma_{zr}^a/(\omega \epsilon)]$, and $\psi$ is any field quantity. Assuming the same condition as Berenger for a reflectionless interface, we let $q_z = \mu_{zr} = \epsilon_{zr}$. Modal propagation will be of the form $\psi = \psi(x, y)e^{-j \beta_z' z}$ where $\beta_z' = \beta_z \sqrt{\mu_{zr} \epsilon_{zr}} = \beta_z q_z$. Substitution into (2.31) gives the wave equation

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \beta_z^2 + \omega^2 \mu \epsilon\right] \psi(x, y) = 0. \quad (2.32)$$

Thus, the governing equation for propagation constants does not change across the normal/PML or PML/PML interfaces. To show that the mode shape is also continuous across the boundary, we write Faraday’s law in the PML medium as

$$-j \omega \mu \overline{H}(x, y) \exp(-j \beta_z' z) = [\nabla_T \times \overline{E}(x, y)] \exp(-j \beta_z' z)$$

$$+ \left(\frac{1}{q_z} \frac{\partial}{\partial z}\right) \times [\overline{E}(x, y) \exp(-j \beta_z' z)]$$

$$-j \omega \mu \overline{H}(x, y) = [\nabla_T \times \overline{E}(x, y)] - \frac{\beta_z q_z}{q_z} [\hat{z} \times \overline{E}(x, y)]. \quad (2.33)$$
where \( \nabla_T \times \) represents the transverse part of the curl operator or

\[
\nabla_T = \frac{\partial}{\partial x} \hat{x} + \frac{\partial}{\partial y} \hat{y}
\]

(2.34)

and \( \times \) is the cross-product operator. Canceling the \( q_z \) terms in (2.33) leads to the same equation as in the non-PML medium. Repeating this analysis for Ampere’s law shows that the equations for the cross-sectional mode shape are identical in the PML and normal regions. The decay rate at any point in the PML is given by

\[
\kappa(z) = \text{Im} \left\{ \beta_z \left( 1 - \frac{j \sigma(z)}{\omega \epsilon} \right) \right\}.
\]

(2.35)

For a real propagation constant and conductivity profile given by (2.22), integration of the decay results in an effective modal reflection coefficient of

\[
R = \exp \left( -\frac{2 \sigma_{\text{max}} \beta_z \Delta z}{\omega \epsilon (n+1)} \right),
\]

(2.36)

which after rearranging becomes

\[
\frac{\sigma_{\text{max}}}{\epsilon_r} = -\frac{(n+1) \ln R \epsilon_0 \omega}{2 \beta_z \Delta z},
\]

(2.37)

representing another way of writing (2.23). For each region of different \( \epsilon_r \) in the waveguide cross section, we will have a different \( \sigma_{\text{max}} \) according to (2.37). This condition is equivalent to that given in [25]. (2.37) suggests that absorption of the guided mode will be difficult for small values of \( \beta_z \), since \( \sigma_{\text{max}} \) will be very large, and the stair stepping of the conductivity gradient rather coarse, leading to numerical reflection. This case is very similar to a plane wave at near grazing incidence. In such circumstances, the PML must be more finely discretized or an alternate ABC employed.

2.2.6 FDTD Volume Averaging

If scatterers are very small compared to the illumination wavelength, many FDTD cells will be required to model the medium. For example, in snow studies at microwave frequencies, ice grains may be as small as 0.01\( \lambda \). In these situations, computer memory is quickly exhausted, and the natural approach is to search for some
method to reduce the resolution of the simulation grid without sacrificing simulation accuracy. Methods for reducing the resolution of physical parameters are closely related to mixing methods, where the effective dielectric constant of a medium is expressed as some kind of average of the dielectric constants of the constituent materials. Rigorous methods exist for finding the effective dielectric constant of certain mixtures (for example, see [27]). An approach which was very useful in this research is obtained using the FDTD equations themselves.

Figure 2.7 shows a basic FDTD Yee cell. Ampere’s law in the $xy$ plane cut by the $E_z$ component is given as

$$\oint \mathbf{H} \cdot d\ell = \frac{d}{dt} \int \int \varepsilon \mathbf{E} \cdot d\Sigma + \int \int \sigma \mathbf{E} \cdot d\Sigma,$$  \hspace{1cm}(2.38)$$

where the integration is over the FDTD cell face. One of the inherent assumptions in FDTD is that each field component is constant in a Yee cell centered about the component. If an integration is added to both sides of (2.38) in the $z$ direction spanning the length of the Yee cell, we obtain

$$\int_{k\Delta z}^{(k+1)\Delta z} \frac{d}{dz} \oint d\ell = \frac{d}{dt} \int_{k\Delta z}^{(k+1)\Delta z} \int \int \varepsilon \mathbf{E} \cdot d\Sigma + \int_{k\Delta z}^{(k+1)\Delta z} \int \int \sigma \mathbf{E} \cdot d\Sigma.$$  \hspace{1cm}(2.39)
Figure 2.8: Geometry used to validate the volume-averaging method. An infinite cylinder is illuminated with a plane wave which travels in the \( \hat{k} \) direction and is polarized along the cylinder axis (\( \hat{z} \)). Far field \( E_z \) was computed as a function of \( \theta \).

When cell sizes are very small compared to the illumination wavelength, the equation can be discretized by assuming the fields are constant in a Yee cell centered about each component, or

\[
\Delta z \left[ H_{y,i+1,j,k}^n \Delta y - H_{x,i,j+1,k}^n \Delta x - H_{y,i,j,k}^n \Delta y + H_{x,i,j,k}^n \Delta x \right] = \\
\left[ E_{z,i,j,k}^{n+\frac{1}{2}} - E_{z,i,j,k}^{n-\frac{1}{2}} \right] \iint e(\tau) dV \\
\frac{H_{y,i+1,j,k}^n - H_{y,i,j,k}^n}{\Delta x} - \frac{H_{x,i,j+1,k}^n - H_{x,i,j,k}^n}{\Delta y} = \\
\frac{1}{\Delta t} \frac{1}{\Delta x \Delta y \Delta z} \iint e(\tau) dV. \tag{2.40}
\]

This equation is identical to the FDTD update equation obtained from the differential form of Ampere’s law, except that the dielectric constant is averaged in the Yee cell about the component. Thus, to reduce simulation resolution, we perform a simple volume average of the physical parameters in each cell.

To test the method, FDTD simulations were performed on an infinite dielectric cylinder of radius 0.01\( \lambda \) as depicted in Figure 2.8 (See Appendix B for exact equations for scattering from infinite dielectric cylinders). The cylinder was illuminated with an incident wave polarized along the cylinder axis and was discretized at 8 cells and 2 cell per diameter. Figure 2.9 compares the resulting scattered far
Figure 2.9: On-axis polarized scattered far fields from the infinite dielectric cylinder at 8 cells per diameter (left) and 2 cells per diameter (right).

fields with results from the exact solution. At 8 cells per diameter, both the volume-averaged and non-volume-averaged cases give a maximum absolute error for scattered field that is less than 2%. When resolution is reduced to 2 cells per diameter, the volume-averaged simulation still gives good results, while the non-volume-averaged simulation has 25% error.

2.3 One-dimensional FDTD PML Solutions

Certain applications may be highly sensitive to error induced by theoretical and numerical reflection off of the PML, and a numerically efficient one-dimensional (1D) solution for the PML is desirable for assessment. This section outlines a 1D method for finding fields as a function of distance along the propagation direction for single-mode operation of the FDTD code. The method requires the modal propagation constant and PML conductivities, and returns the exact $E$ and $H$ fields which are returned by the FDTD simulator for single-mode operation. This 1D method for the analysis of modal propagation in the PML is new. However, similar 1D analyses of the PML for plane waves are available elsewhere (for example, see [28]).

2.3.1 Functional Representation of Fields

Assuming a single mode which propagates in the positive and negative $\hat{z}$ directions, we first require a one-dimensional representation of fields in the $\hat{z}$ direction.
In general, we may write $E$ and $H$ fields as

$$E(x, y, z) = A^+(z)E^+(x, y) + A^-(z)E^-(x, y)$$

$$H(x, y, z) = A^+(z)H^+(x, y) + A^-(z)H^-(x, y),$$

where $A^+(z)$ and $A^-(z)$ are the complex envelopes, $E^+(x, y)$ and $E^-(x, y)$ are the electric field mode profiles, and $H^+(x, y)$ and $H^-(x, y)$ are the magnetic field mode profiles for the forward ($\{\cdot\}^+$) and reverse ($\{\cdot\}^-$) traveling modes. The shape of the forward and reverse traveling modes are identical, except for possible sign reversals.

To relate the functions for forward and reverse traveling modes, consider Equations (2.41). Reversal of the mode direction is equivalent to changing the sign of $\beta_z$. If field profiles $E^+(x, y)$ and $H^+(x, y)$ with propagation constant $\beta_z$ form a solution to (2.1), it is easily verified that

$$E_x^-(x, y) = E_x^+(x, y) \quad H_x^+(x, y) = -H_x^+(x, y)$$
$$E_y^-(x, y) = E_y^+(x, y) \quad H_y^+(x, y) = -H_y^+(x, y)$$
$$E_z^-(x, y) = -E_z^+(x, y) \quad H_z^+(x, y) = H_z^+(x, y)$$

is also a solution for propagation constant $-\beta_z$. Thus, we obtain the simplified equations

$$E_x(x, y, z) = [A^+(z) + A^-(z)] E_x^+(x, y) \quad H_x(x, y, z) = [A^+(z) - A^-(z)] H_x^+(x, y)$$
$$E_y(x, y, z) = [A^+(z) + A^-(z)] E_y^+(x, y) \quad H_y(x, y, z) = [A^+(z) - A^-(z)] H_y^+(x, y)$$
$$E_z(x, y, z) = [A^+(z) - A^-(z)] E_z^+(x, y) \quad H_z(x, y, z) = [A^+(z) + A^-(z)] H_z^+(x, y).$$

A concise representation for the longitudinal variation of the fields is given by the relations $E(z) = A^+(z) + A^-(z)$ and $H(z) = A^+(z) - A^-(z)$, which is used hereafter.

The next step in the one-dimensional solution requires substitution of the one-dimensional representation for the fields into the governing equations for the
PML (of which the normal region is a special case). The governing equations may be written for sinusoidal steady-state excitation as

\[
\begin{align*}
    j\omega\mu H_x &= \frac{1}{\mu z_r} \frac{\partial E_y}{\partial z} - \frac{1}{\mu z_r} \frac{\partial E_z}{\partial y}, \\
    j\omega\mu H_y &= \frac{\partial E_z}{\partial x} - \frac{1}{\mu z_r} \frac{\partial E_x}{\partial z}, \\
    j\omega\mu H_z &= -\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}, \\
    j\omega\epsilon E_x &= \frac{\partial H_y}{\partial z} - \frac{1}{\epsilon z_r} \frac{\partial H_z}{\partial y}, \\
    j\omega\epsilon E_y &= \frac{1}{\epsilon z_r} \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}, \\
    j\omega\epsilon E_z &= \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}.
\end{align*}
\]

(2.45)

where for discrete time stepping, \(\omega \leftarrow \omega \text{sinc}(\omega \Delta t/2)\). Without loss of generality, we assume a mode with \(E_y \neq 0\). The total fields for the \(H_x\) and \(E_y\) components are found by substitution of (2.44) into (2.45) to be

\[
\begin{align*}
    j\omega\mu H^+(x, y)H(z) &= \frac{1}{\mu z_r} E^+(x, y)E'(z) - \frac{\partial E^+(x, y)}{\partial y} H(z) \quad (2.46) \\
    j\omega\mu E^+(x, y)E(z) &= \frac{1}{\epsilon z_r} H^+(x, y)H'(z) - \frac{\partial H^+(x, y)}{\partial x} E(z). \quad (2.47)
\end{align*}
\]

We also know that the forward-propagating mode satisfies Maxwell’s equations in the PML or

\[
\begin{align*}
    j\omega\mu H^+_x(x, y) + j\beta_z E^+_y(x, y) &= -\frac{\partial E^+_y(x, y)}{\partial y} \quad (2.48) \\
    j\omega\epsilon E^+_y(x, y) + j\beta_z H^+_x(x, y) &= -\frac{\partial H^+_x(x, y)}{\partial x}. \quad (2.49)
\end{align*}
\]

where \(\beta_z = \beta'_z \text{sinc}(\beta'_z \Delta z/2)\) for finite resolution in \(\hat{z}\). Substitution of (2.48) and (2.49) into (2.46) and (2.47), and cancellation of appropriate terms leads to the coupled first-order ordinary differential equations

\[
\begin{align*}
    H(z) &= \frac{jE'(z)}{\mu z_r \beta_z} \quad (2.50) \\
    E(z) &= \frac{jH'(z)}{\epsilon z_r \beta_z}, \quad (2.51)
\end{align*}
\]

which may be solved with the same finite-difference scheme as the FDTD equations.

To ensure complete compatibility with FDTD, we need to be sure that we assume both discrete time and spatial stepping. Another subtle consideration concerns the
values we use for $\mu_{zr}$ and $\epsilon_{zr}$. Before, these were assumed to be $\mu_{zr} = [1 - j\sigma_z^*/(\omega\mu)]$ and $\epsilon_{zr} = [1 - j\sigma_z/(\omega\epsilon)]$. However, the split-component FDTD update equations in the PML actually employ effectively different values of $\mu_{zr}$ and $\epsilon_{zr}$. This fact is demonstrated by converting the FDTD PML update equations to the frequency domain, combining the split-field components, and inspecting the values of $\mu_{zr}$ and $\epsilon_{zr}$ used in the equations. To this end, we begin with the time-domain FDTD update equations for $H_{xz}$ and $H_{xy}$ and assume sinusoidal excitation to obtain

$$H_{xz,i,j,k} = \frac{(E_{y,i,j,k+1} - E_{y,i,j,k-1})/\Delta z}{j\omega\mu \text{sinc}(\omega\Delta t/2) + \sigma_z^* \cos(\omega\Delta t/2)}$$

$$H_{xy,i,j,k} = -\frac{(E_{z,i+1,j,k} - E_{z,i,j-1,k})/\Delta y}{j\omega\mu \text{sinc}(\omega\Delta t/2) + \sigma_y^* \cos(\omega\Delta t/2)},$$

where the $\cos(\cdot)$ term arises from the time averaging of $E$ and $H$ fields that is usually required when working with electric and magnetic conductivities in FDTD. Combining (2.52) and (2.53) into a single equation ($H_x = H_{xz} + H_{xy}$) and assuming the only nonzero conductivities to be $\sigma_z$ and $\sigma_z^*$, we obtain

$$j\omega\mu \text{sinc}(\omega\Delta t/2) H_x(x,y) = \frac{E_{y,i,j,k+1} - E_{y,i,j,k-1}}{\Delta z(1 - j\sigma_z^* \cos(\omega\Delta t/2) / \omega \mu \text{sinc}(\omega\Delta t/2))} - \frac{E_{z,i+1,j,k} - E_{z,i,j-1,k}}{\Delta y}.$$  

This expression is equivalent to the equation that would be obtained if the continuous field equations in the PML were cast in the frequency domain and discretized with

$$\mu_{zr} = 1 - j \frac{\sigma_z^* \cos(\omega\Delta t/2)}{\omega \mu \text{sinc}(\omega\Delta t/2)}. \tag{2.55}$$

A similar analysis of any of the FDTD PML update equations involving electric conductivities reveals that FDTD equations effectively use

$$\epsilon_{zr} = 1 - j \frac{\sigma_z \cos(\omega\Delta t/2)}{\omega \epsilon \text{sinc}(\omega\Delta t/2)}. \tag{2.56}$$

Since equations (2.50) and (2.51) were developed from an ideal frequency domain starting point, we must use

$$\mu_{zr} = 1 - j \frac{\sigma_z^* \cos(\omega\Delta t/2)}{\omega \mu \text{sinc}(\omega\Delta t/2)} \tag{2.57}$$

$$\epsilon_{zr} = 1 - j \frac{\sigma_z \cos(\omega\Delta t/2)}{\omega \epsilon \text{sinc}(\omega\Delta t/2)}. \tag{2.58}$$

This adjustment ensures that the new 1D method and FDTD solve precisely the same equations for single mode operation, and are therefore compatible.
Figure 2.10: One-dimensional PML gridding scheme with \( N \) cells. Conductivities are specified in each cell in the same manner as FDTD. The discrete samples of \( E(z) \) and \( H(z) \) fall on the staggered grid as depicted.

### 2.3.2 Solution Method

The following steps summarize the basic method for computing the one-dimensional solution of the FDTD PML:

1. Specify the modal reflection for the PML \( (R) \) and the mode propagation constant \( (\beta_z) \).
2. Compute the maximum electric conductivity with the relation \( (2.23) \).
3. Generate a one-dimensional finite-difference grid (see Figure 2.10) with magnetic and electric conductivities specified at each node in a manner equivalent to FDTD.
4. At each computational node, compute \( \mu_{zr} \) or \( \epsilon_{zr} \) according to \( (2.57) \) and \( (2.58) \). Usually, we assume \( \sigma_z/\epsilon = \sigma^*_z/\mu \). Also, the values of \( \sigma_z \) and \( \sigma^*_z \) are the average of the conductivities on the left and right of the node.
5. Form a matrix equation from the coupled differential equations given by \( (2.50) \) and \( (2.51) \) and invert the relationship to obtain \( E(z) \) and \( H(z) \).
6. The complete three-dimensional fields are now known by applying \( (2.44) \) in combination with the known mode shape.
2.4 Chapter Summary

This chapter outlined the finite-difference methods that were required for successful application of the hybrid technique in this research. The chapter presented a new 2D mode solution method based on a straightforward discretization of Maxwell's equations and a simple iterative linear solution. Development of the decay boundary condition provided a more accurate model for dielectric waveguides. Slight modifications to the method were required to ensure complete compatibility between the mode solutions and FDTD.

Information on FDTD outlined the implementation details of the computer program developed in this research. Novel application of the incident/scattered field formulation to waveguides suggested a new method for reducing modeling error. A new analysis of modal propagation in the PML proved the suitability of the PML technique for waveguide modeling. Finally, the chapter described a 1D technique for obtaining the guided mode PML response in FDTD.
Chapter 3

Radiative Transfer

Initially, radiative transfer theory \cite{2,29} was developed heuristically for use in astrophysical transport problems, but has later found successful application in many important active and passive remote sensing problems. Radiative transfer is suitable for modeling the interaction of propagating waves that have no consistent phase relationship, such as scattering in random media.

To model a random medium with an exact deterministic electromagnetic solver, one would begin by computing one possible realization of the random medium, simulating all of the complex field interactions, and then repeating the simulation over many realizations to obtain an idea of how the medium behaves over the ensemble. This procedure is costly due to the large size of the simulation domain and the many random realizations required.

Radiative transfer, on the other hand, replaces the complicated random medium with an idealized medium that scatters and absorbs power (over the ensemble average) the same as the true random medium (see Figure 3.1). The power flow in the idealized medium is governed by a very simple differential equation known as the equation of transfer. Solving the equation of transfer with respect to appropriate boundary conditions gives a unique solution for the scattering behavior of the medium. The theory is quite easily justified for sparse media, since particles will almost always be in the electromagnetic far field of each other, and will scatter power independently. For dense media, the theory is still useful, but the physical interpretation is more difficult \cite{3}. 

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This chapter provides a basic development of radiative transfer suited for the numerical computation of radiative transfer quantities in Chapter 4. Numerical solutions to radiative transfer are somewhat involved, but may be found in Appendix D by the interested reader.

Although the information in this chapter is not new, other sources generally do not present a unified explanation of radiative transfer, nor do they always indicate the physical interpretation of the equations. This author has attempted to overcome these deficiencies by collecting the important information in a single place and providing explanations that provide physical insight.

### 3.1 Specific Intensity and Stokes Parameters

Radiative transfer models electromagnetic propagation with the *specific intensity* \( I \), often referred to as just *intensity*. Specific intensity is defined in terms of the differential power \( dP \) in a frequency interval \( (\nu, \nu + d\nu) \) flowing through a
surface of area $dA$ in directions confined to an element of solid angle $d\Omega$ as

$$dP = I(\tau, \hat{s}) \cos \theta \ dA \ d\Omega \ d\nu,$$

(3.1)
as depicted in Figure 3.2. In general $I$ is a function of spatial position ($\tau$) and direction $(\hat{s})$. The polarization of propagating waves is defined with the set of modified Stokes parameters, or

$$\begin{bmatrix}
I_v \\
I_h \\
U \\
V
\end{bmatrix} = \frac{1}{\eta} \begin{bmatrix}
|E_v|^2 \\
|E_h|^2 \\
2 \text{ Re } \{E_v E_h^*\} \\
2 \text{ Im } \{E_v E_h^*\}
\end{bmatrix},$$

(3.2)

where $E_v$ and $E_h$ are the complex envelopes of the electric field for vertical and horizontal polarization. For sources which are not strictly monochromatic, the complex
envelopes $E_v$ and $E_h$ vary with time, and the modified stokes parameters are

$$T = \begin{bmatrix} I_v \\ I_h \\ U \\ V \end{bmatrix} = \begin{bmatrix} <|E_v|^2>_t \\ <|E_h|^2>_t \\ 2 \text{ Re} \{<E_v E_h^*>_t\} \\ 2 \text{ Im} \{<E_v E_h^*>_t\} \end{bmatrix}, \quad (3.3)$$

where $<\cdot>_t$ represents a time average. Finally, when independent streams of radiation combine, the Stokes parameters for the resulting stream are the sum of the Stokes parameters for the independent streams.

### 3.2 Equation of Transfer

The equation of transfer defines the attenuation or enhancement of specific intensity, given generally as

$$\frac{dI(\vec{r}, \hat{s})}{ds} = -\bar{k}_e(\vec{r}, \hat{s})I(\vec{r}, \hat{s}) + \bar{J}(\vec{r}, \hat{s}) + \int 4\pi d\Omega' \bar{P}(\vec{r}, \hat{s}, \hat{s}')I(\vec{r}, \hat{s}'). \quad (3.4)$$

The components of the equation of transfer are depicted in Figure 3.1. According to (3.4), incident intensity is attenuated by the extinction ($\bar{k}_e$), enhanced by thermal emission ($\bar{J}$), and enhanced by the scattering of intensity from other directions (dictated by the phase matrix $\bar{P}$). For an isotropic medium, physical quantities are not a function of the propagation direction $\hat{s}$, and $\bar{k}_e$ is not a function of polarization. For a homogeneous medium, the physical quantities are independent of spatial coordinate $\vec{r}$. Thus, for a homogeneous isotropic medium, we have

$$\frac{dI(\vec{r}, \hat{s})}{ds} = -k_e I(\vec{r}, \hat{s}) + J(\vec{r}) + \int 4\pi d\Omega' \bar{P}(\hat{s}, \hat{s}')I(\vec{r}, \hat{s}'), \quad (3.5)$$

where positional dependence of $J$ has been intentionally retained to allow for non-uniform temperature distributions. The following sections describe in detail each component of the equation of transfer as expressed in (3.5).

### 3.3 Extinction Matrix

This section provides a basic definition of the extinction matrix and the isotropic absorption and scattering coefficients. Consult Appendix $E$ for numerical expressions for the extinction coefficients of Rayleigh and Mie dielectric spheres.
Extinction consists of a combination of absorptive and scattering loss. Symbolically, $\bar{k}_e = \bar{k}_a + \bar{k}_s$, where $\bar{k}_a$ is the absorption matrix and $\bar{k}_s$ is the scattering matrix. For isotropic media, the absorption and scattering matrices are the identity matrix multiplied by the scalars $k_a$ and $k_s$, respectively. Figure 3.3 depicts an infinitesimal volume used to define $k_a$ and $k_s$.

![Figure 3.3: Incremental volume used to define radiative transfer quantities](image)

Note that there is a subtle difference between extinction due to absorption and scattering. Intensity which is lost due to absorption is converted into other forms of energy (such as thermal), and the energy does not reappear in (3.4). Intensity which is lost due to scattering reappears as a contribution to the phase matrix integration, and the energy remains in the system.

### 3.3.1 Absorption Coefficient

To define the absorption coefficient, consider an incident intensity of $I$ passing through an area of $dA$ confined to the solid angle $d\Omega$. The reduction in
incident intensity due to absorption is \( dI_a = k_a I \, ds \), and the differential reduction in power passing through the area \( dA \) due to absorption is

\[
dP_a = dI_a \, d\Omega \, dA = k_a I \, ds \, d\Omega \, dA = k_a I \, d\Omega \, dV. \tag{3.6}
\]

\( Id\Omega \) is a differential incident power area density \((dS_i)\), and substitution yields

\[
k_a = \frac{1}{dS_i} \frac{dP_a}{dV}. \tag{3.7}
\]

Thus, the physical interpretation of \( k_a \) is the power absorbed per unit volume per unit of incident power density. For sparse media, the absorption coefficient may be computed by considering single scatterers in isolation. If a single scatterer with parameters \( \zeta \) (size, orientation, shape, etc.) absorbs power \( P_a(\zeta) \) for an incident power density of \( S_i \), a medium of \( N \) scatterers will absorb (on average)

\[
N \, \text{E}\{P_a\} = N \int f(\zeta) P_a(\zeta) d\zeta, \tag{3.8}
\]

where \( f(\zeta) \) is the joint PDF of all the particle parameters. Thus, \( k_a \) may be written as

\[
k_a \approx \frac{1}{S_i} \frac{N \, \text{E}\{P_a\}}{V} = \frac{1}{S_i} n_0 \, \text{E}\{P_a\}, \tag{3.9}
\]

where \( n_0 \) is the number of scatterers per unit volume. For a dense medium, coherent interaction of scattered fields will occur due to the restrictions imposed on the relative particle positions. In this case, \( k_a \) is chosen so that the idealized radiative transfer medium absorbs the same total power (on average) as the physical medium as the medium becomes infinite, or

\[
k_a = \lim_{\Delta V \to \infty} \frac{1}{\Delta V} \frac{\text{E}\{P_a(\Delta V)\}}{S_i}, \tag{3.10}
\]

where \( P_a(\Delta V) \) is the power absorbed by a medium of volume \( \Delta V \) for an incident power density of \( S_i \). Since the ideal radiative transfer medium has no boundary, we require the limit \( (\Delta V \to \infty) \), which removes the effect of the boundary for the true random medium.
3.3.2 Scattering Coefficient

The development of the scattering coefficient is analogous to the absorption coefficient. In this case, we consider the reduction in incident intensity due to scattering \((dI_s = k_s I \, ds)\). The differential reduction in power passing through the area \(dA\) due to scattering is

\[
dP_s = k_s I \, d\Omega \, dV
\]

and

\[
k_a = \frac{1}{dS_i} \frac{dP_s}{dV}.
\]

The physical interpretation of \(k_s\) is the power scattered per unit volume per unit of incident power density. As with the absorption coefficient, for sparse media the scattering coefficient may be computed from the power scattered by a single scatterer \((P_s)\), or

\[
k_s = \frac{1}{S_i} n_0 \, E \{ P_s \}.
\]

For dense media, \(k_s\) is chosen so that the idealized radiative transfer medium scatters the same total power (on average) as the physical medium as the medium becomes infinite, or

\[
k_s = \lim_{\Delta V \to \infty} \frac{1}{\Delta V} \frac{E \{ P_s(\Delta V) \}}{S_i},
\]

where \(P_s(\Delta V)\) is the power scattered by the random medium of volume \(\Delta V\) for an incident power density of \(S_i\).

3.4 Emission Vector

The emission vector represents a forcing source term, due to random thermal emission of the medium. For an isotropic medium, the emission vector may be written as

\[
\overline{J} = \begin{bmatrix} J \\ J \\ 0 \\ 0 \end{bmatrix}
\]
with

\[ J = k_e \frac{K}{\lambda_m^2} T, \tag{3.16} \]

where \( k_e \) is the emission coefficient (for thermal equilibrium, \( k_e = k_a \)), \( K \) is Boltzmann’s constant, \( \lambda_m \) is the wavelength in the medium, and \( T \) is the physical temperature. Emission is usually only important for passive remote sensing, where no coherent source function exists. In this case, casting the equation of transfer in terms of brightness temperature is convenient. Brightness temperature \( (T_B) \) as related to specific intensity is

\[ T_B = \frac{I \lambda}{2 \pi m K}, \tag{3.17} \]

which allows (3.14) to be written as

\[ \frac{dT_B(\tau, \hat{s})}{ds} = -\bar{k}_e(\tau, \hat{s})T_B(\tau, \hat{s}) + \bar{k}_a(\tau, \hat{s})T + \int_{4\pi} d\Omega' \bar{P}(\tau, \hat{s}, \hat{s}')T_B(\tau, \hat{s}'), \tag{3.18} \]

where thermal equilibrium is assumed.

### 3.5 Phase Matrix

This section provides the definition of the phase matrix. For information on actual computation of the phase matrix, consult Appendix E. The phase matrix \( \bar{P}(\hat{s}, \hat{s}') \) relates the incident intensity propagating in direction \( \hat{s}' \) to the scattered intensity propagating in direction \( \hat{s} \). The enhancement in incident intensity due to collected scattering from all propagation directions is

\[ \frac{dI_c}{ds} = \int_{4\pi} d\Omega \bar{P}(\hat{s}, \hat{s}')I(\hat{s}'). \tag{3.19} \]

To gain physical insight into the meaning of the phase matrix, we assume an incident wave with Stokes parameters

\[ T(\hat{s}') = T_i \delta(\hat{s}' - \hat{s}_0), \tag{3.20} \]

which represents a plane wave propagating in the direction \( \hat{s}_0 \). Performing the integration in (3.19) and writing in terms of total power collected passing through the area \( dA \), we obtain

\[ \bar{P}(\hat{s}, \hat{s}_0)T_i d\Omega = \frac{dP_c}{dV}. \tag{3.21} \]
Next, we define the quantity $I_i d\Omega = \hat{I}_i dS_i$, which breaks the incident intensity into Stokes parameters with unit intensity ($\hat{I}_i$) and a differential power density ($dS_i$) that applies the appropriate scaling. The phase matrix relationship becomes

$$\overline{P}(\hat{s}, \hat{s}_0) \hat{I}_i = \frac{1}{dS_i} \frac{dP_c}{dV}.$$ 

(3.22)

The physical interpretation of $\overline{P}(\hat{s}, \hat{s}_0) \hat{I}_i$ is therefore the power collected from direction $\hat{s}_0$ and polarization $\hat{I}_i$ per unit volume per unit of incident power density. As before, for a sparse medium we may compute the phase matrix for a single particle and sum over all particles. For a single particle, we first construct the scattering matrix, which relates scattered far fields to incident fields, or

$$\begin{bmatrix} E_{vs} \\ E_{hs} \end{bmatrix} = \frac{e^{jkr}}{r} \begin{bmatrix} f_{vv} & f_{vh} \\ f_{hv} & f_{hh} \end{bmatrix} \begin{bmatrix} E_{vi} \\ E_{hi} \end{bmatrix},$$

(3.23)

where $k$ is the wavenumber, the subscripts $v$ and $h$ specify vertical and horizontal polarization, and the subscripts $i$ and $s$ specify incident and scattered fields. The Stokes matrix for the single particle relates incident Stokes parameters to scattered Stokes parameters, or

$$\overline{L} = \begin{bmatrix} |f_{vv}|^2 & |f_{vh}|^2 \\ |f_{hv}|^2 & |f_{hh}|^2 \\ 2\text{Re}\{f_{vv}f_{vh}^*\} & 2\text{Re}\{f_{vh}f_{hh}^*\} \\ 2\text{Im}\{f_{vv}f_{hv}^*\} & 2\text{Im}\{f_{vh}f_{hh}^*\} \\
\text{Re}\{f_{vv}f_{vh}^*\} & -\text{Im}\{f_{vv}f_{vh}^*\} \\
\text{Re}\{f_{hv}f_{hh}^*\} & -\text{Im}\{f_{hv}f_{hh}^*\} \\
\text{Re}\{f_{vv}f_{hh}^* + f_{vh}f_{hv}^*\} & -\text{Im}\{f_{vv}f_{hh}^* - f_{vh}f_{hv}^*\} \\
\text{Im}\{f_{vv}f_{hh}^* + f_{vh}f_{hv}^*\} & \text{Re}\{f_{vv}f_{hh}^* - f_{vh}f_{hv}^*\} \end{bmatrix}.$$ 

(3.24)

The phase matrix is then given as

$$\overline{P}(\hat{s}, \hat{s}') = n_0 \int f(\zeta) \overline{L}(\zeta) \, d\zeta.$$ 

(3.25)

In the case of dense random media, coherent interactions will again affect the scattering behavior. The phase matrix is chosen so that the power scattered as a function of
angle in the ideal radiative transfer medium is equal to the average power scattered as a function of angle in the true random medium, or

\[ \overline{P} = \lim_{\Delta V \to \infty} \frac{1}{\Delta V} \mathbb{E}\{\overline{L}(\Delta V)\}, \]  

(3.26)

where \( \overline{L}(\Delta V) \) is the Stokes matrix for a section of the random medium of size \( \Delta V \).

### 3.6 Boundary Conditions

Figure 3.1 depicts the specification of boundary conditions to terminate the radiative transfer domain, and Figure 3.4 depicts a general boundary condition. Each boundary condition must provide a function that relates specific intensity in one region to the specific intensity in adjacent regions. Often, the relation may be cast in the form of an integral expression

\[ I_m(\tau_{m0}, \hat{s}) = \int_{4\pi} d\Omega' \left[ \overline{R}_{mn}(\hat{s}, \hat{s}')T_m(\tau_{m0}, \hat{s}') + \overline{T}_{nm}(\hat{s}, \hat{s}')T_n(\tau_{n0}, \hat{s}') \right], \]  

(3.27)

where \( \overline{R}_{mn} \) is the reflection matrix in region \( m \) looking down into region \( n \), and \( \overline{T}_{nm} \) is the transmission matrix from region \( n \) into region \( m \).

#### 3.6.1 Fresnel Surface

To illustrate the inclusion of boundary conditions, the boundary condition for an ideal Fresnel interface for layered media is presented. The remote sensing
examples in Chapter 4 employ this same boundary condition. In this case, interfaces are treated as ideal planes. The transmission matrix from layer $m$ to layer $n$ is

$$
\mathbf{T}_{mn}(\theta_i) = \frac{\epsilon_n \cos \theta_i}{\epsilon_m \cos \theta_i} \begin{bmatrix}
t_{v, mn} & 0 & 0 & 0 \\
0 & t_{h, mn} & 0 & 0 \\
0 & 0 & \text{Re} \{Y_{mn} X_{mn}^*\} & -\text{Im} \{Y_{mn} X_{mn}^*\} \\
0 & 0 & \text{Im} \{Y_{mn} X_{mn}^*\} & \text{Re} \{Y_{mn} X_{mn}^*\}
\end{bmatrix}
$$

(3.28)

for $\theta_i \in [0, \theta_c]$ ($\theta_c$ is the critical angle), and zero otherwise. The reflection matrix from layer $m$ looking down into layer $n$ is

$$
\mathbf{R}_{mn}(\theta_i) = \begin{bmatrix}
r_{v, mn} & 0 & 0 & 0 \\
0 & r_{h, mn} & 0 & 0 \\
0 & 0 & \text{Re} \{S_{mn} R_{mn}^*\} & -\text{Im} \{S_{mn} R_{mn}^*\} \\
0 & 0 & \text{Im} \{S_{mn} R_{mn}^*\} & \text{Re} \{S_{mn} R_{mn}^*\}
\end{bmatrix}
$$

(3.29)

for $\theta_i \in [0, \pi/2]$ and zero otherwise, where

$$
t_{h, mn} = 1 - |R_{mn}|^2 \quad R_{mn} = \frac{k_{mz} - k_{nz}}{k_{mz} + k_{nz}} = X_{mn} - 1 \\
t_{v, mn} = 1 - |S_{mn}|^2 \quad S_{mn} = \frac{\epsilon_n k_{mz} - \epsilon_m k_{nz}}{\epsilon_n k_{mz} + \epsilon_m k_{nz}} = Y_{mn} - 1 \\
r_{h, mn} = |R_{mn}|^2 \quad k_{mz} = k_0 \sqrt{\epsilon_m \cos \theta_i} \\
r_{v, mn} = |S_{mn}|^2 \quad k_{nz} = k_0 \sqrt{\epsilon_n \cos \theta_i}
$$

(3.30 - 3.33)

and $\epsilon_m$ and $\epsilon_n$ are the dielectric constants in layer $m$ and $n$, respectively. The transmitted angle is found through the relation

$$
\sqrt{\epsilon_n \sin \theta_t} = \sqrt{\epsilon_m \sin \theta_i}.
$$

(3.34)

The critical angle is the incident angle $\theta_c = \theta_i$ at which $\theta_t = \pi/2$. The boundary condition from layer $m$ looking into $n$ may be written as

$$
\mathbf{T}^+_m(\theta_i, \phi_i) = \mathbf{R}_{mn}(\theta_i) \mathbf{T}^-_m(\theta_i, \phi_i) + \mathbf{T}_{nm}(\theta_i) \mathbf{T}^+_n(\theta_t, \phi_i),
$$

(3.35)

where $\mathbf{T}^+$ and $\mathbf{T}^-$ indicate upward and downward traveling intensities. Similarly, the condition from layer $n$ looking up into $m$ is

$$
\mathbf{T}^-_n(\theta_i, \phi_i) = \mathbf{R}_{nm}(\theta_i) \mathbf{T}^+_n(\theta_i, \phi_i) + \mathbf{T}_{mn}(\theta_i) \mathbf{T}^-_m(\theta_t, \phi_i).
$$

(3.36)
3.7 Chapter Summary

This chapter has described the radiative transfer method appropriate for modeling random snow media in Chapter 4. The chapter has defined the key radiative transfer quantities for both sparse and dense media and has provided physical interpretation of these quantities where possible.
Chapter 4

Snow Modeling for Remote Sensing

For several decades, space-borne microwave instruments have monitored the global environment, archiving large sets of active and passive remote sensing data. A continuing arena of important research is concerned with using these data sets to track the temporal evolution of key geophysical parameters that serve as indicators of global status and change. One important example of this effort involves extracting important properties of the earth’s large ice sheets, such as trends in snow accumulation and movement of different zone boundaries [30, 32].

The use of remote sensing data to extract geophysical parameters requires techniques that relate the observed data to the physical parameters. A few empirical studies relating snow and ice parameters to radar data have emerged (for example, see [33, 36]). However, because of the complex nature of snow and ice, full characterization of such media through direct measurement is very difficult. A second approach applies detailed electromagnetic models to correlate radar data with physical parameters. Unfortunately, the complexity of the media, coupled with the large size of the regions under investigation, renders the use of exact numerical electromagnetic techniques prohibitively costly.

One solution for efficiently characterizing the electromagnetic response of large ice sheets is radiative transfer theory [2, 3, 29], a technique that models large regions of random media with macroscopic quantities that tend to be spatially uniform over the illumination area of space-borne remote sensing instruments. Several statistical methods exist for computing the relevant quantities required for radiative transfer:
1. Single particle analytical methods compute the scattering and absorption for a single scatterer. For sparse media, the radiative transfer quantities for the ensemble of particles are the single particle quantities scaled by the number of particles per unit volume. These methods only exist for very simple scatterer geometries and ignore any coherent interaction of particles.

2. Dense-medium analytical methods compute the scattering and absorption of the ensemble of particles, taking into account near-field interaction due to the correlation in particle positions. However, these methods are also limited to very basic geometries and particle correlation functions.

3. Monte Carlo analysis methods may characterize dense media with arbitrary correlation in particle positions. Also, the type of electromagnetic solver may be analytical or numerical, accommodating quite arbitrary particles.

Traditionally, effort has focused on analytical methods [29, 37, 38], although the necessary simplifying assumptions limit their applicability to very basic medium models. More complex media are often accommodated by modifying parameters (e.g. snow grain size, snow density) to make radar observations match model predictions [32, 36, 38].

Recent work has demonstrated a new method that combines Monte Carlo analysis with a T-matrix electromagnetic solver to obtain the radiative transfer quantities for non-penetrating spheres [4]. The method generates many random realizations (or test volumes) and computes the radiative transfer quantities as averages over the realizations. However, the method has two basic drawbacks. First, the T-matrix method limits the application of the technique to very simple media (such as non-penetrating spheres). Second, no analysis of the accuracy of the technique was provided, a component that is critical for determining the required number of Monte Carlo realizations and the required size of the test volumes.

This research overcomes these difficulties by developing a new method that couples Monte Carlo analysis with the finite-difference time-domain (FDTD) technique (see Chapter 2), providing a very powerful tool that can analyze arbitrary
random media. When coupled with a numerical radiative transfer solver, this method captures all of the important near-field and multiple-scattering effects required for accurate electromagnetic characterization of random media. Also, this research presents a new study on the error of the method versus the test volume sizes and the number of random realizations, information which is critical to ensure sufficient accuracy of the method.

Thus, the hybrid method proposed for this problem is (1) FDTD and the Monte Carlo method to obtain extinction coefficients and phase matrices required for radiative transfer, and (2) numerical radiative transfer to compute backscatter coefficients and brightness temperatures. This chapter presents the hybrid FDTD/radiative transfer method with the following steps:

1. Section 4.1 adapts the analytical radiative transfer framework in Chapter 3 to obtain radiative transfer quantities numerically with the Monte Carlo method and FDTD. The results are similar to those given in [4].

2. Section 4.2 presents a study on the effects of finite volume size and finite Monte Carlo realizations. Although these effects have received little or no attention in the past, this section demonstrates that ignoring these effects may lead to large modeling errors.

3. Section 4.3 presents the results of FDTD simulations for sparse and dense distributions of non-penetrating spheres, demonstrating good agreement with existing analytical methods. Next, analysis of a penetrating sphere model demonstrates the power of the new method for modeling arbitrary media, since penetrating spheres cannot be analyzed with any of the existing methods. The large increase in scattering observed with the penetrating sphere model underlines the importance of correct media characterization and the need for these generalized numerical methods.

4. Finally, Section 4.4 shows the utility of the new method by computing the brightness temperature and backscatter of a snow layer overlying a homogeneous
ice layer. The numerical radiative transfer method in Appendix D is used to compute these solutions. The simulations indicate the possible change in predicted data (as measured by space-borne scatterometers and radiometers) as a function of snow depth and the type of physical snow model.

4.1 Numerical Computation of Radiative Transfer Quantities

This section describes the method employed in this research to find extinction coefficients and phase matrices numerically with FDTD and the Monte Carlo method. The basic method is similar to the method presented in [4].

The analytical expressions for the general phase matrix and extinction coefficient given in Chapter 3 involve a volume size which becomes infinite in the limit, which is impossible to model on computers with finite memory and processing power. When the simulation volume is finite, an outside boundary exists which leads to (1) artificial correlation in scatterer positions, and (2) surface scattering due to a change in the effective permittivity.

The only way to mitigate the problem of artificial correlation in scatterer positions is to ensure that the volume is "big enough" so that the number of scatterers near the boundary is small compared to the number of interior scatterers.

Next, As a wave propagates across the boundary enclosing the scatterers, it will experience a change in the effective dielectric constant, leading to surface scattering. The effect of unwanted surface scatter is usually removed from the computation by appropriate Monte Carlo implementation. In this case, the scattered field is decomposed according to the relation

\[ \overline{E}_s = \mathbb{E}\{E_s\} + \overline{\mathcal{E}}_s. \]  

(4.1)

The coherent field \( \mathbb{E}\{E_s\} \) is the average of the scattered field over the Monte Carlo realizations, which for a random medium is due to boundary scattering alone. In an unbounded medium, for example, the scattered field is a combination of many components with random phases, and the average scattered field over the ensemble is zero. The incoherent field \( \overline{\mathcal{E}}_s \) represents the field that differs from the average for
each realization and represents the scattered field for an unbounded random medium. Thus, the boundary scattering effect is removed by utilizing incoherent field quantities in the computations.

Naturally, the effectiveness of the Monte Carlo method depends on both the volume size and the number of Monte Carlo realizations. Section 4.2 outlines a study that examines these issues.

4.1.1 Phase Matrix

To compute the phase matrix, \(3.26\) is adapted by replacing the expectation with an average over \(N\) random realizations of the scattering volume. Also, the scattered field for the infinite volume is replaced with the incoherent scattered field for a finite volume.

Figure 4.1 depicts the basic geometry used to compute the phase matrices. The \(N\) distinct finite test volumes are generated based upon statistical distributions describing snow grain properties. For each realization, two electromagnetic analyses must be performed. First, the volume is illuminated with a vertically polarized plane wave and fields are stored internal to the volume (for absorption computation) and
in the far field. Second, the volume is illuminated with a horizontally polarized plane wave and the same quantities are computed. For isotropic media, only far fields in the plane of incidence need to be stored, since the resulting phase matrix will be invariant to rotation of the test volumes.

Computation of the phase matrix involves correlating combinations of the horizontal and/or vertical components for different scattered directions in space. In the electromagnetic analysis, we must store fields that correspond physically to the same direction for both the horizontal and vertical components. For the isotropic case, for example, we may be tempted to illuminate the test volume with a single incident polarization and then define two different planes of incidence to compute vertical \((V)\) and horizontal \((H)\) components. However, for a random medium, any correlation between \(H\) and \(V\) in this scheme will be lost, and the elements of the phase matrix other than \(P_{11}\) and \(P_{22}\) will tend to zero. Generally, we will require two separate electromagnetic simulations or analyses for the two distinct polarizations.

For the far-field computations, the incoherent field for the \(n\)th realization is given by

\[
\mathcal{E}_{s}^{(n)} = \mathcal{E}_{s}^{(n)} - \frac{1}{N} \sum_{i=1}^{N} \mathcal{E}_{s}^{(i)},
\]

(4.2)

where \(\mathcal{E}_{s}^{(n)}\) is the incoherent scattered field for the \(n\)th realization and \(\mathcal{E}_{s}^{(n)}\) is the scattered field for the \(n\)th realization. The scattering matrix elements for each realization are then obtained from the expression

\[
f_{\beta\alpha} = \frac{\mathcal{E}_{s\gamma}}{E_{\alpha i}} \left( \frac{r}{e^{jkr}} \right) \bigg|_{E_{\gamma i}=0, \gamma \neq \alpha},
\]

(4.3)

where \(\alpha, \beta, \text{ and } \gamma\) can be either \(v\) or \(h\) for vertical or horizontal polarization. The Stokes matrix \(\mathcal{L}^{(n)}\) for the \(n\)th realization is then computed, and the phase matrix is constructed from the expression

\[
\mathcal{P} = \frac{1}{N \Delta V} \sum_{n=1}^{N} \mathcal{L}^{(n)}.
\]

(4.4)
4.1.2 Extinction Coefficients

Absorption and scattering coefficients are computed in a manner similar to the analytical expressions given by (3.10) and (3.14). Again, the expectations are replaced with an average over the \( N \) realizations, and scattered far fields of the infinite volume are replaced with scattered incoherent far fields for the finite volume. The same \( N \) volumetric realizations for computing the phase matrix may be reused. The absorption coefficient is

\[
k_a = \frac{\eta_0}{|E_i|^2 N \Delta V} \sum_{n=1}^{N} \int \int dV \frac{\sigma(\vec{r})}{\Delta V} \left| \vec{E}_s^{(n)}(\vec{r}) \right|^2, \tag{4.5}
\]

where \( \vec{E}_s^{(n)} \) is computed according to (4.2), and the integration is over the scattering volume. The scattering coefficient is

\[
k_s = \frac{\eta_0}{|E_i|^2 N \Delta V} \sum_{n=1}^{N} \int \int dS \left| \vec{E}_s^{(n)}(\vec{r}) \right|^2, \tag{4.6}
\]

where \( S \) denotes an integration surface in the far field.

4.2 Finite Volume and Realization Effects

The previous section described the basic method for numerical computation of radiative transfer quantities via the Monte Carlo method. However, the number of Monte Carlo realizations and the size of the simulation test volumes impact the accuracy of the method. This section provides a detailed study of the effect of finite simulation constraints on the accuracy of the numerical solution. Since using a full-wave solver such as the FDTD method for this study would lead to excessive computational times, a simple Mie scattering technique, which assumes independent summing of the fields from individual snow particles, was developed and used in order to achieve computational efficiency. Performing the study using the assumption of independent scattering allows assessment of the upper bound on required volume size. In other words, if multiple scattering is accounted for, we expect more attenuation in the coherent wave, resulting in shorter interaction distances and therefore a smaller required test volume.
The Mie scattering solution proceeds as follows. A cubical test volume containing a collection of dielectric spheres with center coordinates chosen according to a uniform distribution is generated for a specified size and volume fill fraction. The scattered far fields for a single sphere are calculated using the Mie series as outlined in Appendix C. Assuming independent scattering of fields, the total scattered far field is

$$
\mathbf{E}_{s, \text{total}}(\theta, \phi) = \sum_{n=1}^{N} \mathbf{E}_{s, \text{scat}}(\theta, \phi) \exp \left[ jk \psi(\vec{r}_n) \right],
$$

where

$$
\psi(\vec{r}_n) = x_n \sin \theta \cos \phi + y_n \sin \theta \sin \phi + z_n (\cos \theta - 1),
$$

$\mathbf{E}_{s, \text{scat}}$ is the scattered far-field pattern from a single sphere, and $\vec{r}_n$ is the position of the $n$th sphere center. Once scattered far fields are obtained, the framework developed in Section 4.1 is used directly to obtain phase matrices and extinction coefficients.

In this study, spheres may interpenetrate in the random realizations, which would eliminate any correlation in scatterer positions if no boundary were present. Also, since the analytical solution for independent Mie scattering employs the same assumption, error may be quantified as the difference between the Monte Carlo Mie solution and the analytical solution. The analytical expression for the Mie phase matrix is given in Appendix E.

### 4.2.1 Phase Matrix Convergence

The phase matrix, unlike extinction, contains no integration over observation angles. Thus, the phase matrix should be a more sensitive indicator of error than extinction. In the studies that follow, error is assessed in terms of $P_{11}$ and $P_{22}$, which are two elements of the phase matrix that correspond to vertical and horizontal scatter of the random medium, respectively. Figure 4.2 shows $P_{11}$ (in the plane of incidence) as a function of scattered angle and volume size. This plot reveals that the phase matrix component converges to the analytical solution as the volume becomes large. For the given parameters, a cube with a side length of $5\lambda$ captures most of
Figure 4.2: Plot of $P_{11}$ pattern in the plane of incidence as a function of the length of one side of the test volume cube. Simulation parameters were scatterer radii $a = 0.1\lambda$, fractional volume $f = 10\%$, realizations $N = 256$, and scatterer dielectric constant $\epsilon_s = 3.2\epsilon_0$.

Figure 4.3: Accurate characterization of forward scattering behavior requires a larger test volume size than backscatter due to the nearly equal phase of scattered field components near the forward scattering direction. The behavior. Note that further increase in volume size only reduces error in a small angular neighborhood about the forward scatter direction.

Figure 4.3 provides an explanation of why error in the forward scatter direction is generally higher than the backscatter direction. For a small test volume, scattered fields propagating near the forward direction will have almost identical phase, since only small phase shifts arise from transverse ($\hat{y}$) position of the particles. These waves of equal phase contribute principally to the coherent component, which is removed in the phase matrix computations. In the backscatter direction, however,
longitudinal ($\hat{z}$) variation in particle positions leads to large differences in the phases of the scattered fields, and the correct scattering behavior is adequately captured.

The effect of the number of realizations on the phase matrix for a cubical volume with a side length of $5\lambda$ is depicted in Figure 4.4. These results indicate that the number of realizations impacts the regularity or smoothness of the solution as opposed to changing the level of scattering. The largest number of realizations (256) gives the best results; however, in the FDTD simulations, 32 realizations are used to provide sufficient accuracy but avoid excessive computation time.

4.2.2 Error Quantification

To quantify the error in the phase matrix elements, average and absolute error are defined as

\[
\text{Average Error} = \frac{1}{N} \sum_{n=1}^{N} \frac{P_{n,\text{th}} - P_n}{P_{n,\text{th}}},
\]

\[
\text{Absolute Error} = \frac{1}{N} \sum_{n=1}^{N} \left| \frac{P_{n,\text{th}} - P_n}{P_{n,\text{th}}} \right|,
\]

where $P_n$ is the value of the phase matrix element at the $n$th far-field angle predicted by the Mie scattering code and $P_{n,\text{th}}$ is the corresponding theoretical value. Average
error indicates bias in the phase matrix element, while absolute error indicates the approximate fractional error at each angle. Since the phase matrix elements are already power quantities, mean square error was not considered a useful metric. Figure 4.5 plots the average and absolute error as a function of cubical volume side length for 256 realizations. The figure demonstrates that the average error (or bias) vanishes as the volume size increases. The absolute error also tends to zero, although more slowly. Both curves tend to level off, suggesting a point of diminishing returns.

Figure 4.6 shows the error as a function of the number of realizations for a cube with a side length of $1\lambda$. The average and absolute error both level off at around 256 realizations. This result implies that increasing the number of realizations cannot fully compensate for a small volume size. This behavior is likely due to the substantial correlation in scatterer positions due to the boundary when the test volume is too small. This correlation leads to an increase in the coherent scattered component and a reduction in the incoherent component, which will underpredict the amount of scatter in the radiative transfer computations.

Figure 4.7 shows the error as a function of realizations for a cube with a side length of $20\lambda$. This plot demonstrates the expected downward trend with an increasing number of realizations. Although the error converges to a lower level than
that observed for the 1\(\lambda\) case, a lower bound on the error appears to exist for this test volume as well.

Figure 4.8 plots contours of constant absolute error versus the number of realizations and volume size. For each number of realizations \((N)\) tested, 256 total realizations were run and subdivided into sets of \(N\) realizations, giving \(256/N\) trials. The absolute error across all the trials was then averaged to enhance the smoothness of the plot for low realization counts. The plots for \(P_{11}\) and \(P_{22}\) are slightly different, possibly due to the finite number of test runs, as well as fundamental differences in the shapes of vertical \((P_{11})\) and horizontal \((P_{22})\) scatter. However, the basic trends
Figure 4.8: Plot of absolute error for $P_{11}$ and $P_{22}$ as a function of the number of realizations ($N$) and the volume size. Simulation parameters were scatterer radii $a = 0.1\lambda$, fractional volume $f = 10\%$, and scatterer dielectric constant $\epsilon_s = 3.2\epsilon_0$. Dashed lines in $P_{11}$ indicate contours of constant simulation time for FDTD.

in the two plots are very similar, demonstrating the overall tradeoff between volume size and the number of random realizations.

Figure 4.8 also highlights the care that is required when choosing these simulation parameters. For example, if simulations were run at 8 realizations and a volume size of $2\lambda$, error will drop much faster by increasing the realizations as opposed to the volume size. Generally, the numerical electromagnetic solver employed dictates the ideal number of realizations and volume size for a specified level of error. For example, with FDTD, simulation time is linearly proportional to simulation volume, or proportional to $\ell^3$, where $\ell$ is the side length of the cubical test volume. In most cases, simulation time will also increase linearly with the number of realizations. The dashed lines in the plot of $P_{11}$ indicate contours of constant simulation time for FDTD. If absolute error were the only important metric, we should operate at points where the simulation time contours are parallel to the error contours, thus minimizing absolute error for a fixed simulation time. However, in later FDTD simulations, the average error is also important, so a somewhat larger test volume is used than would be optimal in these plots.

A final important feature of Figure 4.8 is that for small volume sizes and $N \geq 32$, the contours become nearly horizontal, indicating that increasing the number
of realizations will have almost no effect on the error. Only a larger volume size will reduce error significantly at this point. This fact is consistent with Figure 4.2 which shows that accuracy in the forward scattering direction is fundamentally limited when the volume size is too small.

4.3 FDTD Simulations

In order to accurately compute the radiative transfer quantities for a dense medium, the chosen electromagnetic solver must account for coherent interaction of the closely spaced particles. Also, since geophysical media tend to have complex structure, a solver that can accommodate arbitrary media is preferable. This study applied FDTD due to its computational efficiency, ease of implementation, and ability to simulate very complex media.

The basic configuration for the FDTD test volume is depicted in Figure 4.9. A cubical test volume with a side length of of $5\lambda$ was used, consistent with the observations of the convergence study. The sphere size was chosen to be realistic for coarse-grained snow at 14 GHz, with snow grain radii of $a = 0.1\lambda$ and $0.075\lambda$ corresponding to snow grains of 4-mm and 3-mm in diameter (see [30] for a discussion of snow grain size in Greenland). To avoid high computational costs associated with
accurate geometrical modeling of the snow grains, a volume averaging approach was used in the FDTD simulations as discussed in Section 2.2.6.

### 4.3.1 FDTD Phase Matrices

In order to test the FDTD/Monte Carlo method, a sparse distribution of non-penetrating scatterers with a volume fill fraction of 2% was used, allowing comparison against the analytical solution for independent Mie scattering. The results for $P_{11}$ and $P_{22}$ are presented in Figure 4.10.

Recall that the Monte Carlo Mie solution for 256 realizations was very close to the analytical solution (Figure 4.4). For fewer realizations, however, the pattern exhibited more irregularity. The FDTD results in Figure 4.10 for 32 realizations oscillate about the correct solution, which is the expected behavior for this number of realizations. The agreement between the numerical and analytical solutions provides evidence that the hybrid FDTD/Monte Carlo technique is valid.

Next we turn to a more dense medium with a volume fill fraction of 20%. Figure 4.11 shows the resulting components of the phase matrix. In this case the FDTD solution is also compared to the independent Mie scattering solution scaled by the scattering coefficient given by QCA-CP (see Section E.4). As expected, the independent Mie solution predicts scatter which is too high. The FDTD solution compares favorably with the QCA-CP scaled solution. However, apparent in $P_{22}$ is
an upward trend in FDTD as opposed to a downward trend in the QCA-CP scaled solution. This result suggests that the density of a medium affects not only the level of scattering, but also (to a lesser degree) the shape of the phase matrix curves.

4.3.2 Penetrating Spheres

One of the limitations of analytical methods for obtaining the radiative transfer quantities is the need to apply simplifications to the geometry of the scatterers. In FDTD, however, arbitrary media may be simulated within the resolution limits of the simulator. When snow undergoes melt and refreeze cycles, the medium can become very complex, and the ice grains no longer look “non-penetrating.” To show the power of the FDTD method, as well as demonstrate the effect of relaxing simplifying assumptions, the medium is modeled with penetrating spheres.

When generating the realizations for this simulation, spheres are placed according to a uniform distribution as before except that they are allowed to overlap. Enough cells are filled to meet the volume fill fraction requirement, with a given cell being counted only once even if it is contained in two or more spheres.

Figure 4.12 compares the curves of $P_{11}$ and $P_{22}$ resulting from this simulation with the various techniques for analyzing non-penetrating spheres. The results indicate approximately a three fold increase in scattering when a penetrating model is used, which is even higher than the independent scattering solution. In [4], such
Figure 4.12: Phase matrix component given by FDTD simulations for a dense distribution of penetrating spheres. Parameters were $a = 0.075\lambda$, cube length $5\lambda$, $N = 32$, $f = 20\%$, and $\epsilon_s = 3.2\epsilon_0$.

Table 4.1: Comparison of the scattering coefficient resulting from Monte Carlo computations of FDTD simulations with independent and dense media theories. Parameters were $a = 0.075\lambda$, $f = 20\%$, and $\epsilon_s = 3.2\epsilon_0$.

<table>
<thead>
<tr>
<th>Theory/Simulation Type</th>
<th>$k_s (1/\lambda)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Independent Mie Scattering</td>
<td>0.0497</td>
</tr>
<tr>
<td>QCA</td>
<td>0.0116</td>
</tr>
<tr>
<td>QCA-CP (Low Frequency)</td>
<td>0.0152</td>
</tr>
<tr>
<td>FDTD Non-Penetrating</td>
<td>0.0260</td>
</tr>
<tr>
<td>FDTD Penetrating</td>
<td>0.0842</td>
</tr>
</tbody>
</table>

media is modeled with “sticky particles,” where particles tend to clump together to form effectively larger particles. In this case, a dramatic increase in scattering levels was also noted.

4.3.3 Extinction Coefficients

For each of the simulation cases, scattering coefficients were computed to use with the radiative transfer code. Table 4.1 lists the scattering coefficients for the FDTD simulations with non-penetrating and penetrating spheres along with the independent and dense media theories. The scattering coefficients for FDTD for the non-penetrating spheres is slightly higher than QCA-CP in the low frequency limit, which was also the case in [4]. The scattering coefficient for Monte Carlo FDTD simulations with penetrating spheres is about 3.2 times that for non-penetrating spheres.
Figure 4.13: Remote sensing example of perfectly-scattering dry snow overlying a homogeneous ice layer. Physical parameters for the snow layer are scatterer radii \( r = 1:7 \), fractional volume \( f = 20\% \), and scatterer permittivity \( \epsilon_s = 3.2\epsilon_0 \). Backscatter and brightness temperature are computed versus the depth \( d \).

4.4 Remote Sensing Simulations

An important area of research is concerned with computing snow accumulation from a time series of active backscatter \[39\] and passive brightness temperature \[40\]. This section combines the radiative transfer quantities computed in previous sections with the numerical radiative transfer solver (Appendix D) to compute active backscatter and passive brightness temperature as a function of snow depth, demonstrating the utility of the method. Figure 4.13 depicts the basic scenario to be analyzed by the various models. For simplicity, the Mie phase matrix is assumed for each model, with scaling given by the extinction coefficients listed in Table 4.1. The scenario represents a homogeneous layer of ice covered by a perfectly scattering (albedo = 1) layer of dry snow for various accumulation depths. The parameters for the snow layer represent snow grains of diameter 3 mm at 14 GHz or 1.2 mm at 37 GHz. Figure 4.14 plots the co-polarized vertical and cross-polarized response of the snow for various snow depths. The type of model used for the snow strongly affects the level of backscatter, indicating the importance of correctly modeling the snow structure. Figure 4.15 plots the vertical and horizontal brightness temperature as a function of snow depth. In this case, the brightness is proportional to the layer depth, and the overall slope is determined by the scattering coefficient. Again, the
Figure 4.14: Plot of the backscatter coefficient for co-polarized vertical and cross-polarized horizontal illumination of the scenario in Figure 4.13 versus snow layer depth

Figure 4.15: Plot of the vertical and horizontal brightness temperature for the scenario in Figure 4.13 versus snow layer depth

large disparity between the models highlights the importance of correctly modeling the snow structure.

4.5 Chapter Summary

This chapter has presented a method for obtaining inputs to the radiative transfer equation using FDTD and the Monte Carlo technique. In this method the statistical analysis is performed by averaging over many random realizations. Also, certain modifications to the analytical theory are required to remove the finite volume boundary effect.

A convergence study was performed using a simple independent scattering Mie solution. The convergence study demonstrated that care must be taken when applying the Monte Carlo method. If the volume size is too small, the error in
the resulting radiative transfer quantities can be appreciable. If too few realizations are performed, the results may have large irregularity. In general, a tradeoff exists between test volume size and the number of realizations for a given maximum error requirement. However, if the volume size is too small, increasing the number of realizations has virtually no effect on the error. Thus, some sort of convergence study must be applied to use the Monte Carlo method reliably.

Choosing a suitable volume size of $5\lambda$ and 32 realizations, the simulations were run using FDTD for sparse (2% fill) and dense (20% fill) media. For the sparse medium, the FDTD solution was comparable to the values predicted by the independent Mie scattering solution. For the dense medium, the FDTD solution compared favorably with the independent solution scaled by the QCA-CP scattering coefficient. However, the FDTD solution suggests that both the level of scattering and the shape of the phase matrix are affected by the density of the medium. The FDTD method was applied to a dense medium consisting of penetrating spheres, revealing scattering levels comparable to the independent scattering solution.

This new hybrid FDTD/radiative transfer method represents a powerful tool capable of modeling complex geophysical media in a numerically exact manner, rather than resorting to approximate analytical methods. This method has the potential not only to test the accuracy of existing electromagnetic models, but also to generate more reliable models for parameter extraction in remote sensing applications.
Chapter 5

Modeling of an Optical Bragg Resonator

Recent decades have witnessed the development of highly complex optical devices to support the onward expansion of the optical communications infrastructure. Simulation tools that characterize wave propagation in arbitrary guiding structures empower the design engineer with the ability to compare competing designs and avoid faulty designs at the outset. Such tools often reduce the number of prototype and test phases that are required before device manufacturing can take place. Also, in conjunction with the Monte Carlo method, accurate optical modeling tools provide critical information on device yield, which impacts the profitability of proposed designs.

Due to the large electrical size of many optical structures, full-wave three-dimensional (3D) numerical electromagnetic solvers are often precluded, and approximate one-dimensional (1D) analyses are often employed instead. Unfortunately, the approximate 1D analyses ignore much of the physics governing the operation of optical devices. For example, 1D methods overlook the presence of non-guided or radiated fields, which are critical for understanding the efficiency of many devices. Also, the 1D methods generally assume single-mode operation, when due to the complexity of certain devices, multiple modes may actually exist and have a significant effect on device operation. To overcome these shortcomings, this research has developed a new modeling strategy that combines full-wave analysis of propagating modes and waveguide discontinuities with network analysis to obtain very accurate predictions of device response.
Prior work in this area has focused on two-dimensional planar waveguide approximations \([5, 6]\), the approximate beam-propagation method \([7, 8]\), and finite-difference (FD) solutions for propagation constants and mode profiles \([9, 10]\) based on the Helmholtz equation. However, none of these methods provide a framework for modeling arbitrary, electrically large devices with high accuracy.

The new hybrid optical modeling method in this research comprises three basic levels:

1. At the lowest level, modal propagation constants and field profiles are computed with a numerically exact electromagnetic analysis. In this research, a simple FD method based on a straightforward discretization of Maxwell’s equations was employed, as outlined in Section 2.1. This method was chosen for ease of implementation and natural compatibility with subsequent 3D finite-difference time-domain (FDTD) simulations.

2. At the intermediate level, the optical guiding structure is divided into a number of multiport elements which may be characterized in terms of modal transmission and reflection. In general, any waveguide transitions or discontinuities are represented as elements. In this research, three-dimensional FDTD simulations characterize the response of such elements.

3. At the highest level, the elements are connected using network analysis, which in this research was simple S-parameter analysis.

The resulting hybrid FD/FDTD/S-parameter analysis method is a powerful tool for modeling arbitrary guiding structures.

This chapter demonstrates the method by analyzing an electrically large buried-heterostructure Bragg resonator employing a surface-relief grating. The ability of the method to provide realistic results for this numerically sensitive problem provides evidence that the method may be applied to a wide variety of structures.
5.1 Finite Difference Method

At the lowest level, the hybrid method requires computation of modal propagation constants and field profiles for longitudinally homogeneous waveguiding structures. Section 2.1 outlines two basic finite-difference schemes based on a direct discretization of Maxwell’s equations. All numerical values for propagation constants in this chapter were computed assuming a discrete time step of $\Delta t = T/100$ where $T$ is the sinusoidal period. Also, the values listed for $\beta_z$ are propagation constants for a continuous domain in the propagation direction. To convert to the values appropriate for FDTD, relation (2.13) in Chapter 2 must be used.

Since the Bragg resonator under analysis consists of many cascaded sections, the overall response is very sensitive to slight errors in the single section response. The first part of this section considers accuracy of the mode solution by assessing error due to finite-difference approximations and grid truncation conditions. The second part of the section provides the guided-mode solution for the Bragg resonator geometry.

5.1.1 Accuracy of the Mode Solution

In this section, the linear mode solution method is applied to a rectangular dielectric waveguide whose cross-section matches the core of the Bragg resonator to be analyzed later. Accuracy of the modal propagation constants and field profiles is affected by the boundary truncation type, the domain size, and the cell size. The basic geometry under consideration is depicted in Figure 5.1. Figures 5.2 and 5.3 plot the electric and magnetic fields in this structure at the center wavelength of 1550 nm, which was obtained with the mode solution method and the decay boundary condition.

Error in the mode solutions is quantified as fractional deviation of the numerical field profiles and propagation constants from theoretical values. The error in the profile of the $p$th component of the electric field profile is defined as

$$
\epsilon_{E_p} = \frac{E_{\text{num}}^p - E_{\text{th}}^p}{|E_{\text{th}}^p|},
$$

(5.1)
Figure 5.1: Waveguide geometry used to assess error in the propagation constant and field profile found with the FD method. Also shown is the assignment of FD grid indices.

where $E^{\text{num}}$ refers to field for a given numerical experiment, and $E^{\text{th}}$ refers to the theoretical field values. Likewise, error in the propagation constant is defined as

$$
\epsilon_\beta = \frac{\beta^{\text{num}} - \beta^{\text{th}}}{|\beta^{\text{th}}|},
$$

(5.2)

where $\beta^{\text{num}}$ and $\beta^{\text{th}}$ are the numerical and theoretical propagation constants, respectively. Lacking convenient expressions for exact theoretical field profiles and propagation constants, the theoretical values are defined to be the most accurate numerical solution obtained (largest size domain/finest resolution).

Domain Size Dependence

Table 5.1 compares the fractional error in propagation constant due to the zero boundary and decay boundary for various grid sizes, where the cell size is held constant. Figures 5.4 and 5.5 plot the error in the $E_x$ field component for the zero and decay boundary conditions, respectively. This comparison shows that the error produced by the decay boundary is an order of magnitude lower than that produced by the zero boundary. The results also indicate that a modest domain size (4500 nm $\times$ 4800 nm) gives reasonably small error in the propagation constant ($10^{-7}$) and field
Figure 5.2: Transverse vectorial fields in the rectangular dielectric waveguide structure (depicted in Figure 5.1) near the core. Arrow length and direction are proportional to the field intensity and direction, respectively, on a linear scale. The domain size was $84 \times 112$ cells and $6300 \times 6720$ nm, and the decay boundary condition was applied. Dashed lines show the dimensions of the core for reference.
Figure 5.3: Modal field profiles for the rectangular dielectric waveguide. The geometry of the core is superimposed in gray. Plots show contours of constant field for each component of electric and magnetic field.
Table 5.1: Propagation constant value and fractional error for various sizes of the simulation domain.

<table>
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<tr>
<th>Cells</th>
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<th>Zero Bound</th>
<th></th>
<th></th>
<th></th>
<th>Decay Bound</th>
<th></th>
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<td>$N_x$</td>
<td>$N_y$</td>
<td>$x$</td>
<td>$y$</td>
<td>$\beta_x \lambda_0$</td>
<td>Frac. Error</td>
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<td></td>
</tr>
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<tr>
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<td>$3.96 \times 10^{-7}$</td>
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<td>60</td>
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<td>4500</td>
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<td>$6.08 \times 10^{-8}$</td>
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</tr>
</tbody>
</table>

Table 5.2: Propagation constant value and error for various simulation cell sizes.

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>$N_y$</th>
<th>$x$</th>
<th>$y$</th>
<th>$\beta_x \lambda_0$</th>
<th>Frac. Error</th>
</tr>
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<tbody>
<tr>
<td>30</td>
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<td>4800</td>
<td>19.95706883</td>
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<td>60</td>
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<td>4500</td>
<td>4800</td>
<td>19.96163969</td>
<td>$-6.47 \times 10^{-5}$</td>
</tr>
<tr>
<td>90</td>
<td>120</td>
<td>4500</td>
<td>4800</td>
<td>19.96245221</td>
<td>$-2.40 \times 10^{-5}$</td>
</tr>
<tr>
<td>120</td>
<td>160</td>
<td>4500</td>
<td>4800</td>
<td>19.96273238</td>
<td>$-9.92 \times 10^{-6}$</td>
</tr>
<tr>
<td>150</td>
<td>200</td>
<td>4500</td>
<td>4800</td>
<td>19.96286096</td>
<td>$-3.48 \times 10^{-6}$</td>
</tr>
<tr>
<td>180</td>
<td>240</td>
<td>4500</td>
<td>4800</td>
<td>19.96293039</td>
<td>$0.00 \times 10^{0}$</td>
</tr>
</tbody>
</table>

profile ($10^{-3}$). For all further computations, the decay boundary truncation approach will be used.

Cell Size Dependence

Table 5.2 lists the fractional error in the propagation constant for various cell sizes when the domain size is held constant. These values show that the propagation constant is more sensitive to the discretization than the domain size. Figure 5.6 shows the error in the $E_x$ component of the computed field profile for four of the cases considered.
Figure 5.4: Error in the $E_x$ component of the modal field profile for the zero field boundary condition. The solid box denotes the core dimensions, and the dashed box denotes the dimensions of the smallest domain for comparison.
Figure 5.5: Error in the $E_x$ component of the modal field profile for the decay boundary condition. The solid box denotes the core dimensions, and the dashed box denotes the dimensions of the smallest domain for comparison.
Figure 5.6: Error in the $E_x$ component of the field profile for the decay boundary condition for various grid resolutions. The dashed box denotes the dimensions of the core.
5.1.2 Bragg Resonator Guided Mode Solution

Figure 5.7 shows the cross section of the Bragg resonator under consideration. This geometry is based on the buried heterostructure distributed feedback (DFB) device presented in [41] with parameters specified at a physical temperature of $T = 25^\circ\text{C}$ and a wavelength of $\lambda = 1.55\mu\text{m}$. The index of refraction for the cladding (InP) at this temperature is $n_2 = 3.15$ [42] [43]. The core (Ga$_{1-x}$In$_x$As$_y$P$_{1-y}$) was assumed to be matched to the InP lattice with $x = 0.2$ and $y = 0.43$, giving $n_1 = 3.35$ [44].

The refractive index in the grating ($n_3$) is a function of longitudinal position. For the true physical geometry, the grating would have $n_3 = n_1 = 3.35$ and the height would be modulated (surface relief). However, modeling such fine detail significantly increases the memory required for simulation. Instead, $n_3$ assumes the alternating values of 3.35 and 3.33 for the grating modulation, which corresponds to a 10% modulation in the grating height when viewed in terms of an effective permittivity (consistent with the volume averaging approach in Section 2.2.6). Since

Figure 5.7: Waveguide cross section for the Bragg resonator. $n_3$ takes on discrete values in the longitudinal direction.
the longitudinal boundaries for the single grating section will be chosen to cut the \( n_3 = 3.35 \) region, the mode solutions are only required for \( n_3 = 3.35 \).

The eigenvalue/eigenvector method, refined by the linear method was used to obtain propagation constants and mode profiles at 6 different wavelengths. The geometry depicted in Figure 5.7 was assumed with \( n_3 = 3.35 \). The wavelengths and propagation constants are given in Table 5.3. Figures 5.8 and 5.9 depict the shape of the various Cartesian components of the fundamental propagating mode at 1550 nm.

Table 5.3: Propagation constant of the propagating mode versus wavelength

<table>
<thead>
<tr>
<th>( \lambda_0 ) (nm)</th>
<th>( \beta_2 \lambda_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1549.0</td>
<td>20.009476</td>
</tr>
<tr>
<td>1549.5</td>
<td>20.009300</td>
</tr>
<tr>
<td>1550.0</td>
<td>20.009125</td>
</tr>
<tr>
<td>1550.5</td>
<td>20.008949</td>
</tr>
<tr>
<td>1551.0</td>
<td>20.008774</td>
</tr>
<tr>
<td>1551.5</td>
<td>20.008599</td>
</tr>
</tbody>
</table>

5.2 3D Simulations of Bragg Resonator Section

The Bragg resonator is divided into sections, each having the longitudinal geometry depicted in Figure 5.10. The length of the dielectric discontinuity in the grating (referred to here as the “tooth”) is 120 nm, which is approximately \( \lambda/4 \) for the guided mode at the center wavelength. FDTD \([14,15]\) was chosen for simulating the 3D Bragg resonator due to its computational efficiency and ease of implementation. Figure 5.11 depicts the geometry cast into the FDTD simulation framework. The width of each PML is 10 cells and the normal reflection coefficient is specified to be \( R = 1 \times 10^{-5} \). The length of the domain was chosen to be large enough to accommodate a nominal section length of \( \ell_s = 243 \) nm and provide adequate buffer space between the discontinuity and the PML.
Figure 5.8: Transverse vectorial fields in the Bragg resonator waveguide geometry (depicted in Figure 5.7) near the core. Arrow length and direction are proportional to the field intensity and direction, respectively, on a linear scale. Dashed lines show the dimensions of the core and grating for reference.
Figure 5.9: Modal field profiles for the Bragg resonator waveguide. The geometry of the core and grating is superimposed on the contour plots in gray. The plots show contours of constant field for each of the electric and magnetic field components.
Figure 5.10: Unit section of the Bragg resonator to be modeled with 3D full-wave analysis. The dashed lines at A and B denote the extent of the unit section, $\ell_t$ and $\ell_s$ are physical lengths of the “tooth” and Bragg section, and $\theta$ is the angular length of the section in radians at $\lambda_0 = 1550$ nm.

Figure 5.11: Geometry of the Bragg resonator for the FDTD analysis

FDTD is generally well-suited for free-space propagation and scattering problems. When applied to the Bragg resonator, important considerations include

1. Discrete stepping in time and finite resolution in the propagation direction will lead to a slightly different mode than that given by (2.2) where exact derivatives have been assumed in time and propagation direction.
2. The fields scattered by the 3D geometry will be very weak compared to the incident wave, giving rise to large dynamic range requirements.

3. The error induced by the absorbing boundary condition (ABC) must be acceptably low. This is particularly important as the Bragg resonator frequency response can be highly sensitive to errors in the computed fields.

These issues are treated in Sections 5.2.2, 5.2.3, and 5.2.4, respectively.

5.2.1 Mode Extraction

The analysis that follows requires the extraction of complex mode envelopes from steady-state fields. Because of mode orthogonality, the complex envelope of the mode with electric field shape $M_{ij}$ can be extracted from the fundamental frequency component of the FDTD simulation $E_{ijk}$ using the expression

$$A_{zk} = \frac{\sum_{ij} E_{ijk} M_{ij}^*}{\sum_{ij} |M_{ij}|^2},$$

where $A_{zk}$ is the complex mode envelope, $i$ and $j$ represent indices in the transverse directions, $k$ is the index in the propagation direction, and $z_k$ is the $z$ position corresponding to the $k$th index.

5.2.2 Finite Difference Approximations

The method outlined in Section 2.1.6 was used to ensure complete compatibility of modes supported by the 2D FD mode computations and the 3D FDTD simulations. Although the FD and FDTD simulations are compatible, the propagation constant used may deviate from the real propagation constant for the physical medium, which is continuous in time and space. The propagation constant changes by $-1.7 \times 10^{-4}$ due to finite temporal stepping (100 steps per period) and by $6.9 \times 10^{-4}$ due to finite propagation direction resolution (10 nm/cell). In Section 5.3.1 these values will be used to assess the accuracy of the complete Bragg solution.
5.2.3 Dynamic Range

For many waveguide geometries, such as a small section of a Bragg resonator, the field scattered by the obstacle may be significantly weaker than the incident field. In these situations, finite precision arithmetic may produce unacceptable error. To minimize the dynamic range requirements as well as remove the need to absorb the strong incident field at the domain boundaries, the scattered field formulation outlined in Section 2.2.3 was applied.

5.2.4 ABC Performance

In this research, PML-based methods were used to absorb both the guided mode and radiated fields. The PML presents two basic difficulties. First, the guided mode traveling in the propagation direction will reflect off of the PML, introducing error in the reflection and transmission coefficient computations. Second, PML on the transverse walls will tend to distort the mode shape. The following sections quantify the error introduced by these two effects.

Propagation PML

The reflection of the guided mode off of the PML in the propagation direction was quantified with the 1D single-mode solution given in Section 2.3. Figure 5.12 shows the basic setup for testing the PML. The source is a forced electric wall at \( z = 0 \) with unit amplitude. The propagation constant in the medium is \( \beta_z \) at the center wavelength of 1550 nm as given in Table 5.3. Also, time stepping and resolution in the \( \hat{z} \) direction match the FDTD simulations. Figure 5.13 plots the amplitude of the steady-state solution as a function of distance along the propagation direction. For a reflectionless surface, only the incident mode with unit amplitude would be present. However, due to numerical reflection off of the PML, a standing wave pattern is present. The amplitude of the modulation compared to the unit incident wave indicates the degree of reflection from the PML, which is approximately \( 5 \times 10^{-5} \). As will be seen, this value is small compared to other sources of error.
Figure 5.12: Geometry and parameters for computing 1D solutions for PML modal reflection. The parameters listed are propagation direction step $\Delta z$, time step $\Delta t$, propagation constant $\beta_z$, and the specified normal modal PML reflection $R$.

\[
\begin{align*}
\Delta z & = 10 \text{ nm} \\
\Delta t & = T/100 \\
\beta_z & = 20.009125\lambda_0 \\
R & = 1 \times 10^{-5}
\end{align*}
\]

Figure 5.13: One-dimensional solution for reflection from the PML to be used for absorbing the incident mode. The figure on the left shows the electric field amplitude for the complete structure. The figure on the right shows an enlargement of fields in just the normal region. The reflected mode is on the order of $5 \times 10^{-5}$.
Figure 5.14: FDTD simulation domain for assessing the impact of transverse PMLs

Transverse PML

In order to absorb fields radiated from waveguide discontinuities, PMLs are placed on the transverse sides ($\hat{x}$ and $\hat{y}$) of the simulation volume. The Helmholtz equation given by (2.29) and (2.30) will be different in the normal and transverse PML regions, leading to aberrations in the mode shape. However, if modal fields are weak near the transverse PML boundary, the effect will be small.

To demonstrate the small impact of the transverse PML, FDTD simulations were run with the volume depicted in Figure 5.14. The simulation cross section is equivalent to the Bragg resonator waveguide shown in Figure 5.7 with $n_3 = 3.35$. Also, the parameters in the propagation direction are equivalent to those in the 1D simulation depicted in Figure 5.12. The truncation condition in the $+\hat{z}$ direction is the usual perfect electrical conductor condition. In the transverse directions, simulations were run with either a perfect conductor or the decay boundary condition (the condition used to obtain FD mode solutions as described in Section 2.1.2). The source for the simulations is an electric wall at the left side of the volume that is forced to the known mode. The steady-state fields are extracted by taking the FFT of a complete period and using the sample corresponding to the fundamental frequency.
By comparing the modal fields of the FDTD simulations with those of the ideal 1D solution (depicted in Figure 5.13), the impact of the transverse PMLs is assessed. The FDTD and 1D modal simulations were compared in two ways: (1) with the complex envelope of the $E_x$ field component along the center of the simulation domain (on the line $x = 0, y = 0$), and (2) with the complex modal envelopes using (5.3). Figure 5.15 plots the error in these fields and mode envelopes for the various cases considered.

Figure 5.15(a) represents a scenario that attempts to match the ideal mode solution. Fields in the FDTD domain were initialized to the known field values at $t = 0$. The grid was terminated with the decay boundary condition, and no transverse PML was present to distort the mode shape. The difference between the ideal 1D mode solution and the FDTD simulation is very small, even after $20T$, validating the mode propagation constant, field profile, and the 1D mode solution. Figure 5.15(b) depicts the same basic scenario with a perfectly conducting boundary in the transverse direction. In this case the error is on the order of $1 \times 10^{-5}$ for the mode envelope.

In Figures 5.15(c) and 5.15(d), the fields were initialized to zero and a Gaussian ramp function with a 99% rise time of $3T$ was applied to avoid initial transients. This case is more realistic, since in true simulations the initial fields will not be known. For the decay boundary condition, modal error drops below $5 \times 10^{-6}$ after $5T$. For the conducting boundary condition, error is below $2 \times 10^{-5}$ after $5T$.

Figures 5.15(e) and 5.15(f) show the result of adding PML in the transverse directions. The PML increases the error to $1 \times 10^{-5}$ for the decay boundary condition. Interestingly, the conducting boundary with PML exhibits the same amount of error, suggesting that the PML absorbs distortions caused by the imperfect truncation condition.

The conclusion to be drawn from this section is that distortion of the mode due to the transverse PML accounts for about $1 \times 10^{-5}$ error for either a conducting or decaying truncation condition on the transverse walls. In subsequent simulations, the decay boundary condition is employed for slightly better accuracy. However, the perfectly conducting boundary would also have sufficed.
Figure 5.15: Fractional deviation of FDTD simulations from the ideal 1D mode solution due to imperfect transverse truncation, initial transient response, and transverse PML. The transverse truncation was the decay condition (Decay) or a perfect conductor (Cond.). Fields were set at $t = 0$ to known modal values (Initialized), or to zero (Uninitialized).
Table 5.4: Reflection and transmission of the single Bragg section. Also listed are the propagation constants at each wavelength.

| $\lambda_0$ (nm) | $\beta_0\lambda_0$ | $|R_0|$ | $\angle R_0$ (deg) | $|T_{0,0} - 1|$ | $\angle(T_{0,0} - 1)$ (deg) |
|-----------------|-------------------|-------|-----------------|-------------|-----------------|
| 1549.0          | 20.009476         | 2.7232 x $10^{-4}$ | 1.27          | 4.2981 x $10^{-4}$ | 90.0379         |
| 1549.5          | 20.009300         | 2.7222 x $10^{-4}$ | 1.30          | 4.2952 x $10^{-4}$ | 90.0375         |
| 1550.0          | 20.009125         | 2.7212 x $10^{-4}$ | 1.33          | 4.2922 x $10^{-4}$ | 90.0372         |
| 1550.5          | 20.008949         | 2.7202 x $10^{-4}$ | 1.36          | 4.2893 x $10^{-4}$ | 90.0368         |
| 1551.0          | 20.008774         | 2.7192 x $10^{-4}$ | 1.39          | 4.2864 x $10^{-4}$ | 90.0364         |
| 1551.5          | 20.008599         | 2.7182 x $10^{-4}$ | 1.42          | 4.2834 x $10^{-4}$ | 90.0360         |

5.3 Bragg Resonator Response

FDTD simulations were run for the wavelengths given in Table 5.4 using the simulation volume depicted in Figure 5.11. Fields were stored at $z = 0$ (for reflection) and $z = 120$ nm (for transmission) and the corresponding complex envelope ($A_0$ and $A_{120}$) of the propagating mode was found. In the following discussion, the reflection coefficient at plane $z$ is represented as

$$R_z = \frac{A_z}{A_i},$$

(5.4)

where $z$ is a coordinate in the propagation direction, and $A_i$ and $A_z$ are the incident and scattered complex mode envelopes computed according to (5.3) at the propagation coordinate $z$. Similarly, the transmission coefficient from plane $z = z_i$ to plane $z = z_t$ is represented as

$$T_{z_i,z_t} = \frac{A_{z_t} + A_{z_t}^i}{A_{z_i}^i},$$

(5.5)

where the incident mode had the functional form

$$A_i^i = e^{-j\beta_i z_i}.$$

(5.6)

Table 5.4 lists the reflection and transmission coefficients at $z = 0$ (where $A_0^i = 1$), which were computed from

$$R_0 = A_0,$$

(5.7)

$$T_{0,0} = A_{120} \exp(j\ell_t \beta_z) + 1.$$

(5.8)
To compute the response of the Bragg section at planes A and B, the equations are

\[ R_A = R_0 \exp[j\beta_z(\ell_t - \ell_s)] \]  
\[ T_{A,B} = T_{0,0} \exp(j\beta_z \ell_s). \]

The physical section length (\( \ell_s \)) in these computations was chosen to give an angular length (\( \theta \)) of \( \pi \) radians at the center wavelength of 1550 nm, or \( \ell_s = 243.362 \) nm.

Since the FDTD simulations only allow computation of the reflection and transmission coefficients at discrete wavelengths, some type of interpolation is required to obtain response for the intermediate wavelengths. Figure 5.16 plots propagation constant obtained by the 2D mode solution method, and \( R_0 \) and \((T_{0,0} - 1)\) obtained with the FDTD simulations. Also plotted is a linear regression of the discrete data points. Due to the linearity of the data, the linear regression was used for interpolation.

Once the reflection and transmission behavior of the single Bragg section is known for a fixed wavelength, the single-section S-parameter matrix is formed as

\[
\begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix}
\begin{bmatrix}
R_A \\
T_{A,B}
\end{bmatrix}.
\]

The single section ABCD matrix is then obtained from the S-parameter matrix as

\[
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}
\]

where

\[
A = \frac{(1 + S_{11})(1 - S_{22}) + S_{12}S_{21}}{2S_{21}}
\]
\[
B = \frac{(1 + S_{11})(1 + S_{22}) - S_{12}S_{21}}{2S_{21}}
\]
\[
C = \frac{(1 - S_{11})(1 - S_{22}) - S_{12}S_{21}}{2S_{21}}
\]
\[
D = \frac{(1 - S_{11})(1 + S_{22}) + S_{12}S_{21}}{2S_{21}}.
\]

Next, the ABCD matrix for the complete \( N \) section Bragg resonator is

\[
\begin{bmatrix}
A
\end{bmatrix} = \begin{bmatrix}
A
\end{bmatrix}^N,
\]

95
Figure 5.16: Propagation constant, \( R_0 \), and \( T_{0,0} \) versus wavelength. Also shown in a linear regression for each of the quantities.
and converting back to S-parameters, we have

$$ S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = \frac{1}{\Delta} \begin{bmatrix} A + B - C - D & 2(AD - BC) \\ 2 & -A + B - C + D \end{bmatrix}, \quad (5.18) $$

where

$$ \Delta = A + B + C + D. \quad (5.19) $$

Thus, the complex modal reflection and transmission of the matched $N$ section Bragg resonator is given by $S_{11}$ and $S_{21}$, respectively. Another important quantity is the power balance of the Bragg resonator, or

$$ P_{\text{bal}} = |S_{11}|^2 + |S_{21}|^2. \quad (5.20) $$

If each section of the Bragg resonator were lossless, this quantity would be unity. However, a small amount of power will be lost in each section due to radiation. Also, high irregularity of power balance may indicate error in the solution. Neglecting any sources of error, the $N = 10^4$ section Bragg resonator response is plotted in Figure 5.17. Figure 5.18 plots the corresponding power balance, which is better than 98%. The slight positive power balance (representing gain) is likely due to small phase errors, which will be discussed in Section 5.3.1 below.

### 5.3.1 Error Quantification

Small amounts of error in the single section response may cause more appreciable error in the complete Bragg response. Table 5.5 lists the primary sources of error and their estimated values. The numbers in boldface in the table represent error values that are most significant: increased mode amplitude due to finite FD grid resolution and an increase in $\beta_z$ due to finite FDTD resolution in the propagation direction. The effect of these sources of error is discussed below.

**Error Source: Increased Mode Amplitude**

The finite resolution of the FD method leads to a mode amplitude which is too high in the region of the waveguide discontinuity. Since we are applying the
Figure 5.17: Reflection and transmission of the Bragg resonator. All sources of error have been ignored.

Figure 5.18: Power balance of the Bragg resonator. All sources of error have been ignored.
Figure 5.19: Deviation in Bragg response due to mode shape error. The single section reflection and transmission are perturbed by -0.2%. Plots show the resulting complete Bragg reflection, transmission, and power balance and the difference between the perturbed and unperturbed solutions.
Table 5.5: Sources of error in the Bragg resonator and approximate values.

<table>
<thead>
<tr>
<th>Error Source</th>
<th>Fractional Error in $\beta_z$</th>
<th>Mode Shape</th>
<th>$R$ and $T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FD Grid Truncation</td>
<td>$6.1 \times 10^{-8}$</td>
<td>$1.0 \times 10^{-6}$</td>
<td>-</td>
</tr>
<tr>
<td>FD Grid Resolution</td>
<td>$-6.5 \times 10^{-5}$</td>
<td>$2.0 \times 10^{-3}$</td>
<td>-</td>
</tr>
<tr>
<td>PML Reflection (Guided Mode)</td>
<td>-</td>
<td>-</td>
<td>$5.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>PML Reflection (Radiated Fields)</td>
<td>-</td>
<td>-</td>
<td>$1.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>Finite Time Step</td>
<td>$-1.7 \times 10^{-4}$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Finite Resolution in $\hat{z}$</td>
<td>$6.9 \times 10^{-4}$</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

scattered field formulation and the error is nearly constant over the waveguide discontinuity, the scattered fields will increase linearly with the amount of error. To assess the impact of this effect, we reduce the magnitude of the complex mode envelopes extracted from the FDTD simulations by the given 0.2% and again plot the response. Figure 5.19 depicts the change in the complete Bragg reflection and transmission response. Also, fractional change in the reflection and transmission response is less than 2% and 1%, respectively.

**Error Source: Increase in $\beta_z$**

The propagation constant for discrete sampling in the propagating direction is about 0.07% higher than the ideal continuous space solution. At the value of $\beta_z$ for $\lambda_0 = 1550$ nm, the amount of phase error over the discontinuity length of 120 nm is $0.06^\circ$. The resulting error in the phase of $A_0$ and $A_{120}$ is uncertain due to the multiple reflections in the discontinuity. However, we may explore the effect of phase error by assuming independent distributions on the phase error for $A_0$ and $A_{120}$ and produce a number of Monte Carlo realizations. Plotting the response for several random values will provide an indication of the distribution of the error.

The error in phase for $A_0$ and $A_{120}$ is assumed to be uniformly distributed on $[-0.06^\circ, 0.06^\circ]$, since the true distribution is unknown. Figures 5.20 and 5.21 plot the magnitude and phase response of 32 Monte Carlo realizations along with the mean of the realizations. Figure 5.20 shows that the transmission behavior is fairly
insensitive to the phase error. The maximum deviation in transmission amplitude and phase is only about 0.001 and 0.03°, respectively. Figure 5.21 plots the reflection response. The maximum amplitude deviation is still only about 0.003. The reflection phase, however, is very sensitive around the regions of resonance, since the reflection is nearly zero. Figure 5.22 shows the power balance curves for the 32 realizations. The ideal unity power balance curve falls within the bounds of the 32 realizations, which indicates that a slight phase adjustment accounts for the aberration in power balance. Additionally, the plot suggests that the radiated power is quite small.

5.4 Chapter Summary

This chapter has outlined a method for simulating complex optical devices with a hybrid method encompassing three basic modeling tools: (1) a 2D FD mode
Figure 5.21: Bragg reflection response for 32 Monte Carlo realizations with phase for $A_0$ and $A_{120}$ uniformly distributed on $[-0.06^\circ, 0.06^\circ]$. The mean is plotted in gray.

Figure 5.22: Bragg resonator power balance for 32 Monte Carlo realizations with phase for $A_0$ and $A_{120}$ uniformly distributed on $[-0.06^\circ, 0.06^\circ]$. 
solution technique for finding modes in arbitrary guiding structures, (2) 3D full-wave FDTD analysis of waveguide discontinuities, and (3) network analysis employing a 1D transmission line model. Using the method a large ($10^4$ sections) Bragg resonator was simulated, with results showing very good accuracy. Natural extensions include the simulation of DFB lasers by incorporating gain into the 3D full-wave FDTD simulator and multimode analysis. Also, the transmission structures analyzed need not be 1D in nature. The recursive Green’s function method (RGFM) [46], for example, provides an efficient framework for obtaining the response of a complete structure when the response of individual cells is known. 2D mode analysis and 3D FDTD analysis may be performed on each cell, and RGFM may be applied to the composite structure for 2D or 3D interconnection, allowing efficient simulation of very complex structures.
Chapter 6

MIMO Measurement System

Recent years have witnessed unprecedented growth in the area of personal wireless communications. Broadband networking hardware for wireless LAN is also making its debut. An understanding of the radio propagation channel is crucial when developing today’s wireless communications systems. Figure 6.1 depicts a theoretical indoor/outdoor communications environment. Cellular phone users communicate with outdoor base stations or possibly indoor access points. Broadband wireless LAN hardware can communicate on a peer-to-peer basis or with access points connected to a campus network. As information-carrying electromagnetic signals propagate in

Figure 6.1: A complex indoor/outdoor wireless communications environment involving many types of wireless communications devices. Signals from a single transmitter to receiver travel along multiple paths, giving rise to multipath fading.
such an environment, often no direct line-of-sight (LOS) path exists from transmitter
to receiver. Also, the same electromagnetic signal may travel along distinct paths in
the environment. When these signals with random phase combine at the receiver,
the resulting signal experiences random power fluctuation, referred to as multipath
fading.

Many systems have been proposed to combat difficulties associated with
multipath fading. Since all of the multipath components do not arrive at the same
time, temporal channel equalization can somewhat mitigate the effect in wide-bandwidth
systems [47]. For narrowband systems, antenna diversity has had significant success
in mitigating multipath effects [48, 49]. Recent work has demonstrated that the use
of multiple antennas on both sides of a communications link allows multipath to be
exploited to increase transmission rates [11] [50, 51]. Conceptually, multiple transmit
antennas allow independent data to be sent on the various multipath components.
Multiple receive antennas then allow the receiver to discriminate between the vari-
ous multipath channels and receive the independent data streams. These multiple
antenna systems are referred to as multiple-input multiple-output (MIMO) systems.

The development of complex wireless systems can benefit from accurate
electromagnetic channel models. As with other areas of engineering, accurate model-
ing allows system performance assessment in the design stage, rather than after costly
prototyping, testing, and deployment. Previous analysis of the MIMO wireless chan-
nel has focused on very simple analytical models that tend to be inaccurate, very
complex ray-tracing studies which are computationally expensive and site specific,
and empirical models based on data alone. In this research, a new hybrid modeling
approach is adopted that combines full-wave electromagnetic analysis of antenna ar-
rays with a statistical description of multipath propagation. Direct measurement of
representative indoor MIMO wireless channels provides evidence that validates the
method.

The following three chapters present this new hybrid model for MIMO
wireless channels. This first chapter outlines the hardware and signal processing
required to measure MIMO channels. Next, Chapter 7 presents the data collected
with the MIMO measurement system in terms of channel capacity and correlation statistics. Finally, Chapter 8 utilizes observations from the data to develop a hybrid model that combines full-wave electromagnetic analysis with the Saleh Valenzuela model.

In this chapter, Section 6.1 describes the hardware that was developed as part of this research, and Section 6.2 outlines the signal processing required to obtain channel matrices from raw data.

6.1 Hardware

For this and later discussions, the \( N_R \) receive by \( N_T \) transmit narrowband channel matrix \( \overline{H} \) relates the transmit (\( \overline{x} \)) and receive (\( \overline{y} \)) complex baseband vectors as

\[
\overline{y} = \overline{H} \overline{x} + \overline{\eta},
\]

where \( \overline{\eta} \) is the independent and identically distributed (i.i.d.) white complex Gaussian receiver noise vector. The MIMO measurement platform must collect channel response data, from which \( \overline{H} \) may be accurately estimated. The MIMO measurement system had the following key requirements:

1. Modularity. The system should have the ability to be reconfigured to accommodate new measurement scenarios. Antennas, RF modules, and signal modulation components should all be easily replaceable.

2. Frequency Range. The system must be able to probe any frequency bands of current interest. The range 1 to 10 GHz was considered sufficient.

3. Raw Data Storage. As much as possible, collected data must be processed offline in software. Storage of raw data avoids wasted data collection time due to faulty real-time algorithms, since faulty software may easily be corrected and rerun on the same raw data.

4. Multiple Channels. The system should have the ability to simultaneously probe up to 16 transmit and 16 receive channels.
5. **Non-tethered.** The transmit and receive systems should be completely separate, and not require a dedicated local-oscillator cable, which could preclude long-range outdoor and mobile measurements.

6. **Range.** Transmit power should be sufficient to measure typical campus-wide scenarios with at least 20 dB SNR.

7. **Fast Development.** When possible, off-the-shelf components should be used to reduce system development time.

8. **Cost.** The budget for this initial system was limited to about $50,000.

The following subsections provide a detailed description of the hardware that met these goals.

### 6.1.1 High-level System Diagram

Figure 6.2 depicts a high-level block diagram of the system. The system must probe an arbitrary channel by measuring the complex gain from each of $N_T$ transmit antennas to each of $N_R$ receive antennas, forming an $N_R \times N_T$ channel matrix. This measurement is accomplished by generating $N_T$ independent BPSK streams, each of which is up-converted with a programmable microwave generator to a specified carrier frequency. BPSK modulation was chosen due to its simplicity, as well as the...
availability of dedicated digital pattern generator instruments with wide buses. The $N_T$ independent signals are amplified and fed to the $N_T$ transmit antennas.

At the receiver, the signal from each of the $N_R$ receive antennas is amplified and down-converted to a convenient intermediate frequency (IF). The $N_R$ IF signals are then sampled and stored in parallel via a PC-based data-acquisition system. Storage of the raw IF signals allows all significant data processing to occur off-line in software. The transmit and receive systems may be synchronized (mainly for system calibration) with an optional 10-MHz signal.

6.1.2 Hardware Components

This section describes the hardware components chosen to realize Figure 6.2. The transmit and receive hardware were housed on carts for mobility. Figure 6.3(a) depicts the transmit subsystem. The microwave source is a synthe-
sized microwave generator, programmable from 2 to 18 GHz with a maximum output power of 0 dBm. The BPSK signals are generated with a Tektronix digital pattern generator, capable of driving up to 24 loads with an impedance of 50 Ω. The digital outputs assume the discrete values $\pm V$, where $V$ is programmable from 1 to 5 volts. The pattern memory is deep enough to store 64K bits per channel. The maximum bit rate of the instrument is 200-Mb/s, allowing probing with a very large bandwidth if required. The high-frequency signal from the microwave source and the $N_T$ baseband BPSK signals from the pattern generator are fed into a custom RF chassis, where up-conversion, signal amplification, and power amplification take place. The RF chassis is described in Section 6.1.3. The resulting $N_T$ output signals are then fed to the antenna array.

Figure 6.3(b) depicts the receive subsystem. The receive system employs a 0 to 26 GHz synthesized microwave generator with a maximum output power of 7 dBm. The $N_R$ signals are received on the antenna array and fed into the RF chassis, where signal amplification, down-conversion, filtering, and IF amplification occur. The resulting $N_R$ IF signals are fed to a PC containing a National Instruments data acquisition card, capable of multiplexed acquisition of 16 parallel channels, with a maximum combined sample rate of 1.25 MS/s.

6.1.3 RF Chassis

Two custom RF chassis were developed as part of this research. The transmit and receive chassis employ the same basic modular design. Figure 6.4 shows the transmit chassis. An ordinary AT computer power supply provides switched $\pm 5$ volt and $\pm 12$ volt supplies to the chassis. The heart of the transmit chassis is a broadband backplane that supplies power, LO, and BPSK signals to the $N_T$ transmit cards. The $N_T$ BPSK signals from the pattern generator (with a code rate of $f_c$) are fed via dual-inline pin (DIP) connectors at the rear of the chassis to the backplane. The backplane also accepts the master LO signal (with a frequency of $f$) from the microwave source. The output of each transmit card is fed through holes in the front of the chassis to the $N_T$ transmit antennas.
Figure 6.4: Custom RF transmit chassis. The boxed items show external connections and the unboxed items label the various components. $f$ is the measurement carrier frequency, and $f_c$ is the code rate (equivalent to the bit rate on each channel) of the BPSK signals.

The receive chassis in Figure 6.5 is nearly identical to the transmit chassis. The receive array feeds the $N_R$ receive cards that are connected to an identical backplane as employed in the transmit chassis. The backplane provides LO and power, and feeds the $N_R$ IF signals from the receive cards to an IF board for filtering and amplification. These signals are then fed to a 68-pin high-density sub-D connector at the back of the chassis, the native interface of the National Instruments data acquisition board in the PC. The PC also supplies digital signals to the IF board for gain control.

**Broadband Backplane**

Figure 6.6 depicts the backplane used in the transmit and receive chassis. The backplane and transmit/receive cards employed grounded coplanar waveguide (GCPW) with metal vias to equalize potential at the top and bottom ground planes. The backplane supplies LO to each card via a surface mount SMA connector, and low-frequency signals and power via an edge-card connector. The transmission lines depicted in Figure 6.6 are 50 Ω. Each resistive split is accomplished with the circuit
Figure 6.5: Custom RF receive chassis. The boxed items show external connections, and the unboxed items label the various components. $f$ is the measurement carrier frequency, $f_{IF}$ is the desired IF, and $f_s$ is the sample rate of the data acquisition card.

Figure 6.6: Picture of the broadband backplane used in the transmit and receive RF chassis. The backplane employs resistive power division to supply LO to up to 16 transmit/receive cards. Power, baseband, and IF signals are provided via the edge-card connectors.
Figure 6.7: Resistive network for equal power division. Power is fed into port A. The power exiting ports \( B_1 \) and \( B_2 \) is 6 dB lower than the input power. \( P_{in} \) is the input power and \( P_i \) is the power dissipated by resistor \( i \).

depicted in Figure 6.7, as described in [52]. This placement of resistors ensures that each port sees a match to \( Z_0 \). The power rating on the resistors should be chosen to be a third of the maximum input power. Resistive power division has the advantage of allowing broadband operation (the usable bandwidth of this backplane is 0 to 10 GHz). The two disadvantages of the resistive division are the 3 dB loss in power per two-way split and poor isolation in the presence of return signals. Thus, the LO port of the transmit/receive cards should present a good match to 50 \( \Omega \). Also, unused LO output ports must be terminated.

Transmit Card

The transmit card is depicted in Figure 6.8(a) along with the external connections to the backplane and transmit antenna. Devices on the card were chosen to allow operation in the 1 to 3 GHz range. Figure 6.8(b) provides a schematic diagram of the transmit card. The LO is amplified and mixed with the BPSK signal. The modulated signal is further amplified by a signal amplifier and a power FET. Output power delivered to each transmit antenna is approximately 0.5 W.
Figure 6.8: The 1 to 3 GHz transmit card and schematic representation. The diagram in (a) depicts the transmit card and connections to the backplane. The transmit card schematic in (b) shows important component values. The boxed numbers give the nominal signal power throughout the circuit.
Receive Card

The receive card is depicted in Figure 6.9 (b) along with external connections to the backplane and receive antenna. Devices on the card were chosen to allow operation in the 1 to 3 GHz range. Figure 6.9 (b) provides the schematic of the receive card. The receive signal is amplified by two ERA-3SM stages, providing approximately 40 dB of gain. The amplified local oscillator is mixed with the RF signal, producing an IF signal that is fed to the backplane.

IF Board

The IF board in the receive chassis provides simple filtering and digitally controlled gain of up to 16 receive channels with approximately 70 kHz of available bandwidth per channel. The complete IF board is depicted in Figure 6.10. The IF board receives the 16 IF signals from the backplane (one from the IF mixer pin on each receive card). Each signal passes through two gain and two filter stages. Gain control is accomplished with digital signals that specify a gain of 1, 10, or 100 for each amplifier, allowing gains from unity to 10,000. The gains on the channels are tied together so that one gain value is set for all 16 channels. Channel-by-channel gain adjustment is available on the data-acquisition board. The filter stages are simple RC networks with a corner frequency of 72 kHz. The 100 kΩ resistors provide the necessary amplifier bias current.

6.1.4 Antennas

Two types of antennas were used in the arrays required for channel measurement. The first type of antenna is a dual-polarized patch, allowing assessment of both polarization and directivity effects on the channel. The second type of antenna is a simple monopole antenna, allowing close spacing and the assessment of mutual-coupling effects.
Figure 6.9: The 1 to 3 GHz receive card and schematic representation. The diagram in (a) depicts the receive card and connections to the backplane. The schematic in (b) shows important component values and the signal power throughout the circuit.
Figure 6.10: Board providing digitally controlled amplification and basic low-pass filtering of the IF signals. Subfigure (a) shows the basic components of the board, and (b) provides a schematic for each of the 16 channels. $V_{g1}$ and $V_{g2}$ are 2 bit digital signals from the PC, specifying gains of 1, 10, or 100 for each amplifier.
Figure 6.11 shows the basic layout of the patch antenna, fabricated on 60 mil substrate (GIL Technologies part number GML1000). The design strategy in

![Diagram of Patch Antenna](image)

Figure 6.11: Single patch antenna. Dimensions are in mils. The thin transmission line containing the curved section is nominally $3/4\lambda$.

was used to obtain the initial dimensions of the patch, and the dimensions were later refined by simulation with the Momentum package by Agilent Technologies to obtain a center frequency of 2.45 GHz. The input impedance seen by the orthogonal feeds is approximately 402 Ω, requiring a quarter-wave line with a characteristic impedance of 142 Ω for matching. Use of a single quarter-wave section resulted in the wide 50 Ω lines being too close to the patch, which distorted the radiation pattern. The length of the matching section was therefore extended to $(3/4)\lambda$, which reduced the effect of the feeds on the radiation pattern, but also narrowed the bandwidth.
The small amount of mismatch due to coupling in the curved section was tuned out by slightly adjusting the transmission line length.

Figure 6.12: Input impedance, reflection, and port coupling of the patch antenna

Figure 6.12 plots the input impedance, the reflection coefficients, and the coupling of the ports as a function of frequency resulting from Momentum simulations. Figure 6.13 plots the radiation patterns for the patches in the horizontal and vertical plane for excitation of port 1 (vertical polarization) and port 2 (horizontal polarization).

**Monopole Antennas**

Figure 6.14 shows the basic layout of a single monopole antenna. The monopole is fabricated by soldering a copper whip to the center of a standard SMA bulkhead connector (Johnson part number 142-0901-401). Adequate extension of the coaxial feed above the ground plane allows a good match to 50 Ω. This particular antenna was designed for a center frequency of 2.42 GHz. Chief advantages of the monopole antennas are the ability to achieve close spacing and array reconfigurability. Spacing as low as λ/10 for a center frequency of 2.42 GHz can theoretically be achieved with this design. Also, the 33 × 33 grid depicted in Figure 6.15 was fabricated to allow many different array configurations to be created. FDTD simulations were run on the
Figure 6.13: Radiation pattern of the dual-polarized patch antenna at 2.45 GHz. Either port 1 (vertical pol) or port 2 (horizontal pol) is excited, and the radiation pattern in either the horizontal or vertical plane is plotted in dB.
Figure 6.14: Single monopole antenna layout. Solid lines show the exact dimensions of the physical antenna. The dashed lines show modifications to the antenna shape to allow FDTD simulations with a fixed cell size.

Figure 6.15: Grid plate for reconfigurable monopole arrays
Figure 6.16: Input impedance and reflection coefficient of the isolated monopole antenna. Plots were obtained from FDTD simulations.

Figure 6.17: Radiation patterns of the monopole antenna in the horizontal and vertical planes in dB at 2.42 GHz. Plots were obtained from FDTD simulations.

single monopole antenna, yielding the input impedance and input reflection coefficient plots in Figure 6.16. The radiation patterns for the vertical field component in the horizontal and vertical planes are depicted in Figure 6.17. Details on the FDTD simulations are given in Chapter 8.
6.1.5 Calibration Procedure

Due to variation in transmit/receive card fabrication and the microwave devices, the response of one card deviates from that of another. The effect may be removed by measuring the response of each card, and then applying the proper correction to collected data. In general, we may write the measured channel matrix $\overline{H}_M$ as

$$\overline{H}_M = \overline{R} \overline{H} \overline{T},$$

(6.2)

where $\overline{R}$ is the receiver response matrix, $\overline{T}$ is the transmit response matrix, and $\overline{H}$ is the ideal channel matrix. Assuming we can measure the response matrices of the receive and transmit systems, we can compute the true channel matrix from the measured channel matrix as

$$\overline{H} = \overline{R}^{-1} \overline{H}_M \overline{T}^{-1}.$$

(6.3)

In practice, obtaining exact values for $\overline{R}$ and $\overline{T}$ is difficult. The following sections outline some methods for estimating these quantities.

Amplitude Calibration

When inter-channel coupling is small, phase error in the measurement system leads to a distinct random phase shift applied to each row and column of the channel transfer matrix. Capacity is invariant to this type of phase shift, since the singular values of $\overline{H}$ remain unchanged (only the left and right singular vectors are altered). Also, computation of the correlation coefficient of two of the elements of the channel matrix is equal to the true correlation coefficient with a random phase shift. The magnitude of the correlation coefficient, however, will be unaltered. Thus, for studies on capacity and the magnitude of the correlation coefficient, phase error may be ignored and amplitude correction of the data is sufficient. Figure 6.18 shows the setup for measuring the magnitude of $\overline{T}$, requiring the calibration card depicted in Figure 6.19. If coupling may be neglected among the transmit cards, the transmit signals may be left unmodulated and one card at a time is connected as depicted in Figure 6.18 with the other transmit cards terminated. If the $n$th sample of the
Figure 6.18: Setup for amplitude calibration of transmit system. Each transmit card is connected as depicted, allowing computation of relative output amplitude.

Figure 6.19: Image of the calibration card, containing a mixer for down-conversion, a 6 dB attenuator section, and DC blocking capacitors
IF signal stored for the $k$th connected card is $y_k[n]$ and the corresponding average sinusoidal amplitude is $y_k$, the transmit response matrix is

$$T_{ij} = y_i \delta_{ij},$$

which may be scaled by an arbitrary constant. If coupling between the transmitters needs to be measured, the carriers of the transmitters should be modulated with the independent BPSK codes. As before, one card at a time is connected to the calibration setup with the other cards terminated, and the IF waveform $y_k[n]$ is stored, where $k$ is the transmit card connected, and $n$ is the sample number. The method in Section 6.2 can be used to compute the $1 \times N_T$ channel matrix for each case, denoted as $\mathcal{H}_k$. Finally, the magnitude of the calibration matrix is

$$|T| = \begin{bmatrix} |\mathcal{H}_1| \\ |\mathcal{H}_2| \\ \vdots \\ |\mathcal{H}_{N_T}| \end{bmatrix}.$$  

(6.5)

Although having the amplitude of the complete transmit response matrix indicates coupling between the transmitters, the coupling cannot be removed without phase information.

The amplitude of the receive response matrix can be obtained using the setup in Figure 6.20. In this case, the calibration card is not required. A microwave source at a low test power drives one receive card at a time with the other receive cards terminated. The IF signal for all receivers is $y_{\ell k}[n]$, where $\ell$ is the receiver being sampled, $k$ is the excited (or connected) receiver, and $n$ is the sample number. The magnitude of the receive response matrix is then formed as

$$\mathcal{R} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1,N_R} \\ y_{21} & y_{22} & \cdots & y_{2,N_R} \\ \vdots & \vdots & \ddots & \vdots \\ y_{N_R,1} & y_{N_R,2} & \cdots & y_{N_R,N_R} \end{bmatrix},$$

(6.6)
Figure 6.20: Setup for amplitude calibration of receive system. Each receive card is connected at depicted, allowing computation of relative receive amplitude.

where $y_{ij}$ is the average sinusoidal amplitude of the signal $y_{ij}[n]$. As with the transmit calibration measurement, having the magnitude of the receive response matrix only indicates coupling and does not contain sufficient information to remove the coupling.

When coupling at the transmit and receive is small (the off-diagonals of $T$ and $R$ are nearly zero), we perform an amplitude only correction to the data by setting the off-diagonal elements of $|T|$ and $|R|$ to zero and applying relation (6.3).

**Phase Calibration**

The setups in Figure 6.18 for transmit and Figure 6.20 for receive may be modified to obtain the phase of the response matrix as depicted in Figures 6.21 and 6.22. In this case the sample clock of the data-acquisition board is disciplined to the same 10 MHz oscillator that synchronizes the transmit and receive microwave sources. Also, the 10 MHz reference is divided by 10,000 to obtain a 1 kHz signal to trigger the beginning of each sample data record. If the IF is an integer multiple of 1 kHz, sampling always begins at the same point on the IF sinusoid, and the beginning of the record represents an absolute time (and therefore phase) reference.

A simple divide-by-10K circuit is depicted in Figure 6.23. The transistor acts as an inverter and converts the $\pm 1$ V reference to 0 V and 5 V. The four divide-by-10 stages then generate the 1 kHz signal. Care should be taken that the 74390 is chosen from a sufficiently fast logic family to handle the 10 MHz reference.
Figure 6.21: Setup for amplitude and phase calibration of the transmit system. Each transmit card is connected as depicted, allowing computation of relative output amplitude and phase.

Figure 6.22: Setup for amplitude and phase calibration of the receive system. Each receive card is connected as depicted, allowing computation of relative receive amplitude and phase.

Figure 6.23: Simple divide by 10,000 trigger circuit. The circuit accepts a 10 MHz reference and supplies a 1 kHz reference which can be used to trigger the start of sample records.
Unfortunately, the author encountered some difficulty in synchronizing the National Instruments data acquisition board in this manner. On the order of 10 to 20° of phase shift could occur over a calibration cycle. Alternatively, all channels may be sampled simultaneously, which is covered in the next subsection.

Simultaneous Phase Calibration

Figure 6.24 depicts a power splitter or combiner. The circuit uses resistive power division with an additional 35-dB attenuation section for each port. In connection with the resistive power divider (24 dB of attenuation), a signal from input to output experiences about 60 dB of attenuation. This circuit may be used to combine the signals from all transmitters into a single receive channel, or split a single source signal and feed all receive channels. By simultaneously measuring the transmit channels or receive channels, relative phase is preserved.

The transmit calibration setup is depicted in Figure 6.25(a). All $N_T$ transmit channels are fed to the power combiner and the unused ports are terminated. The signal processing schemes in Section 6.2 are then used to compute the $1 \times N_T$ channel matrix, or $\bar{H}_T$ in vector form. Neglecting any transmitter coupling, the transmit

![Figure 6.24: Image of the calibration power combiner/divider that was used for simultaneous phase calibration](image-url)
Figure 6.25: Simultaneous phase calibration setups for transmit and receive. A power combiner/divider is used to sample all transmit/receive channels at once, allowing measurement of relative phase.
response matrix is

\[ T_{ij} = H_{Ti} \delta_{ij}. \]  \hfill (6.7)

The receive calibration setup is depicted in Figure 6.25(b). A single microwave source drives the input on the power divider to create \( N_R \) phase coherent signals. These signals then drive the \( N_R \) receivers, and the \( N_R \times 1 \) channel matrix is computed, or \( \bar{H}_R \) in vector form. Neglecting any receiver coupling, the receiver response matrix is

\[ R_{ij} = H_{Ri} \delta_{ij}. \]  \hfill (6.8)

In order to apply this method, the complex multiport response of the power divider/combiner must also be known. Instead of measuring the entire \( 17 \times 17 \) S-parameter matrix for the device, only the forward and reverse response from the input port to each of the 16 output ports was measured, terminating the unused ports. The rest of the elements of the S-parameter matrix were assumed to be zero. Taking into account the response of the power divider/combiner and assuming reciprocity, the transmit and receive response matrices are

\[ T_{ij} = H_{Ti}/S_{i0} \delta_{ij} \]  \hfill (6.9)

\[ R_{ij} = H_{Ri}/S_{i0} \delta_{ij}. \]  \hfill (6.10)

Agreement between the amplitude of the response matrices with this procedure and those using the amplitude only procedure was poor, possibly due to inaccurate characterization of the power splitter/combiner. As a compromise, the amplitude calibration procedure was used to compute amplitude correction, and the simultaneous phase method was used to compute the phase correction.

### 6.1.6 Antenna Pattern Coverage

Since the MIMO measurement platform excites the transmit array with phase coherent signals, concern may arise over the phased-array interpretation of the transmitter. For example, for a single bit of the BPSK codewords, the transmit antennas are excited with sinusoids having a phase of either 0 or 180°. The resulting
beam pattern has strong lobes in certain directions and nulls in others. For adequate probing of the channel, power must be sent in all possible propagation directions.

The ability of the array to illuminate the channel adequately rests on the degree of orthogonality of the transmit modulation signals. If the signals are exactly orthogonal, the average radiation pattern of the array of elements is the same as that for a single element (ignoring mutual coupling effects).

![Figure 6.26: Arbitrary transmit array configuration. For orthogonal BPSK transmit modulation on the transmit antennas, the average far-field radiation pattern of the array is identical to the single elements.](image)

Considering the arbitrary transmit array in Figure 6.26 and assuming BPSK modulation of the transmit signals, we write the average far-field radiation pattern in direction $\hat{s}$ as

$$P_{\text{avg}}(\hat{s}) = \frac{1}{NK} \sum_n \left| \sum_k a_{kn} E(\hat{s}) e^{j\hat{s} \cdot \bar{r}_k} \right|^2,$$

(6.11)

where $N$ is length of the codewords, $K$ is the number of transmit antennas, $a_{kn}$ is the $n$th bit ($\pm 1$) of the BPSK codeword modulating the signal on antenna $k$, $E(\hat{s})$ is a far field component of a single antenna element (assumed to be identical for all elements in the array), and $\bar{r}_k$ is the displacement of the $k$th antenna. With some
manipulation, and assuming orthogonality of the BPSK codes, we have

\[
P_{\text{avg}}(\hat{s}) = \frac{1}{NK} |E(\hat{s})|^2 \sum_{k_1} \sum_{k_2} e^{j \hat{s}(\tau_{k_1} - \tau_{k_2})} \sum_{n} a_{k_1,n} a_{k_2,n}^* N \delta_{k_1,k_2}
\]

\[= |E(\hat{s})|^2 = P(\hat{s}), \quad (6.12)
\]

where \(P(\hat{s})\) is the single element radiation pattern. In many cases, the use of codes which are not exactly orthogonal is convenient, such as pseudo-random sequences generated with a shift register. In this case, (6.12) does not strictly hold. However, we may compute the average radiation pattern by computing (6.11) directly for a given array configuration and BPSK codes. The BPSK codes used in this research were generated using the maximum-length generating polynomial

\[p(x) = 1 + x^{10} + x^{30} + x^{31}. \quad (6.13)
\]

The codes were generated using a 32-bit shift register with all bits initially set to 1. The first antenna used bits 1-1000 of the resulting sequence, the second antenna used bits 1000-1999, the third antenna used bits 1999-2998, etc. The one bit overlap was for convenience since the next codeword can be generated by seeding the shift register with the contents from the last codeword. The codes were stored in parallel in the pattern memory of the digital pattern generator. Thus, the bit patterns for all of the antennas form the matrix

\[
\begin{bmatrix}
    b_1 & b_2 & \cdots & b_{1000} \\
    b_{1000} & b_{1001} & \cdots & b_{1999} \\
    b_{1999} & b_{2000} & \cdots & b_{2998} \\
    \vdots & \vdots & \ddots & \vdots 
\end{bmatrix}, \quad (6.14)
\]

where \(b_i\) is the \(i\)th bit in the pseudo random code sequence, and rows and columns of \(\overline{A}\) correspond to antenna and time indices, respectively. Figure [6.27] shows the average radiation pattern for a 10-element monopole array with \(\lambda/4\) spacing employing these codewords (mutual coupling has been neglected). The radiation pattern is still very close to uniform. The effects of non-orthogonality of the codes are removed using the procedure in Section [6.2].
Figure 6.27: Average radiation pattern for a 10 element linear monopole array with $\lambda/4$ spacing for pseudo-random BPSK modulation. The array is oriented along the $\hat{x}$ axis.

6.2 Signal Processing

The hardware platform described in Section 6.1 excites the channel with the BPSK codewords and stores the raw IF waveforms from each receive element. This section describes the signal processing required to estimate the channel matrix $\overline{H}$ from the raw data. Figure 6.28 shows the basic steps required to estimate $\overline{H}$, each of which is covered in the following subsections.

![Signal processing steps](image)

Figure 6.28: Signal processing steps
6.2.1 Data Storage Format

The raw data is stored according to the National Instruments NI-DAQ standard. The 12-bit samples are stored as signed 16-bit words in little-endian format. The 16-bit integer $i$ is converted to a sample voltage $v$ as

$$v = 5 \left( \frac{i \cdot g_r \cdot g_f}{2^{11}} \right),$$

(6.15)

where $g_r$ is the rough gain applied to all channels on the IF board (1, 10, 100, 1000), and $g_f$ is the fine gain applied to each individual channel. The gains are stored in a separate file during data acquisition so that the correct voltage may be computed.

6.2.2 Code Search

Estimation of the channel first requires determination of the proper alignment of the codewords in the raw data. In this research, the BPSK codes were pseudorandom sequences, which are nearly orthogonal with respect to shifts of themselves. The signal from each receiver (neglecting noise) is of the form

$$y[n] = \sum_{\ell=1}^{N_T} A_\ell \cdot p_\ell[n] \cos(\Omega_1 n + \phi_\ell),$$

(6.16)

where $y[n]$ is the $n$th sample of a received IF signal, $A_\ell$ and $\phi_\ell$ are the magnitude and phase of the signal sent by the $\ell$th transmitter, $p_\ell[n]$ is the $n$th sample of the baseband BPSK code sent by the $\ell$th transmitter, and $\Omega_1$ is the discrete IF. If we multiply this receive signal against a properly-aligned codeword, we have

$$z[n] = y[n]p_i[n]$$

$$= p_i^2[n]A_i \cos(\Omega_1 n + \phi_i) + \sum_{\ell \in [1, N_T], \ell \neq i} p_i[n]p_\ell[n]A_\ell \cos(\Omega_1 n + \phi_\ell)$$

$$\equiv z_1[n] + z_2[n].$$

(6.17)

The first term ($z_1[n]$) is very close to the unmodulated signal from transmitter $i$ (shifted to the IF), which has been recovered by multiplying a known codeword against the same codeword in the IF data. This operation is referred to as despreading in CDMA parlance, and the resulting signal is known as the despread signal. The second
term \( z_2[n] \) represents interference due to the other codewords. Taking the discrete-time Fourier-transform (DTFT) of the first term gives

\[
Z_1(\Omega) = \mathcal{F}\{z_1[n]\} = \frac{1}{2} \mathcal{F}\{p_i^2[n]\} \ast \left[ A_i \delta(\Omega - \Omega_1) + A_i^* \delta(\Omega + \Omega_1) \right], \tag{6.18}
\]

where \( \ast \) is a convolution operation, \( \mathcal{F}\{\cdot\} \) is the DTFT, and \( A_i = A_i \exp(j\phi_i) \). The DTFT of the squared BPSK modulation is

\[
\mathcal{F}\{p_i^2[n]\} = \sum_n p_i^2[n] e^{-j\Omega n} \approx \delta(\Omega), \tag{6.19}
\]

since \( p_i^2[n] = 1 \) (note that \( p_i^2[n] \approx 1 \) if pulse shaping is applied), and the expression becomes

\[
Z_1(\Omega) \approx \tilde{A}_i \delta(\Omega - \Omega_1) + \tilde{A}_i^* \delta(\Omega + \Omega_1), \tag{6.20}
\]

representing an infinite peak at the IF. The second (interference) term is

\[
Z_2(\Omega) = \mathcal{F}\{z_2[n]\} = \sum_{\ell \in [1,N_T], \ell \neq i} \mathcal{F}\{p_i[n]p_\ell[n]\} \ast \left[ \tilde{A}_i \delta(\Omega - \Omega_1) + \tilde{A}_i^* \delta(\Omega + \Omega_1) \right], \tag{6.21}
\]

where

\[
\mathcal{F}\{p_i[n]p_\ell[n]\} = \sum_n p_i[n]p_\ell[n] e^{-j\Omega n}. \tag{6.22}
\]

In a small neighborhood of \( \Omega = 0 \) the DTFT expression is

\[
\mathcal{F}\{p_i[n]p_\ell[n]\} \approx \sum_n p_i[n]p_\ell[n] \approx 0, \tag{6.23}
\]

where the second approximation is equality for perfectly orthogonal codes. Therefore, \( Z_2(\Omega) \approx 0 \) in a neighborhood of \( \Omega = \Omega_1 \), and

\[
Z(\Omega) \approx Z_1(\Omega) \approx \tilde{A}_i \delta(\Omega - \Omega_1) + \tilde{A}_i^* \delta(\Omega + \Omega_1), \tag{6.24}
\]

which illustrates that the spectrum of the receive signal multiplied by a codeword will exhibit a sharp peak at the IF.

With these concepts in hand, a simple alignment procedure can be developed as depicted in Figure 6.29. The IF signal from the \( k \)th receive channel is \( y_k[n] \),
Figure 6.29: Code alignment procedure. The optimal codeword alignment for the $k$th receive channel is given by $s_{k}^{\text{start}}$.

where $n$ is a sample index. The signal $y_k[n]$ is multiplied by the $i$th baseband codeword shifted by $s$ samples, or $p_i[n-s]$. When the shifted baseband code and the codeword in the data are properly aligned, the FFT exhibits a peak at the center frequency of the IF signal. The ideal shift for each channel is determined by computing

$$s_{k}^{\text{start}} = \arg\max_s \left( \max_f |g_{ki}[s, f]| \right),$$

(6.25)

where $g_{ki}[s, f] = \text{FFT}(y_k[n]p_i[n-s])$, and $f$ is a frequency bin index. The $\max(\cdot)$ operation should only cover a small neighborhood of the nominal IF, determined by the accuracy of the microwave sources.

The algorithm in this research used a number of modifications to the approach suggested by (6.25):

1. An adaptive procedure was used where the initial codewords are shortened to one-quarter of the length of the full codes, speeding up the multiplication and FFT operations. Full-length codes are used for later refinement.

2. Shifts are first searched in increments of one-half of the bit time, rather than all possible one-sample shifts. Once this rough alignment is found, the optimal alignment is determined by finding (6.25) with the full-length code over a narrow sample range (at least ±1 bit time).
3. Ideally, (6.25) is also maximized over all transmit codewords to find the strongest transmit signal at each receiver. This addition increases the search time, but improves robustness of the algorithm.

4. For a given receive stream, once two codewords are found that give the same location for optimal alignment, the search for all remaining receivers and codewords is limited to a small neighborhood of this location (such as ±5 bit times).

Since the data acquisition card in this research uses a multiplexed scheme without simultaneous sample-and-hold hardware, there may be as much as a one sample range in the optimal alignment of the channels. Also, since the receive data acquisition hardware is not synchronized with the transmit modulation, the alignment is refined for every block (complete codeword) of data, since optimal alignment may change over time.

6.2.3 Carrier Recovery

Once proper alignment of the codewords is obtained, the carrier may be recovered in two steps:

1. An estimate of the frequency of the IF is obtained with an optimization loop.

2. The long-term phase evolution of the carrier is tracked.

Figure 6.30 depicts algorithmically how the carrier frequency is estimated. An initial guess is chosen for $\Omega_1$. Next, the despread signal from one of the receivers is correlated against the current estimate of the IF. The IF is adjusted in accordance with some type of search procedure to determine the value of $\Omega_1$ that maximizes this correlation. This operation is equivalent to finding the peak of the DTFT of the despread signal. Mathematically, we are finding

$$\Omega_1^\text{opt} = \arg\max_{\Omega_1} \left| \sum_n y_k[n] p_\ell[n] e^{-j\Omega_1 n} \right|,$$

(6.26)

where the transmitter ($\ell$) and receiver ($k$) indices are generally chosen to be the pair yielding the strongest signal.
Figure 6.30: Carrier frequency recovery algorithm

Figure 6.31: Carrier phase recovery algorithm

Figure 6.31 shows the method for computing the time evolution of the phase. The despread signal from one of the receivers is correlated against the I and Q carrier components at the estimated IF. Taking the inverse tangent of the components results in a raw phase estimate. To reduce the effect of noise and interference from other codewords, the resulting phase estimate may be convolved with a suitable smoothing window.

6.2.4 Channel Estimation

When the code alignment, carrier frequency, and carrier phase are known, the channel transfer matrix can be estimated. The observed $n$th sample of the signal
on the $k$th receiver may be written as

$$y_k[n] = \sum_\ell A_k\ell \ p_\ell[n] \cos(\Omega_1 n + \phi_n + \phi_{k\ell}) + \eta_k[n], \quad (6.27)$$

where $A_k\ell$ and $\phi_{k\ell}$ are the amplitude and phase of the $k\ell$th element of channel transfer matrix ($H_{k\ell} = A_k\ell \exp[j\phi_{k\ell}]$), $p_\ell[n]$ is the aligned baseband codeword for transmitter $\ell$, $\Omega_1$ is the estimated IF, $\phi_n$ is the estimated carrier phase, and $\eta_k[n]$ is additive white Gaussian receiver noise. The maximum likelihood (ML) estimate of the $k$th row of $\overline{H}$ is given by

$$\overline{H}_{k}^{\mathrm{ML}} = \arg\max_{\overline{H}_k} f(y_k[n] \mid \overline{H}_k), \quad (6.28)$$

where $f(y_k[n] \mid \overline{H}_k)$ is the probability density function of the observed sequence $y_k[n]$ given that the $k$th row of the channel transfer matrix is $\overline{H}_k$. The conditional PDF is found by fixing $\overline{H}_k$ and computing the PDF of $y_k[n]$, as given in (6.27). Adding a constant to $\eta_k[n]$ shifts the mean of the Gaussian random variable, or

$$f(y_k[n] \mid \overline{H}_k) = \prod_n \frac{1}{\sqrt{2\pi \sigma_\eta}} \exp\left[\frac{-(y_k[n] - \mu_{kn})^2}{2\sigma_\eta^2}\right] = \left(\frac{1}{\sqrt{2\pi \sigma_\eta}}\right)^N \exp\left[-\frac{1}{2\sigma_\eta^2} \sum_n (y_k[n] - \mu_{kn})^2\right], \quad (6.29)$$

where each mean $\mu_{kn}$ is given by

$$\mu_{kn} = \sum_\ell A_k\ell \ p_\ell[n] \cos(\Omega_1 n + \phi_n + \phi_{k\ell})$$

$$= \sum_\ell A_k\ell \ p_\ell[n] \left[\cos(\Omega_1 n + \phi_n) \cos(\phi_{k\ell}) - \sin(\Omega_1 n + \phi_n) \sin(\phi_{k\ell})\right]$$

$$= \sum_\ell p_\ell[n] \left[H_{k\ell}^R c_n - H_{k\ell}^I s_n\right], \quad (6.30)$$

where $H_{k\ell}^R$ and $H_{k\ell}^I$ are the real and imaginary parts of $H_{k\ell}$, $c_n = \cos(\Omega_1 n + \phi_n)$, and $s_n = \sin(\Omega_1 n + \phi_n)$. The necessary condition for a local maximum of $f(y_k[n] \mid \overline{H}_k)$ is that partial derivatives with respect to $H_{R,k\ell'}$ and $H_{I,k\ell'}$ must vanish at the maximum for all $\ell'$, or

$$\frac{\partial f}{\partial H_{k\ell'}^{[R,I]}} = \left(\frac{1}{\sqrt{2\pi \sigma_\eta}}\right)^N \exp\left[-\frac{1}{2\sigma_\eta^2} \sum_n (y_k[n] - \mu_{kn})^2\right] \times \sum_n (-1/\sigma_\eta^2)(y_k[n] - \mu_{kn}) \left(-\frac{\partial \mu_{kn}}{\partial H_{k\ell'}^{[R,I]}}\right), \quad (6.31)$$
where
\[
\frac{\partial \mu_{kn}}{\partial H^R_{k\ell'}} = p_{\ell'}[n] \cos(\Omega_1 n + \phi_n) \tag{6.32}
\]
\[
\frac{\partial \mu_{kn}}{\partial H^I_{k\ell'}} = -p_{\ell'}[n] \sin(\Omega_1 n + \phi_n). \tag{6.33}
\]

The only way to make \((6.31)\) identically zero is to make
\[
\sum_n (y_k[n] - \mu_{kn}) \frac{\partial \mu_{kn}}{\partial H^{[R,I]}_{k\ell'}} = 0. \tag{6.34}
\]

First, setting \(\frac{\partial f}{\partial H^R_{k\ell'}} = 0\) gives
\[
0 = \sum_n \left\{ y_k[n] - \sum_{\ell} p_{\ell}[n] \left[ H^R_{k\ell} c_n - H^I_{k\ell} s_n \right] \right\} p_{\ell'}[n] c_n
\]
\[
\sum_n y_k[n] p_{\ell'}[n] c_n = \sum_n \sum_{\ell} p_{\ell}[n] p_{\ell'}[n] \left[ H^R_{k\ell} c_n^2 - H^I_{k\ell} s_n c_n \right]
\]
\[
= \frac{1}{2} \sum_n \sum_{\ell} p_{\ell}[n] p_{\ell'}[n] \left[ H^R_{k\ell}(1 + c'_n) - H^I_{k\ell} s'_n \right], \tag{6.35}
\]
where \(c'_n = \cos[2(\Omega_1 n + \phi_n)]\) and \(s'_n = \sin[2(\Omega_1 n + \phi_n)]\). Next, setting \(\frac{\partial f}{\partial H^I_{k\ell'}} = 0\) gives
\[
0 = \sum_n \left\{ y_k[n] - \sum_{\ell} p_{\ell}[n] \left[ H^R_{k\ell} c_n - H^I_{k\ell} s_n \right] \right\} p_{\ell'}[n] s_n
\]
\[-\sum_n y_k[n] p_{\ell'}[n] s_n = \sum_n \sum_{\ell} p_{\ell}[n] p_{\ell'}[n] \left[ H^I_{k\ell} s_n^2 - H^R_{k\ell} c_n s_n \right]
\]
\[
= \frac{1}{2} \sum_n \sum_{\ell} p_{\ell}[n] p_{\ell'}[n] \left[ H^I_{k\ell}(1 - c'_n) - H^R_{k\ell} s'_n \right]. \tag{6.36}
\]

For a fixed value of \(k\), Equations \((6.35)\) and \((6.36)\) can be formed into a block matrix equation as
\[
\begin{bmatrix}
\overline{R}_R \\
\overline{R}_I 
\end{bmatrix} =
\begin{bmatrix}
\overline{B}_{RR} & \overline{B}_{RI} \\
\overline{B}_{IR} & \overline{B}_{II} 
\end{bmatrix}
\begin{bmatrix}
H^R \\
H^I
\end{bmatrix}, \tag{6.37}
\]
where
\[
\{\overline{R}_R\}_{\ell'} = \sum_n y_k[n] p_{\ell'}[n] c_n
\]
\[
\{\overline{B}_{RR}\}_{\ell'\ell} = \frac{1}{2} \sum_n p_{\ell}[n] p_{\ell'}[n](1 + c'_n)
\]
\[
\{\overline{B}_{RI}\}_{\ell'\ell} = -\frac{1}{2} \sum_n p_{\ell}[n] p_{\ell'}[n] s'_n. \tag{6.38}
\]
Simple matrix inversion yields $H_k$. To compute the complete channel matrix, the operation is performed for each receiver $k$. In this research, the range of samples $n$ in the summations was chosen to be all the samples associated with a complete 1000-bit codeword. However, larger or smaller ranges can also be used depending on the application.

Note that this estimation scheme can be obtained by casting the problem into the well known ML method that solves the problem

$$ \bar{Y} = \bar{H} \bar{S} + \bar{\eta}, $$

(6.40)

where $\bar{Y}$ is the receive signal matrix, $\bar{H}$ is the channel matrix, $\bar{S}$ is the known transmit signal matrix, and $\bar{\eta}$ is a matrix of i.i.d. Gaussian noise samples. In this case, the ML estimate of the channel $H$ is given by

$$ \bar{H}_{\text{ML}} = \bar{Y} \bar{S}^H (\bar{S} \bar{S}^H)^{-1}, $$

(6.41)

where $\{\cdot\}^H$ is the Hermitian operator. The estimation problem here may be cast into this framework by letting the signal matrix be

$$ S_{\ell n}^R = p_\ell[n] \cos(\Omega_1 n + \phi_n) $$

$$ S_{\ell n}^I = -p_\ell[n] \sin(\Omega_1 n + \phi_n) $$

(6.42)

and

$$ \bar{S} = \begin{bmatrix} \bar{S}_R^T \\ \bar{S}_I^T \end{bmatrix}^T, $$

(6.43)

where $\{\cdot\}^T$ is the transpose operator. Similarly, the channel matrix is defined as

$$ \bar{H}^T = \begin{bmatrix} \bar{H}_R^T \\ \bar{H}_I^T \end{bmatrix}^T, $$

(6.44)
where $\overline{H}_R$ and $\overline{H}_I$ are the real and imaginary parts of the complex channel matrix. Finally, the receive signal matrix is given as

$$Y_{kn} = y_k[n].$$  \hfill (6.45)

Insertion of these definitions into (6.41) yields the same solution as that given by (6.37) for a single receive channel. One may be tempted to conclude, however, that processing one row at a time is actually sub-optimal. However, inspection of (6.41) reveals that the estimation operator only operates on one row of $\overline{Y}$ at a time to yield a single row of $\overline{H}$. Thus, estimation can take place one row at a time without sacrificing optimality.

### 6.2.5 Estimation Error

Knowledge of the length of codes required for a specific amount of estimation error is useful. Dividing the total received signal from one receiver into a signal part and a noise part, we have

$$y[n] = \hat{y}[n] + \eta[n],$$  \hfill (6.46)

where $\hat{y}[n]$ is the signal that would be measured if there were no noise. Next, the real correlation term becomes

$$\overline{R}_R = \sum_n (\hat{y}[n] + \eta[n])\overline{p}[n]c_n$$

$$= \sum_n \hat{y}[n]\overline{p}[n]c_n + \sum_n \eta[n]\overline{p}[n]c_n$$

$$\equiv \overline{R}_R + \overline{N}_R,$$  \hfill (6.47)

where $\{\overline{p}[n]\}_\ell = p_\ell[n]$. Likewise, the imaginary correlation term is

$$\overline{R}_I = -\sum_n (\hat{y}[n] + \eta[n])\overline{p}[n]s_n$$

$$= -\sum_n \hat{y}[n]\overline{p}[n]s_n - \sum_n \eta[n]\overline{p}[n]s_n$$

$$\equiv \overline{R}_I + \overline{N}_I.$$  \hfill (6.48)
Also, we have the relations
\[ R = \overline{B} \, H^{\text{ML}} \quad \mathcal{R} = \overline{B} \, H. \] (6.49)

Defining the error as the difference between the ML estimate of the channel matrix and the true channel matrix gives
\[ \overline{\xi} = \mathcal{H}^{\text{ML}} - \mathcal{H} = \overline{B}^{-1}(R - \mathcal{R}) = \overline{B} \, \mathcal{N}, \] (6.50)
where \( \overline{B} = \overline{B}^{-1} \) and \( \mathcal{N} = R - \mathcal{R} \). \( \overline{\xi} \) is described with the multivariate joint Gaussian distribution since it is a linear combination of Gaussian random variables. The mean and covariance matrices are given by
\[ \mathbb{E}\{\overline{\xi}\} = \overline{B} \, \mathbb{E}\{\xi\} = 0 \] (6.51) and
\[ \overline{K}_\xi = \mathbb{E}\{\overline{\xi}\,\overline{\xi}^T\} = \mathbb{E}\{(\overline{B} \, \mathcal{N})(\overline{B} \, \mathcal{N})^T\}
= \overline{B} \, \mathbb{E}\{\mathcal{N}\,\mathcal{N}^T\}\overline{B}^T \equiv \overline{B} \, \overline{K}_N \overline{B}^T. \] (6.52)

The covariance of the summed noise vector \( \mathcal{N} \) is found as
\[ \overline{K}_\mathcal{N} = \mathbb{E}\left\{ \begin{bmatrix} \mathcal{N}_R \\ \mathcal{N}_I \end{bmatrix} \begin{bmatrix} \mathcal{N}_R^T \\ \mathcal{N}_I^T \end{bmatrix} \right\} = \mathbb{E}\left\{ \begin{bmatrix} \mathcal{N}_R \mathcal{N}_R^T & \mathcal{N}_R \mathcal{N}_I^T \\ \mathcal{N}_I \mathcal{N}_R^T & \mathcal{N}_I \mathcal{N}_I^T \end{bmatrix} \right\}. \] (6.53)

The components of this covariance matrix are found as
\[ \mathbb{E}\{\mathcal{N}_R \mathcal{N}_R^T\} = \mathbb{E}\left\{ \left( \sum_{n_1} \eta[n_1] \overline{p}[n_1] c_{n_1} \right) \left( \sum_{n_2} \eta[n_2] \overline{p}^T[n_2] c_{n_2} \right) \right\}
= \sum_{n_1} \sum_{n_2} \overline{p}[n_1] \overline{p}^T[n_2] c_{n_1} c_{n_2} \mathbb{E}\{\eta[n_1] \eta[n_2]\}
= \sigma^2_{\eta} \sum_n \overline{p}[n] c_n^2 = \sigma^2_{\eta} \overline{B}_{RR} \] (6.54)
\[ \mathbb{E}\{\mathcal{N}_R \mathcal{N}_I^T\} = \mathbb{E}\{\mathcal{N}_I \mathcal{N}_R^T\} = \sigma^2_{\eta} \sum_n \overline{p}[n] c_n s_n = \sigma^2_{\eta} \overline{B}_{RI} \] (6.55)
\[ \mathbb{E}\{\mathcal{N}_I \mathcal{N}_I^T\} = \sigma^2_{\eta} \sum_n \overline{p}[n] s_n^2 = \sigma^2_{\eta} \overline{B}_{II}, \] (6.56)
where \( \overline{p}[n] = \overline{p}[n]\overline{p}^T[n] \). Therefore, we have

\[
K_N = \sigma^2 \bar{B}^T \quad \quad K_\xi = \sigma^2 \overline{\bar{B}}^T = \sigma^2 \overline{\bar{B}}^{-1}.
\]

(6.57)

Thus, we have an exact expression for the error covariance for a given set of codewords and a known carrier. Later we use the average RMS error, defined as

\[
\epsilon = \frac{1}{N_T} \sqrt{\sum_{i} \left\{ K_\xi \right\}_{ii}},
\]

(6.58)

which represents a combined RMS error for the real and imaginary parts, averaged over all transmit streams. Next, we consider the case of orthogonal codes, where

\[
\sum_n \overline{p}[n] = N\bar{T}.
\]

(6.59)

If we have several samples per period of the IF, we find that

\[
\sum_n c_n^2 \approx \sum_n s_n^2 \approx N/2
\]

\[
\sum_n c_n s_n \approx 0.
\]

(6.60)

Also, if the IF is an integer multiple of the bit-rate, we have the relations

\[
\sum_n \overline{p}[n]c_n \approx \sum_n \overline{p}[n]s_n \approx \frac{1}{2} \sum_n \overline{p}[n]
\]

\[
\sum_n \overline{p}[n]c_n s_n \approx 0.
\]

(6.61)

Thus, the simple approximate expression for \( \overline{\bar{B}} \) is

\[
\overline{\bar{B}}_{RR} \approx \frac{1}{2} N\bar{T}
\]

\[
\overline{\bar{B}}_{RI} = \overline{\bar{B}}_{IR} \approx 0
\]

\[
\overline{\bar{B}}_{II} \approx \frac{1}{2} N\bar{T}
\]

(6.62)

and therefore \( \overline{\bar{B}}^{-1} = (2/N)\bar{T} \). From (6.57), the covariance of the error in the real and imaginary parts of the channel matrix elements becomes

\[
K_\xi = \sigma_\eta^2 \overline{\bar{B}}^{-1} = \frac{2\sigma_\eta^2}{N} \bar{T}.
\]

(6.63)
Adding the variances associated with the real and imaginary parts for each element gives the total error variance

\[ \sigma_H^2 = \frac{4\sigma_n^2}{N}. \]  

(6.64)

### 6.2.6 Simulations

This section validates the methods presented in Section 6.2 by running the algorithms on simulated data. For each simulation, raw IF data was generated with the parameters in Table 6.1. A single 10 × 10 channel matrix was generated assuming a unit variance i.i.d. multivariate complex normal distribution on the elements. A block of data consisted of all of the samples for a single codeword (10,000 samples). Codewords were pseudo-random bit sequences generated with a shift register operating on the polynomial \( 1 + x^{10} + x^{30} + x^{31} \), as described in Section 6.1.6. 21 blocks were generated to allow 20 estimates of the channel matrix (one estimate per complete block). \( N - 1 \) estimates are obtained rather than \( N \), because the first complete codeword does not start right at the first sample. The average RMS error for the channel matrix elements was defined as

\[ \epsilon_H = \sqrt{\frac{1}{N_T N_R N} \sum_n \| e^{j\phi} \hat{H}_n^{ML} - \overline{H} \|_F^2}, \]  

(6.65)

where \( \| \cdot \|_F \) is the Frobenius norm, and \( \phi \) was chosen in such a manner to rotate the phases of the elements of the estimated channel matrix to best fit the ideal channel matrix. This rotation is necessary, since the estimation procedure only preserves
the relative phases of the channel matrix elements. For each channel matrix, $\phi$ is calculated from

$$\cos \phi = \frac{1}{N_R N_T} \sum_i \sum_j \left( \text{Re} \{ H_{ij}^{\text{ML}} \} \text{Re} \{ H_{ij} \} + \text{Im} \{ H_{ij}^{\text{ML}} \} \text{Im} \{ H_{ij} \} \right)$$

$$\sin \phi = \frac{1}{N_R N_T} \sum_i \sum_j \left( \text{Re} \{ H_{ij}^{\text{ML}} \} \text{Im} \{ H_{ij} \} - \text{Im} \{ H_{ij}^{\text{ML}} \} \text{Re} \{ H_{ij} \} \right).$$

A number of important cases were considered:

1. The carrier frequency and phase were either known exactly (know carrier), or the carrier frequency was estimated and the phase recovered (unknown carrier).

2. Drift of the carrier phase was simulated by applying a very low frequency FM component of either 0 Hz (constant phase) or 0.1 Hz (varying phase).

3. The code rate was set to one that evenly divides the sample rate ($f_c = 12500$), or one that did not ($f_c = 12500.25$). Setting an uneven code rate tests the ability of the algorithms to handle slippage of the code with respect to the sample rate, a realistic case for an unsynchronized system.

4. Different cases of additive receiver noise were tested. The proper amount of noise was added to obtain average receiver SNRs of $\infty$ (no noise), 20 dB, 10 dB, or 0 dB. For each level of SNR, the expected RMS error ($\epsilon$) was computed from (6.57).

Table 6.2 shows the RMS error for the various combinations of parameters. Also tabulated is the computed average RMS error for noise only ($\epsilon$) from (6.57). For the case of no noise and a known carrier, the error is $5 \times 10^{-12}$, most likely due to the error of finite-precision arithmetic. Next, for a known carrier with additive noise, the simulated error is very close to the exact expression given by (6.57). The uneven code rate does not change the results significantly. Even in the noiseless case, not knowing the carrier leads to about 0.4% RMS error. This error is mainly due to the difficulty in estimating the carrier phase using a single despread transmit channel, since the sinusoid is slightly corrupted by other transmit codes. This error could be reduced in a number of ways:
Table 6.2: RMS error for channel estimation simulations. $\epsilon$ is the expected RMS error computed from (6.57).

<table>
<thead>
<tr>
<th>$f_c$</th>
<th>SNR</th>
<th>$\epsilon$</th>
<th>Known Carrier</th>
<th>Unknown Carrier</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>FM: 0 Hz</td>
<td>FM: 0.1 Hz</td>
</tr>
<tr>
<td>12500</td>
<td>$\infty$</td>
<td>0</td>
<td>$5 \times 10^{-12}$</td>
<td>$5 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>20 dB</td>
<td>0.00198</td>
<td>0.000201</td>
<td>0.000202</td>
</tr>
<tr>
<td></td>
<td>10 dB</td>
<td>0.00627</td>
<td>0.00639</td>
<td>0.00642</td>
</tr>
<tr>
<td></td>
<td>0 dB</td>
<td>0.01982</td>
<td>0.02017</td>
<td>0.02020</td>
</tr>
<tr>
<td>12500</td>
<td>$\infty$</td>
<td>0</td>
<td>$5 \times 10^{-12}$</td>
<td>$5 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>20 dB</td>
<td>0.00198</td>
<td>0.00197</td>
<td>0.00201</td>
</tr>
<tr>
<td></td>
<td>10 dB</td>
<td>0.00627</td>
<td>0.00636</td>
<td>0.00622</td>
</tr>
<tr>
<td></td>
<td>0 dB</td>
<td>0.01982</td>
<td>0.01969</td>
<td>0.02001</td>
</tr>
</tbody>
</table>

1. The phase estimates from several despread transmit channels could be averaged to obtain a better estimate.

2. The channel could be estimated in a two-step procedure. In the first step, the carrier is estimated blindly as before and an initial channel estimate is obtained. On the second step, the initial channel estimate is used to null the effect of all but a single transmit channel at a time, giving a better phase estimate.

3. A maximum likelihood scheme could be developed that estimates the carrier and channel matrix elements in a joint fashion.

4. Exactly orthogonal codes could be used to minimize cross correlation.

For the purposes of this research, RMS error less than 1% was deemed sufficient, avoiding the need for more sophisticated channel estimation.

6.3 Chapter Summary

This chapter has introduced MIMO wireless systems as a method of increasing system transmission rates without increasing bandwidth. Understanding of true channel behavior requires a system capable of direct measurement of the channel. This chapter presented the hardware and software for a flexible $16 \times 16$ channel
measurement system, suitable for narrowband channel probing. Representative sim-
ulations were provided to validate the data processing methods.
Chapter 7

MIMO Data Collection

This chapter presents data that was collected with the MIMO measurement platform described in Chapter 6. Data was collected in a number of important scenarios to assess the impact of antenna spacing, antenna directivity, antenna polarization, and multipath richness on the measured channel.

The organization of the chapter is as follows. Section 7.1 describes the locations and measurement parameters for each location. Section 7.2 plots marginal PDFs for the data sets, showing that the single-element subchannels are marginally complex Gaussian. Sections 7.3 and 7.4 present measured spatial and temporal correlation functions, suggesting the required antenna separations and channel stationarity. Sections 7.5, 7.6, and 7.7 study capacity versus the number of antenna elements, antenna polarization, and antenna directivity, respectively. Section 7.8 explores the tradeoff between multipath richness and average SNR, and the overall impact on capacity.

This presentation provides new insight into the behavior of MIMO wireless channels. Although the single-element subchannels exhibit marginal Rayleigh fading, the subchannels are not independent except for very wide antenna spacings. The capacity gains are more modest than simple independent multivariate complex normal models would suggest. Antenna design and array configuration affect the multipath richness (and therefore capacity) of the channel. However, multipath richness usually comes at the loss of average receive SNR, which cannot be ignored.
7.1 Measurement Locations and Parameters

This section describes the indoor locations for the data collection and the associated measurement parameters. The data in this research can be organized into a hierarchy of collections, locations, and data sets. At the highest level, a collection encompasses data taken in a single day, usually to study a single phenomenon. Next, a collection consists of several probing locations. A location refers to a specific configuration of transmit and receive. For each location, a number of sets may be collected, each of which is a 10-second record of MIMO channel data. Table 7.1 provides an overview of the data collections and basic measurement configurations. Subsections that follow describe each data collection in detail. The majority of the measurement scenarios are on the 4th floor of the Clyde building, as depicted in Figure 7.1.

Table 7.1: MIMO measurement locations, antenna types, and number of ten-second records collected. Antenna array types are four single-pol patches (4SP), two dual-pol patches (2DP), and ten monopoles (10SP).

<table>
<thead>
<tr>
<th>Collection</th>
<th>Transmit</th>
<th>Receive</th>
<th>Antenna Type</th>
<th>Records</th>
</tr>
</thead>
<tbody>
<tr>
<td>4×4(a)</td>
<td>Room 484</td>
<td>Several Rooms</td>
<td>4SP</td>
<td>233</td>
</tr>
<tr>
<td>4×4(b)</td>
<td>West Hall</td>
<td>Room 400</td>
<td>2DP</td>
<td>165</td>
</tr>
<tr>
<td>10×10(a)</td>
<td>West Hall</td>
<td>Room 400</td>
<td>10SP</td>
<td>474</td>
</tr>
<tr>
<td>10×10(b)</td>
<td>Room 484</td>
<td>Room 400</td>
<td>10SP</td>
<td>274</td>
</tr>
<tr>
<td>10×10(c)</td>
<td>Several Rooms</td>
<td>Several Rooms</td>
<td>10SP</td>
<td>109</td>
</tr>
</tbody>
</table>

The rationale behind the data collection configurations was the desire to model plausible communications systems as closely as possible. In this discussion, server refers to a wireless base station or wireless LAN server, and client refers to a mobile wireless user or a wireless LAN client. Three basic scenarios seem very likely:

1. A high power server would be placed in the center of a building (room 484) to serve clients on an entire floor. This configuration corresponds to collections 4×4 (a) and 10×10(b).
Figure 7.1: Locations on the fourth floor of the Clyde Building. Rooms and hallways which fall in one of data collections are shaded.
2. A lower power server would be placed in a hallway to serve clients in rooms attached to the hallway. This configuration corresponds to collections 4×4(b) and 10×10(a).

3. Clients could communicate on a peer-to-peer basis without any central server. This configuration corresponds to collection 10×10(c).

The measurements employed a number of basic antenna types. Antenna configurations 4SP, 2DP, and 10SP refer to four single-polarized patches, two dual-polarized patches, and ten single-polarized monopole antennas, respectively. Figure 7.2 depicts the 4-element patch array. The patches were spaced λ/2 apart (center to center). For collections labeled with 4SP, the vertical ports (2_V, 4_V, 6_V, and 8_V) were excited or measured. For collections labeled with 2DP, all ports of the center two patches (3_H, 4_V, 5_H, 6_V) were excited or measured.

Figure 7.2: 4-element patch antenna array. Ports are numbered from right to left, with the subscript indicating the polarization. On each patch, the right or the bottom is excited for horizontal or vertical polarization. The arrow indicates the array orientation for later top-view diagrams.
Figure 7.3: 10-element monopole antenna array. Ports are numbered from right to left. The arrow indicates the array orientation for later top-view diagrams.

<table>
<thead>
<tr>
<th>Table 7.2: Common data collection parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carrier Frequency</td>
</tr>
<tr>
<td>Intermediate Frequency</td>
</tr>
<tr>
<td>Code Bit Rate</td>
</tr>
<tr>
<td>Code Length</td>
</tr>
<tr>
<td>Sample Rate</td>
</tr>
</tbody>
</table>

Table 7.2 gives the common parameters for all of the collections. The IF and code rates were chosen to evenly divide a convenient sample rate supported by the data-acquisition card. The pseudo-random codes were obtained from the polynomial

\[ p(x) = 1 + x^{10} + x^{30} + x^{31} \]  

as described in Section 6.1.6. The following subsections describe each of the data collections in detail.

### 7.1.1 Collection 4×4(a)

In data collection 4×4(a), the transmitter was placed in room 484, and the receiver was placed in several different rooms on the fourth floor and a single room on the fifth floor. The transmit and receive locations are depicted in Figures 7.3 and
Data was collected during a summer term late in the afternoon, so activity was very low.

### 7.1.2 Collection 4×4(b)

In data collection 4×4(b), two dual-polarization patches were employed on each side of the link to explore the benefits of systems with multiple polarization. In this case, the transmitter was placed at several locations in the west hallway and the receiver was placed at several locations in room 400 (see Figure 7.6). Every combination of transmit and receive location was probed to obtain a good sample of the statistical ensemble. Activity in the hallway containing the transmitter was moderate.

### 7.1.3 Collection 10×10(a)

In data collection 10×10(a), closely-spaced (λ/4) monopole antennas were employed at each side of the link. The transmitter was placed at four locations in the west hallway and the receiver was placed at six different locations in room 400 (see Figure 7.7). Every combination of transmit and receive location was probed. Data was collected in the early evening when activity was very low.

### 7.1.4 Collection 10×10(b)

Figure 7.8 depicts the measurement location for data collection 10×10(b), where the monopole arrays were again employed. For location 1, the transmitter was fixed in the middle of room 484, and the receiver was moved in discrete 1-ft steps between the data sets. For location 2, the transmitter was fixed and the receiver moved continuously across the room at the rate of about 0.13 ft/s. For location 3, the receiver was fixed, and the transmitter was moved in 1-ft steps. However, the movement was not synchronous with the receiver data acquisition, so movement usually occurred inside of a data set. For location 4, the receiver was fixed, and the transmitter moved in 1-ft steps. For location 5, the transmitter was placed in the
Figure 7.4: Specific measurement locations for collection 4×4(a). Room 421 was probed in part 3 and room 420 in part 4.
Figure 7.5: Specific measurement locations for collection 4×4(a) (continued)
Figure 7.6: Specific measurement locations for collection 4×4(b). Locations are denoted as $\text{loc}_{\{\text{xmit}\}}_{\{\text{recv}\}}$ where $\{\text{xmit}\}$ is one of the six transmit locations and $\{\text{recv}\}$ is one of the six receive locations.

Figure 7.7: Specific measurement locations for collection 10×10(a). Locations are denoted as $\text{loc}_{\{\text{xmit}\}}_{\{\text{recv}\}}$ where $\{\text{xmit}\}$ is one of the four transmit locations and $\{\text{recv}\}$ is one of the six receive locations.
Figure 7.8: Specific measurement locations for collection 10×10(b). For locations 1-4, either the transmitter or receiver moved. Movement was in discrete steps for locations 1, 3, and 4, and continuous for location 2. For location 5, the receiver was moved in discrete 3-foot steps along the west hallway. In each case, a set is a single step along one of the paths.
west hall, and moved in 3-foot steps between the data sets along the noted path. Data was collected in the early evening when activity was very low.

### 7.1.5 Collection 10×10(c)

In data collection 10×10(c), a peer-to-peer communications environment was simulated with the 10-element monopole arrays. A number of discrete positions were set for transmit and receive (see Figure 7.9), and several combinations were probed. This data collection was also very useful for understanding the tradeoff between multipath richness and SNR. Table 7.3 provides the positions and orientations of transmit and receive for each probed location. Data was collected from the morning to early afternoon on a Friday before a 3-day holiday weekend, and activity was low.

### 7.2 Marginal PDFs

For an indoor communications environment with no direct line-of-sight (LOS), we expect a large number of independent multipath components, leading to Rayleigh fading at the receiver. In this case, the PDF for the amplitude and phase of the received signal are

\[
f(r) = \frac{r}{\sigma^2} \exp \left( -\frac{r^2}{2\sigma^2} \right), \quad r \geq 0 \tag{7.2}\]

\[
f(\phi) = \frac{1}{2\pi}, \quad \phi \in [-\pi, \pi], \tag{7.3}\]

where \( f(r) \) is the standard Rayleigh PDF with parameter \( \sigma \). Marginal PDFs may be computed from the channel matrix data by performing a histogram operation on the amplitude and phase of the \( H \) matrix elements over all of the sets in a data collection. Specifically,

\[
f[r] \approx \frac{1}{N_T N_R \Delta r} \text{HIST} |H_{ij,n}| \tag{7.4}\]

\[
f[\phi] \approx \frac{1}{N_T N_R \Delta \phi} \text{HIST} \angle H_{ij,n}, \tag{7.5}\]

where \( f[r] \) and \( f[\phi] \) are discrete samples of the measured amplitude and phase PDFs and \( \text{HIST}(\cdot) \) represents a one-dimensional histogram of the quantity in the argument,
Figure 7.9: Measurement locations for collection 10×10(c) are specified by the circled numbers. Transmitter and receiver could assume these seven possible positions, and several combinations were probed. Distances are in specified in feet.

Table 7.3: Positions and orientations for data collection 10×10(c)

<table>
<thead>
<tr>
<th>Name</th>
<th>Transmit Loc</th>
<th>Transmit Orient</th>
<th>Receive Loc</th>
<th>Receive Orient</th>
</tr>
</thead>
<tbody>
<tr>
<td>loc1a</td>
<td>#4</td>
<td>N</td>
<td>#2</td>
<td>S</td>
</tr>
<tr>
<td>loc1b</td>
<td>#4</td>
<td>N</td>
<td>#2</td>
<td>E</td>
</tr>
<tr>
<td>loc2a</td>
<td>#3</td>
<td>W</td>
<td>#2</td>
<td>E</td>
</tr>
<tr>
<td>loc2b</td>
<td>#3</td>
<td>W</td>
<td>#2</td>
<td>S</td>
</tr>
<tr>
<td>loc3a</td>
<td>#7</td>
<td>W</td>
<td>#2</td>
<td>S</td>
</tr>
<tr>
<td>loc3b</td>
<td>#7</td>
<td>W</td>
<td>#2</td>
<td>E</td>
</tr>
<tr>
<td>loc4a</td>
<td>#7</td>
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<td>#3</td>
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</tr>
<tr>
<td>loc4b</td>
<td>#7</td>
<td>S</td>
<td>#3</td>
<td>W</td>
</tr>
<tr>
<td>loc5a</td>
<td>#6</td>
<td>E</td>
<td>#3</td>
<td>W</td>
</tr>
<tr>
<td>loc5b</td>
<td>#6</td>
<td>E</td>
<td>#3</td>
<td>S</td>
</tr>
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<td>loc6a</td>
<td>#4</td>
<td>N</td>
<td>#3</td>
<td>S</td>
</tr>
<tr>
<td>loc6b</td>
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<td>N</td>
<td>#3</td>
<td>W</td>
</tr>
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<td>S</td>
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</table>
taken over the specified indices. To obtain a PDF, the histogram is scaled by the
number of transmitters ($N_T$), the number of receivers ($N_R$), the number of channel
matrix measurements ($N$), and the histogram bin size ($\Delta r$ or $\Delta \phi$). In order to
compare the various data sets, the channel matrices must be normalized. For the
computation of the marginal PDFs, each channel matrix was normalized to give unit
SISO channel gain, as described in Appendix H. Figure 7.10 plots the marginal PDFs
for element magnitude and phase for the various data sets. All of the data sets conform
quite well to the ideal distributions for Rayleigh fading. The dual-pol measurements
deviate somewhat, due to the fact that the cross-pol channels are deterministically
weak compared to the co-pol channels.

At first glance, the good fit to the Rayleigh and uniform distributions
suggests that a simple multivariate complex normal distribution (Appendix G) may
be applied to model the channel. However, Chapter 8 will demonstrate that capacity
statistics of the data and physical path-based models do not agree well with the
multivariate complex normal models. Thus, even though the channels are marginally
complex normal, there is no guarantee that the joint distribution is multivariate
complex normal.

7.3 Spatial Correlation

Another important characteristic of the channel is the spatial correlation at
transmit and receive as a function of transmit and receive position. For the complex
normal distribution, uncorrelated channels are also statistically independent, which is
desirable to achieve high capacity. For channels which are not multivariate complex
normal, however, the interpretation is not as precise. The channels are assumed to
have separable and shift-invariant correlation functions as described in Appendix G.
Thus, the correlation coefficient at transmit and receive may be plotted as a one-
dimensional function versus element separation.

Figure 7.11 plots the magnitude of the correlation coefficient for trans-
mitt and receive at the discrete points sampled by the antennas. Also plotted is
Jakes’ model for comparison. The correlation functions compare favorably with Jakes’
Figure 7.10: Marginal PDFs on element magnitude and phase. Measured PDFs are compared with the ideal Rayleigh PDF and uniform PDF for magnitude and phase.
Figure 7.11: Spatial correlation for each data collection
model, suggesting that antennas need to be separated by a few wavelengths to achieve statistical independence. The only collection that seems to deviate significantly from Jakes’ model is $10 \times 10(b)$, and then only for the larger spacings. Figure 7.12 plots the correlation for the five locations making up the set. For location 1 and 2, the receiver moves across room 400, and the results compare better with Jakes’ model. For the sets where the transmitter moves and the receiver is stationary, we see high correlation at the receiver. The higher correlation may be due to two factors: (1) when only the transmitter is moving, the receiver sees nearly the same incoming ray structure for the various transmit positions, and (2) the limited amount of variation at the receiver may violate the separability argument.

### 7.4 Temporal Correlation

Temporal correlation of the indoor channel indicates how quickly the elements of the channel matrix change. The average temporal covariance of the channel matrix elements may be defined as

$$X^k_{ij}[\ell] = \frac{1}{N} \sum_n H^k_{ij}[n] H^{k*}_{ij}[n+\ell], \quad (7.6)$$

where $k$ is a set number, $\ell$ is the temporal sample separation, and $H^k_{ij}[n]$ is the time evolution of the $ij$th channel matrix element. When computing (7.6), the channel is left unnormalized to avoid altering the temporal statistics. The correlation coefficients of all of the elements of the channel matrix may be averaged to obtain

$$\rho_\ell = \frac{1}{N_T N_R K} \sum_{i,j,k} X^k_{ij}[\ell] X^k_{ij}[0], \quad (7.7)$$

where $K$ is the number of data sets. In all of the collections, each set was processed to give a 10-second time evolution of the channel matrix. Figure 7.13 plots the temporal correlation for each of the considered data collections over a 5-second interval. For all of the collections, the average correlation coefficient is above 0.9 over the 5-second interval, suggesting that the indoor channel with fixed transmitter and receiver is very stationary.
Figure 7.12: Spatial correlation for each location in data collection 10×10(b). Cases where only the transmitter moved exhibited a high receive correlation for larger antenna spacings.
The correlation coefficient for collection 4×4(b) is the lowest due to two factors: (1) in the dual-polarization setup, the weak cross-pol subchannels are more sensitive to slight changes in the channel, and (2) the transmitter was in a hallway with moderate activity. Figure 7.14 plots the average correlation coefficients for the co-pol and cross-pol subchannels, demonstrating the shorter stationarity of the more sensitive cross-pol subchannels.

Collection 10×10(b) has the next lowest temporal correlation, due mainly to movement of the transmitter or receiver during each data set. Figure 7.15 plots the average correlation coefficient for each of the locations making up collection 10×10(b). For locations 1, 4, and 5, movement occurred in discrete steps between the data sets, and the temporal correlation is very high. For location 2, the receiver covered a distance of about 20 feet in 160 seconds, giving an average velocity of 0.13 ft/s.
Figure 7.15: Comparison of temporal correlation for individual locations in 10×10(b). The locations where movement occurred between sets show very high correlation. Those involving movement inside of the sets were less stationary.

For location 3, the transmitter moved in discrete steps, but the steps were not synchronous with the receiver’s acquisition times. Therefore, the discrete movements usually occurred somewhere inside of a data set.

7.5 Capacity Per Channel

In this chapter, capacity for the flat-fading channel is defined using the water-filling solution, as described in Appendix I with an assumed average SISO SNR of 20 dB. For the complex normal i.i.d. channel model, capacity may grow linearly when antenna elements are added to both sides of the transmission link. For real communications systems, however, the positions of antenna elements will likely be constrained to a finite aperture. Correlations between the elements will become large as more and more elements are packed into a finite space. To see the impact of antenna correlation on capacity, subsets of the channel matrix data from collection 10×10(a) were analyzed to effectively form linear arrays with 2, 4, and 10 elements. Each array had a total length of 2.25λ. Referring to Figure 7.13, elements 1 and 10 were used for the 2×2 case, elements 1, 4, 7, and 10 were used for the 4×4 case, and all of the elements were used for the 10×10 case. For comparison, Monte Carlo simulations with 10^5 channel realizations were run for the same array sizes assuming the i.i.d. complex normal model. Figure 7.16 plots capacity per channel complimentary cumulative distribution functions (CCDFs) for each case.
Figure 7.16: Capacity per channel (number of transmit or receive antennas) for collection 10×10(a). Solid lines are computed CCDFs for measured data (M) for various array sizes, and the broken lines are the result of Monte Carlo simulations (S) for 10⁵ i.i.d. complex normal channels with the same array sizes.

For the 2×2 case, wide separation of the antennas ensures fairly uncorrelated transmit and receive signals, and the measured and modeled capacity curves are very close. As more antennas are packed into the same array length, however, correlation between the elements increases and the capacity is degraded from the ideal linear increase predicted by the i.i.d. complex normal model.

7.6 Capacity vs. Polarization

Arrays constructed with dual-polarization elements may be able to accommodate more antenna elements in the same aperture than single-polarization arrays. Also, since depolarization is small for structures built mostly with right-angle geometries, the two orthogonal polarizations will be nearly independent in a deterministic sense. Data collection 4×4(b) explores the benefits and drawbacks of dual-polarization systems by measuring the channel with arrays consisting of 2 dual-polarized elements. The channel matrices from 4×4(b) were divided into a number of important subchannels, exploiting various types of polarization. Figure 7.17 plots the capacity CCDF for various normalized subchannels. For the measured channels, single polarization (SP) has the lowest performance, followed by dual-pol without separation (DP) and dual-pol with separation (DPS). The figure also shows capacity CCDFs for two different Monte Carlo simulations of 10⁵ channel matrices. The
Figure 7.17: Capacity CCDFs versus various types of array polarizations. Subsets of collection 4×4(b) were used to form the various 2×2 array types. Each of the 2×2 channel matrices was normalized.

first represents simulations assuming full i.i.d. complex normal channels (IID). In the second case, the channels are diagonal, and the diagonal elements are i.i.d. complex normal (DIAG). Although the measured dual-polarized channels are nearly diagonal due to the low depolarization, there is some channel coupling. Therefore, we expect the capacity CCDFs for dual-polarization to fall between the IID and DIAG cases.

In this analysis, the channel matrices for each array type were normalized to obtain 20 dB average SISO SNR. With normalization, the same amount of receive power is available for both the full and diagonal cases, and the diagonal channel will yield a higher capacity. This type of normalization is generally unwarranted, however, because a diagonal channel will usually mean less average receive power.

To analyze the problem realistically, the following normalization procedure was applied. For fixed receiver noise, each complete channel matrix is scaled by the appropriate constant to fix the average SNR for the co-polarized SISO channels only. The subchannels are then created after this normalization. This method avoids unrealistic inflation of the dual-polarized subchannels. Monte Carlo simulations are performed assuming a channel with i.i.d. complex normal co-pol SISO channels, and cross-pol SISO channels with zero gain, thus simulating a channel with zero depolarization. The same normalization procedure is then applied to the simulated channels. The resulting CCDFs are plotted in Figure 7.18. In this case, the conclusions are different from those drawn from Figure 7.17. First, the ideal i.i.d. single-pol channel
Figure 7.18: Capacity CCDFs versus various types of array polarizations. In this case, the complete channel matrix was normalized with respect to the average power of the co-pol channels only.

(SP) is the clear winner, highlighting the loss in receiver power which occurs due to a diagonal channel (DP). For the measured channels, however, the dual-pol case (DP) still outperforms the single-pol case (SP) where the elements have nonzero correlation. Thus, the increase in capacity due to the orthogonal channels outweighs the loss due to reduced SNR.

This section demonstrates that for the case of low depolarization, dual-polarization is well suited for small arrays. For arrays where antennas may be far apart, correlation will be low, and the single-pol array will give higher capacity. This basic result is solidified in Chapter 8 through channel simulation.

7.7 Capacity vs. Directivity

Ideally, the monopole antennas depicted in Figure 7.3 radiate uniformly in the horizontal plane. The patch antennas in Figure 7.2 are more directive and only radiate into a half space. Comparison of the data taken with the two antenna types indicates the effect of antenna directivity on capacity. Unfortunately, data was not taken in the exact same locations for the patch array and the monopole array, and data collections 10×10(a) and 4×4(a) will have to suffice. The 10×10(a) data consists of 10-element linear arrays with λ/4 spacing. On the other hand, the 4×4(a) data consists of 4-element linear arrays with λ/2 spacing. To provide a fair comparison, 4-element monopole arrays with λ/2 spacing are formed using element indices [1 3 5 7]
Figure 7.19: Capacity versus antenna directivity. The capacity of a 4×4 patch array is compared to the capacity of a 4×4 monopole array. The capacity for the 4×4 array is also plotted with a 3 dB SNR boost to demonstrate antenna gain.

and [4 6 8 10], and averaging the capacity results. Figure 7.19 plots the capacity CCDFs for the 4-element patch array and 4-element monopole array. The capacity CCDFs for the two antenna types are nearly identical, suggesting that the patch array sees virtually the same amount of multipath as the monopole array.

When comparing the two antenna types, the normalization may again be unwarranted. For an environment where multipath components are mainly in the half space illuminated/received by the patch array, we would expect an approximate doubling of power for both transmit and receive over the monopole arrays. To see the effect, Figure 7.19 also shows the capacity increase for the patch antennas with a 3 dB boost in SNR.

Chapter 8 presents a more detailed study on effect of antenna directivity on capacity. The study shows that directive antennas are beneficial when proper orientation is possible, allowing a boost in the SNR. For very large arrays, however, directive antennas may limit system capacity by limiting the apparent multipath.

7.8 Multipath Richness vs. SNR

Studies on the capacity of the MIMO channel often focus on the gains due to multipath interference and ignore the reduction in SNR due to path loss. In a hypothetical indoor wireless MIMO system, as separation between transmit and receive
increases, capacity increases due to increased channel complexity (multipath). However, path loss also increases, leading to lower SNR and therefore reduced capacity. This interesting tradeoff deserves some attention \[54\].

To highlight the importance of path loss, collection 10×10(c) was analyzed giving the capacity results plotted in Figure 7.20. Each arrow in the figure represents a single scenario with the arrow pointing from transmit location to receive location. The top number in the box on each arrow gives the channel capacity when each individual channel matrix is normalized for 20 dB average SISO SNR. This first normalization removes the effect of path loss. The bottom number (in italics) gives the capacity when all of the channel matrices in the collection are scaled by the same constant, such that the average SISO SNR over all of the measurements is 20 dB. This later value includes the effect of path loss.

Figure 7.20: The effect of path loss on capacity. Arrows connect transmit location to receive location for a single scenario. The boxed numbers are the capacity ignoring path-loss (top) and including path loss (bottom, italics).
Several of the cases with large separation (5→3, for example) exhibit a high capacity without path loss (due to large multipath), but suffer greatly when path loss is included. Other cases where transmit and receive are in closer proximity (7→4 most notably) exhibit the opposite effect due to the high SNR observed. These results demonstrate the importance of including both path loss and multipath richness when comparing the performance of different channels.

7.9 Chapter Summary

This chapter has described representative data that was collected with the hardware platform in Chapter 6. The data was processed to obtain channel matrices for three important scenarios: a centralized server, a server in a hallway, and no server with peer-to-peer communications. The data was interpreted in terms of marginal PDFs, spatial and temporal correlation functions, and capacity. The marginal PDFs show that the individual SISO channels exhibit Rayleigh fading. The spatial correlation functions compare well with Jakes’ model, and the temporal correlation functions show a very high correlation coefficient ($\geq 0.9$) over a 5-second interval. The effect of number of channels, polarization, directivity, and path loss on capacity statistics was studied. In the next chapter, a realistic statistical path-based model coupled with electromagnetic antenna simulations provides a more in-depth treatment of these phenomena.
Chapter 8

MIMO Channel Modeling

Chapters 6 and 7 presented a measurement system for multiple-input multiple-output (MIMO) wireless channels along with representative data collected in typical indoor environments. The results demonstrated the capacity gains that are possible with advanced MIMO systems. The development of these advanced systems relies on accurate models that can adequately match measured data. This chapter explores the topic of MIMO wireless channel modeling and develops a new hybrid modeling strategy.

The grid in Figure 8.1 shows many strategies for modeling the indoor MIMO wireless channel. Generally, a system designer desires statistics of the system performance over all realistic operation scenarios. This statistical information may be in the form of theoretical quantities like capacity PDFs, or more real-world system performance metrics like average bit-error rate (BER).

Deterministic models analyze system performance for a single channel at a time. The Monte Carlo approach provides statistical information by combining the results of deterministic simulations on many channels, which have been selected according to some statistical distribution. Deterministic models may exist in closed form for very simple channels (a two-path signal model, for example). Such models are usually too restrictive to represent any real communications environment. Direct measurement of the channel matrix provides an exact empirical model for the measured scenarios, but characterization of all types of channels by measurement is difficult due to the vast amount of data required. Deterministic physical models apply an electromagnetic simulation tool (such as ray tracing [55]) to obtain nearly exact
Figure 8.1: Approaches to modeling the indoor MIMO wireless channel. The grid shows a number of important combinations of model types.

propagation characteristics of a fixed environment. However, detailed simulations can be time-consuming, and capturing sufficient detail of real buildings into a computer model may be non-trivial.

Statistical models may often be less complex than the deterministic models, and yet provide sufficiently accurate channel information. Consider a system designer who requires capacity statistics for a proposed antenna array in a certain type of building. The designer could use a ray tracing tool to capture the entire building with the exact placement of all pertinent walls, furniture, duct work, etc. Many realizations could be simulated with various orientations and locations of transmitter and receiver, combinations of opened and closed doors, people placed randomly in the channel, etc. However, macroscopic quantities (such as capacity and channel matrices) essentially sum the perturbations due to these small effects. If the perturbations are random in nature, they will tend to average out over the ensemble. Thus, a much simpler statistical description of the channel is usually possible. Statistical models provide savings by modeling the macroscopic behavior of the random channel, rather than the very complex microscopic behavior.

Similar to their deterministic counterparts, statistical models may also be closed form, empirical, or physical. Approximate closed-form expressions have
been obtained for capacity for the i.i.d. complex normal channel [11], but the i.i.d. assumption is invalid for many real scenarios. Empirical models can be formed by assuming a statistical distribution on the channel matrix elements, and computing the required statistical moments from measured data. However, convenient probability distributions (such as the multivariate complex normal) may not match real channels. Also, even if the chosen distribution is correct, the empirical statistical moments may only apply to the specific measurement scenario. Finally, statistical models based on the basic physics of wave propagation are particularly attractive. These physical models have the ability to provide accurate statistical information, without the complexity of detailed deterministic approaches.

Most modeling effort to date has either focused on the approximate closed-form models, or very complex ray-tracing studies. Also, in most cases, antennas have been treated as ideal, ignoring mutual-coupling effects. To overcome some of the drawbacks of existing methods, this research develops a new hybrid approach that combines the accuracy of full-wave electromagnetic analysis with the efficiency of a statistical description of the multipath. Full-wave analysis of the antenna arrays ensures that the correct far-field radiation behavior and array network characteristics are captured. This type of analysis allows the designer to answer questions about the effect of antenna spacing on capacity, for example, a study which is not possible when antennas are treated as ideal omnidirectional radiators. Multipath is efficiently simulated with the Saleh-Valenzuela model, allowing an overall statistical assessment of system performance and requiring far less simulation time than complicated ray-tracing studies. Thus, the hybrid method has two basic components: (1) an electromagnetic simulation (FDTD or MOM) to characterize the array network response and far-field radiation patterns, and (2) the Saleh-Valenzuela model to obtain random channel matrices, correlation functions, and capacity statistics.

This new method relies heavily on past developments of the Saleh-Valenzuela model [56], a statistical channel model based on the basic principles of wave propagation for wireless communications channels. This model relates the random impulse response of the channel to the random arrival and decay of multipath components.
The initial model only described the time impulse response of the channel. Later work extended the model to include the random spatial or angle-of-arrival (AOA) response of the channel \[57, 59\]. In this research, angle-of-departure (AOD) statistics are also included, and the model is referred to as the SVA model (Saleh-Valenzuela model with AOA/AOD).

The chapter is organized as follows. Section 8.1 explains the electromagnetic analyses required to obtain network response and far-field radiation patterns for the 4-element dual-polarized patch array and the 10-element monopole array. Section 8.2 provides a detailed description of the SVA model, simplifies the model appropriate for the narrowband case, and relates the model directly to more simple multivariate complex normal models. The results show that multivariate complex normal models have difficulty matching capacity and covariance statistics generated by the more complex SVA model. Section 8.3 demonstrates a simple method for extending existing models to account for dual-polarization. Finally, Section 8.4 provides realistic channel simulations to better understand the phenomena discovered in Chapter 7.

8.1 Antenna Characterization

This section describes the electromagnetic simulations required to compute the network characteristics and far-field radiation patterns of the 4-element dual-polarized patch array and the 10-element monopole array.

8.1.1 Patch Array

As described in Section 6.1.4, patch antennas are planar printed circuits. Although FDTD could have been used for this structure, the MOM technique \[1\] is more efficient. Thus, the Momentum package by Agilent Technologies (a MOM solver) was used to compute the necessary network characteristics and far-field radiation patterns. Figure 8.2 shows the antenna geometry under analysis.

Table 8.1 lists the S-parameters for the 4-element patch array in dB. The return loss from any individual element is about -19 dB. Isolation between the hori-
Figure 8.2: Layout of the 4-element dual-polarized patch array and the network port assignments. Elements are separated by $\lambda/2$ at the center frequency of 2.45 GHz.

Table 8.1: Magnitudes of the S-parameters for the 4-element patch array in dB

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<td>-29.9</td>
<td>-18.6</td>
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</table>

Horizontal and vertical ports for a given element is better than 25 dB. Isolation between co-polarized adjacent elements is better than about 15 dB. For simplicity, the patch array network will be considered ideal, so that the reflection looking into any port is zero and the isolation between different ports is infinite. Figure 8.3 plots the far-field radiation patterns at 2.45 GHz. For each curve, one of the ports is excited and the others are terminated. The plots demonstrate aberrations in the radiation patterns due to adjacent elements. These simulated radiation patterns are coupled with the SVA model in Section 8.4.
Figure 8.3: Far-field radiation patterns in the horizontal plane for the patch array at 2.45 GHz, relative to an omnidirectional dipole. Each curve shows the far-field response in the horizontal plane when the specified port is excited, and the others are terminated in 50 Ω.
8.1.2 Monopole Array

The non-planar geometry of the monopole array was simulated with a detailed FDTD simulation. Figure 8.4 depicts the exact dimensions of a single monopole antenna along with slightly modified dimensions appropriate for FDTD simulations with a fixed cell size. With the exception of the special treatment of the curved metal surfaces (see Appendix J), the FDTD antenna simulations used the basic techniques outlined in Chapter 2 to simulate the single monopole element and the monopole array. The following subsections describe in detail the steps which were required.

Coaxial Feed

First, the FDTD simulations required an adequate representation of the coaxial feed to each monopole antenna. The coaxial feed could be modeled a number of different ways, but this research employed a straightforward stairstep approximation. The mode in the coax could be computed from exact analytical expressions. However, to remain compatible with the FDTD simulations, the modes were solved with the linear FD mode solution (Section 2.1.4). Since the mode is TEM, the propagation constant is already known, and only a single iteration is required to compute
Table 8.2: Physical parameters and FD simulation parameters for the monopole coaxial feed

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<tr>
<td>$Z_{0\text{ideal}}$</td>
<td>Analytical impedance</td>
<td>52.61 $\Omega$</td>
</tr>
</tbody>
</table>

the mode profiles. Table 8.2 lists the physical parameters of the coaxial feed and parameters for the FD simulation. The exact analytical expression for the impedance of the coaxial line is

$$
Z_0 = \frac{\eta_0}{2\pi\sqrt{\epsilon_r}} \ln \left( \frac{r_2}{r_1} \right),
$$

(8.1)

where $\eta_0$ is the free-space wave impedance. For the FD simulation, the metal surfaces were approximated in a manner similar to that in Appendix J. Figure 8.5 plots the field components considered inside or on the surface of a conductor. These components were forced to zero in the FD mode solver. The resulting E and H cross-sectional fields are plotted in Figure 8.6. Voltage and current were computed with appropriate line and contour integrals, and the ratio gave an impedance of $Z_0^{FD} = 52.27\ \Omega$.

To test correct operation of the coaxial feed, FDTD simulations of the coax were run as depicted in Figure 8.7. An additive source with the mode shape given by the FD solution was placed at the source plane. After 5 sinusoidal periods, the fields were stored at the field storage plane. The fields at this plane were virtually identical to those in the FD mode solution. Voltage and currents were computed as in the FD simulation, and the computed impedance was $52.27 - j0.34\ \Omega$. 

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Figure 8.5: Metal surfaces of the coaxial feed were simulated by forcing field components inside of or tangential to metal surfaces to zero. This figure shows only those field components on the staggered grid which were set to zero to simulate these metal surfaces.

Figure 8.6: Coax TEM mode solution from the linear FD mode solver
Single Antenna Simulations

Next, FDTD simulations were run for the single monopole antenna in isolation. Figure 8.8 plots the dimensions of the FDTD domain and the nominal dimensions of the antenna structure. To compute the input impedance of the antenna at plane B, an additive source was placed at plane A whose temporal variation was a sinusoid at 2.42 GHz modulated by a Gaussian pulse function \( g(t) \), given by

\[
g(t) = \exp \left[ -\frac{(t - t_0)^2}{\tau^2} \right], \quad (8.2)
\]

where the lag time was \( t_0 = T \), the pulse half-width was \( \tau = 0.4T \), and \( T \) is the sinusoidal period. The source assumed the spatial variation dictated by the coaxial FD mode solution. The simulation was run for 10\( T \), by which time the fields had decayed essentially to zero. An FFT was taken of the E and H fields at plane B. Note that the E and H fields are actually one-half cell apart, and the phase of H was adjusted to account for this fact. Voltages and currents were computed with the proper line and contour integrations on E and H for each FFT component. The expression

\[
Z(\omega_k) = \frac{V(\omega_k)}{I(\omega_k)}, \quad (8.3)
\]
Figure 8.8: Domain for single antenna FDTD simulations. The coax mode is excited at plane A. Fields are stored at B to compute antenna impedance. Box C is used for the far-field integration.

where $V$ and $I$ are the FFT of voltage and current, gives the impedance as a function of the discrete frequency samples $\omega_k$ returned by the FFT. Figure 8.9 plots the resulting input impedance and reflection coefficient. The best match occurs very near the design frequency of 2.42 GHz.

The radiation pattern of the antenna was obtained with an additional simulation employing an additive sinusoidal source with the known mode shape at plane A. The source was modulated with a Gaussian ramp function to avoid initial transients. After $5T$, the fields had basically reached sinusoidal steady-state variation. The FFT of the fields on box C were used to compute the far-field radiation pattern. Note that special treatment of the ground plane is required. Appendix K shows that the far fields may be obtained by integrating the fields on box C (omitting the face at $z = 0$) in the standard way to obtain $E_1^0(\theta, \phi)$. The physical far-field $E$ field in the
Figure 8.9: Input impedance and reflection coefficient of the isolated monopole antenna

top half-space is then given by

\[ E_\theta(\theta, \phi) = E^1_\theta(\theta, \phi) + E^1_\theta(\pi - \theta, \phi) \]  \hspace{1cm} (8.4)

\[ E_\phi(\theta, \phi) = E^1_\phi(\theta, \phi) - E^1_\phi(\pi - \theta, \phi). \] \hspace{1cm} (8.5)

Figure 8.10 plots the radiation patterns for the vertical component \( E_\theta \) in the horizontal and vertical planes. The antenna exhibits the familiar dipole radiation pattern.

**Antenna Array**

Next, the complete array was simulated as depicted in Figure 8.11. In each simulation, one of the elements was excited at plane A with a sinusoidal source at 2.42 GHz and the others were terminated. Storage of the fields for all elements at plane B allowed computation of the self and mutual impedances of the entire array. Note that even though there are 10 elements, only five simulations were required due to symmetry. These simulations were run for 5\( T \) time units, and the number of PML cells was reduced from 10 to 6 due to the very large domain. Table 8.3 lists the S-parameters of the network obtained from the simulations. The table shows that the reflection coefficient has risen significantly from the \(-20 \) dB level of the isolated antenna case. However, even more apparent is the coupling of power from one port to
Figure 8.10: Radiation patterns of the monopole antenna for the vertical component in the horizontal and vertical planes. The excitation frequency is 2.42 GHz, and the patterns are plotted in dB.

Table 8.3: S-parameters of the 10-element monopole array for $Z_0 = 52.27 \ \Omega$. The S-parameters not shown are obtained by symmetry of the array.

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>-15\degree 83°</td>
<td>-8\degree -81°</td>
<td>-15\degree 175°</td>
<td>-19\degree 75°</td>
<td>-22\degree -24°</td>
</tr>
<tr>
<td>2</td>
<td>-9\degree -81°</td>
<td>-11\degree 77°</td>
<td>-8\degree -76°</td>
<td>-14\degree -178°</td>
<td>-18\degree 82°</td>
</tr>
<tr>
<td>3</td>
<td>-15\degree 175°</td>
<td>-8\degree -76°</td>
<td>-11\degree 80°</td>
<td>-8\degree -77°</td>
<td>-14\degree 180°</td>
</tr>
<tr>
<td>4</td>
<td>-19\degree 75°</td>
<td>-14\degree -178°</td>
<td>-8\degree -77°</td>
<td>-11\degree 78°</td>
<td>-8\degree -77°</td>
</tr>
<tr>
<td>5</td>
<td>-22\degree -24°</td>
<td>-18\degree 82°</td>
<td>-14\degree 180°</td>
<td>-8\degree -77°</td>
<td>-11\degree 79°</td>
</tr>
<tr>
<td>6</td>
<td>-24\degree -118°</td>
<td>-21\degree -16°</td>
<td>-18\degree 80°</td>
<td>-14\degree 180°</td>
<td>-8\degree -77°</td>
</tr>
<tr>
<td>7</td>
<td>-27\degree 146°</td>
<td>-23\degree -111°</td>
<td>-21\degree -19°</td>
<td>-18\degree 80°</td>
<td>-14\degree 180°</td>
</tr>
<tr>
<td>8</td>
<td>-29\degree 64°</td>
<td>-26\degree 154°</td>
<td>-23\degree -114°</td>
<td>-21\degree -19°</td>
<td>-18\degree 80°</td>
</tr>
<tr>
<td>9</td>
<td>-31\degree -19°</td>
<td>-28\degree 75°</td>
<td>-26\degree 154°</td>
<td>-23\degree -111°</td>
<td>-21\degree -16°</td>
</tr>
<tr>
<td>10</td>
<td>-32\degree -109°</td>
<td>-31\degree -19°</td>
<td>-29\degree 64°</td>
<td>-27\degree 146°</td>
<td>-24\degree -118°</td>
</tr>
</tbody>
</table>
Figure 8.11: Domain for FDTD simulations of the complete 10-element monopole array. For each simulation one antenna is excited at plane A and the others are terminated. Fields are stored on plane B to compute network characteristics. Fields on box C (excluding the face at \( z = 0 \)) are used to compute the far-field radiation pattern for each element.
Table 8.4: Power balance for the 10-element monopole array. This table lists the total power supplied to the excited port for each of the five simulations. Power is either reflected, coupled into adjacent ports, or radiated. The balance should ideally be zero.

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{\text{tot}}$</td>
<td>9.57 mW</td>
<td>9.57 mW</td>
<td>9.57 mW</td>
<td>9.57 mW</td>
<td>9.57 mW</td>
</tr>
<tr>
<td>$P_{\text{refl}}$</td>
<td>0.30 mW</td>
<td>0.82 mW</td>
<td>0.70 mW</td>
<td>0.72 mW</td>
<td>0.71 mW</td>
</tr>
<tr>
<td>$P_{\text{coup}}$</td>
<td>1.95 mW</td>
<td>3.73 mW</td>
<td>4.17 mW</td>
<td>4.30 mW</td>
<td>4.36 mW</td>
</tr>
<tr>
<td>$P_{\text{rad}}$</td>
<td>7.20 mW</td>
<td>4.78 mW</td>
<td>4.45 mW</td>
<td>4.31 mW</td>
<td>4.25 mW</td>
</tr>
<tr>
<td>Balance</td>
<td>0.11 mW</td>
<td>0.23 mW</td>
<td>0.25 mW</td>
<td>0.23 mW</td>
<td>0.24 mW</td>
</tr>
</tbody>
</table>

another. Table 8.4 accounts for the power sent to the excited port in each simulation. For elements near the center of the array, nearly half of the power is coupled into other elements rather than being radiated. Therefore, use of this array without a very sophisticated matching network will result in lost transmit power. Also, by reciprocity, the receiver will experience reduced sensitivity.

The radiation patterns for the array were obtained by integrating over box C in Figure 8.11 (excluding the $z = 0$ face) and using the method in Appendix K to compute far fields. Figure 8.12 plots the radiation patterns for the vertical E-field component in the horizontal plane. The radiated fields are drawn relative to an ideal monopole that radiates power uniformly in the horizontal plane. Clear from the plot is the deviation in level and shape of the radiation patterns from that of the ideal dipole due to the mutual coupling. These far-field patterns will be coupled with the SVA model in Section 8.4 to explore the effect of this mutual coupling on capacity.

8.2 SVA Model

This section presents the Saleh-Valenzuela model with AOA/AOD (referred to as the SVA model for brevity). A simplified model for the narrowband channel is also presented, which is easily related to the multivariate complex normal distribution. A study on simulated 4×4 and 8×8 channels demonstrates that joint
complex normal models have difficulty matching the statistics of the physical path-based models. Results in the next section demonstrate the ability of the SVA model to match capacity and pairwise joint PDF statistics of measured data for realistic model parameters.

### 8.2.1 Full Model

The SVA model characterizes the channel by representing each multipath component in terms of its amplitude, arrival time, and AOA/AOD. Based upon experimental observations, these arrivals or rays arrive in clusters in both space and time. Figure 8.13 shows the model parameters for a single cluster in the SVA model. For this discussion, the departure and arrival of multipath components are limited to the horizontal plane. However, the model could be easily extended to the three-dimensional case by adding elevation angle. The directional and temporal channel impulse response arising from $L$ clusters and $K$ rays per cluster is

$$h(\theta^R, \theta^T, t) = \sum_{\ell=0}^{L-1} \sum_{k=0}^{K-1} \beta_{\ell k} \delta(t - \tau_\ell - \tau_{k\ell}) \delta(\theta^T - \Theta^T_\ell - \omega^T_{k\ell}) \delta(\theta^R - \Theta^R_\ell - \omega^R_{k\ell}), \quad (8.6)$$

with the parameter definitions listed in Table 8.5. In the general model, the param-
Figure 8.13: Transmit and receive cluster parameters for a single cluster in the SVA model.

Parameters $\omega_{kI}^T$, $\omega_{kI}^R$, $\tau_{kI}$, $\tau_{I}$, and $\beta_{kI}$ are random variables. Also, the number of rays $K$ is typically set to only include rays with amplitudes above some threshold.

Measurement of the indoor channel with an omnidirectional transmit antenna and a directional receive antenna has demonstrated a close fit of AOA statistics to a two-sided Laplacian distribution [59]. Also, the mean cluster arrival angles were essentially independent and uniform on $[0, 2\pi]$. For a system where the transmit configuration is identical to the receive configuration, the distributions on AOA and AOD should be the same. From previous indoor measurements and the symmetry of transmit and receive, the AOA/AOD distributions for transmit and receive are given by the double-sided Laplacian PDF, or

$$f^P(\omega) = \frac{1}{\sqrt{2}\sigma_P} \exp \left( - \left| \sqrt{2} \omega / \sigma_P \right| \right), \quad (8.7)$$

where $P \in \{T, R\}$ for transmit or receive, $\omega$ is an angle relative to the mean cluster arrival or departure angle, and $\sigma_P$ is the standard deviation of angle in radians. Also, cluster mean AOA/AOD are assumed to be independent and uniform on $[0, 2\pi]$. 

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Table 8.5: Parameters for the SVA model channel response defined by (8.6)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\ell$</td>
<td>Cluster number</td>
</tr>
<tr>
<td>$k$</td>
<td>Arrival number within a cluster</td>
</tr>
<tr>
<td>$\theta^T$</td>
<td>Transmit angle of departure</td>
</tr>
<tr>
<td>$\theta^R$</td>
<td>Receive angle of arrival</td>
</tr>
<tr>
<td>$\Theta^T_\ell$</td>
<td>Mean angle of departure of rays in the $\ell$th cluster</td>
</tr>
<tr>
<td>$\Theta^R_\ell$</td>
<td>Mean angle of arrival of rays in the $\ell$th cluster</td>
</tr>
<tr>
<td>$\omega^T_{k\ell}$</td>
<td>Angle of departure of the $k$th transmit ray in the $\ell$th cluster, relative to $\Theta^T_\ell$</td>
</tr>
<tr>
<td>$\omega^R_{k\ell}$</td>
<td>Angle of arrival of the $k$th receive ray in the $\ell$th cluster, relative to $\Theta^R_\ell$</td>
</tr>
<tr>
<td>$\tau_\ell$</td>
<td>Arrival time of the $\ell$th cluster</td>
</tr>
<tr>
<td>$\tau_{k\ell}$</td>
<td>Arrival time of the $k$th ray in the $\ell$th cluster, relative to $\tau_\ell$</td>
</tr>
<tr>
<td>$\beta_{k\ell}$</td>
<td>Complex gain of the $k$th ray in the $\ell$th cluster</td>
</tr>
</tbody>
</table>

The cluster arrival times are distributed according to the conditional exponential waiting-time distribution

$$f(\tau_\ell | \tau_{\ell-1}) = \Lambda e^{-\Lambda(\tau_\ell - \tau_{\ell-1})}, \quad \tau_{\ell-1} < \tau_\ell < \infty,$$

where $\Lambda$ is a cluster arrival rate, and $\tau_0$ is an arbitrary arrival time of the first cluster. Likewise, the arrival times of rays (relative to the cluster arrival times) are distributed as

$$f(\tau_{k\ell} | \tau_{k-1,\ell}) = \lambda e^{-\lambda(\tau_{k\ell} - \tau_{k-1,\ell})}, \quad \tau_{k-1,\ell} < \tau_{k\ell} < \infty, \tau_{0\ell} = 0,$$

where $\lambda$ is the ray arrival rate. The ray amplitudes ($|\beta_{k\ell}|$) are assumed to be Rayleigh distributed, and the mean power of each ray is related to its arrival time. The mean ray power decays according to the product of two exponentials, where the first describes the mean power decay with respect to the cluster arrival time, and the second describes the decay with respect to the ray arrival time within the cluster. Specifically,

$$E\{|\beta_{k\ell}|^2\} = E\{|\beta_{00}|^2\} \exp\left(-\frac{\tau_\ell}{\Gamma}\right) \exp\left(-\frac{\tau_{k\ell}}{\gamma}\right),$$

where $\Gamma$ and $\gamma$ are parameters.
where $\Gamma$ and $\gamma$ are the cluster and ray decay time constant, and $E\{|\beta_{00}|^2\}$ is defined by the path loss for a given scenario. The phase of the rays within each cluster are assumed to be independent and uniformly distributed on $[0, 2\pi]$. Figure 8.14 shows one realization of the SVA model.

For any given realization of the SVA model, the $mn$th element of the time-dependent channel response matrix may be written as

$$h_{mn}(t) = \int_{2\pi}^{2\pi} d\theta R d\theta T W_m^R(\theta_R) h(\theta_R, \theta_T, t) W_n^T(\theta_T).$$

(8.11)

The steering vectors are defined as

$$W_m^R(\theta) = g_m^R(\theta) \exp\left[j\psi_m^R(\theta)\right]$$
$$W_n^T(\theta) = g_n^T(\theta) \exp\left[j\psi_n^T(\theta)\right],$$

(8.12)

where $g_m^R(\theta)$ and $g_n^T(\theta)$ are gain patterns associated with the $m$th receive antenna and the $n$th transmit antenna. The phase function $\psi$ is given by

$$\psi_m^R(\theta) = k_0 \left(x_m^R \cos \theta + y_m^R \sin \theta\right)$$
$$\psi_n^T(\theta) = k_0 \left(x_n^T \cos \theta + y_n^T \sin \theta\right),$$

(8.13)

where $k_0$ is the free-space wavenumber, and $(x_m^R, y_m^R)$ and $(x_n^T, y_n^T)$ are the coordinates of the $m$th receive antenna and $n$th transmit antenna, respectively.

### 8.2.2 Narrowband Simplifications

For the narrowband case, the multipath delay spread is small compared to the symbol time. The multipath components can therefore be summed, yielding a directional response of the form

$$h(\theta_R, \theta_T) = \int_0^\infty dt \ h(\theta_R, \theta_T, t),$$

(8.14)

and the corresponding channel matrix

$$h_{mn} = \sum_{\ell=0}^{L-1} \sum_{k=0}^{K-1} \beta_{k\ell} W_m^R(\Theta_\ell^R + \omega_{k\ell}) W_n^T(\Theta_\ell^T + \omega_{k\ell}).$$

(8.15)
Figure 8.14: Example realization of the SVA model. The model parameters were $\Gamma = 1$, $\Lambda = 0.5$, $\gamma = 0.3$, $\lambda = 20$, $\sigma = 26^\circ$, and $E \{|\beta_{00}|^2\} = 1$. 

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Although time does not appear explicitly in (8.15), the ray and cluster arrival times are still significant since they control the mean power of the various multipath components. For the narrowband case, the absolute time scale is not significant and may be normalized to a unit cluster arrival rate ($\Lambda = 1$).

Since we expect the rays in different clusters to vary more than rays in the same cluster, the model can be simplified by assuming a constant average ray power within each cluster, or

$$E\{|\beta_{k\ell}|^2\} = E\{|eta_{\ell}|^2\} = \exp\left(-\frac{\tau_{\ell}}{\Gamma}\right), \quad (8.16)$$

thus eliminating the parameters $\lambda$ and $\gamma$. In this case, we require a normalization factor of $K^{-1/2}$ to allow the number of rays to become large without increasing the overall received power. The simplified channel matrix is given by

$$h_{mn} = \frac{1}{\sqrt{K}} \sum_{\ell=0}^{L-1} \sum_{k=0}^{K-1} \beta_{k\ell} W_m^R(\Theta_{\ell}^R + \omega_{k\ell}^R) W_n^T(\Theta_{\ell}^T + \omega_{k\ell}^T). \quad (8.17)$$

The resulting simplified SVA model only has two independent parameters: $\Gamma$ and $\sigma$.

### 8.2.3 Complex Normal Approximation

$\mathbf{H}$ may be generated directly by computing (8.17) for each realization of the SVA model. An alternate method computes channel matrices according to a complex normal distribution for each fixed set of cluster statistics. This latter method reduces computational time and links the model to simpler complex normal models.

For a fixed set of cluster statistics ($\Theta_{\ell}^T, \Theta_{\ell}^R, E\{|\beta_{\ell}|^2\}$) and ray arrival angles ($\omega_{k\ell}^T, \omega_{k\ell}^R$), $h_{mn}$ is a weighted sum of zero-mean complex normal random variables, resulting in a correlated complex normal distribution. If the angular spread on $\omega$ is small, the $h_{mn}$ will look closely complex normal even if the $\omega_{k\ell}^T$ and $\omega_{k\ell}^R$ are allowed
to vary. In this case, we find the average covariance matrix $E\{\mathbf{R}\}$ as

$$E \{ R_{m_1n_1,m_2n_2} \} = E \left\{ h_{m_1,n_1} h_{m_2,n_2}^* \right\}$$

$$= E \left\{ \left( \frac{1}{\sqrt{K}} \sum_{\ell_1=0}^{K-1} \sum_{k_1=0}^{L-1} \beta_{k_1 \ell_1} W_{m_1}^R (\Theta_{\ell_1} + \omega_{k_1 \ell_1}^R) W_{m_1}^T (\Theta_{\ell_1}^T + \omega_{k_1 \ell_1}^T) \right) \right\}$$

$$\times E \left\{ \left( \frac{1}{\sqrt{K}} \sum_{\ell_2=0}^{K-1} \sum_{k_2=0}^{L-1} \beta_{k_2 \ell_2}^* W_{m_2}^R (\Theta_{\ell_2}^R + \omega_{k_2 \ell_2}^R) W_{m_2}^T (\Theta_{\ell_2}^{T*} + \omega_{k_2 \ell_2}^{T*}) \right) \right\}$$

$$= \frac{1}{K} \sum_{\ell_1} \sum_{\ell_2} \sum_{k_1} \sum_{k_2} E \left\{ \beta_{k_1 \ell_1} \beta_{k_2 \ell_2}^* \right\}$$

$$\times E \left\{ W_{m_1}^R (\Theta_{\ell_1} + \omega_{k_1 \ell_1}) W_{m_2}^{R*} (\Theta_{\ell_2}^{R*} + \omega_{k_2 \ell_2}^{R*}) \right\}$$

$$\times E \left\{ W_{n_1}^T (\Theta_{\ell_1}^T + \omega_{k_1 \ell_1}^T) W_{n_2}^{T*} (\Theta_{\ell_2}^{T*} + \omega_{k_2 \ell_2}^{T*}) \right\}.$$

where independence of complex ray gain, AOA, and AOD has been assumed. The complex gains of rays in different clusters are independent. Also, the complex gains of distinct rays in the same cluster are independent, such that

$$E \left\{ \beta_{k_1 \ell_1} \beta_{k_2 \ell_2}^* \right\} = \delta_{k_1 k_2} \delta_{\ell_1 \ell_2} E \left\{ |\beta_{\ell_1}|^2 \right\}; \quad (8.19)$$

and the expression for average covariance becomes

$$E \left\{ R_{m_1n_1,m_2n_2} \right\} = \frac{1}{K} \sum_{\ell} E \left\{ |\beta_{\ell}|^2 \right\} \sum_k E \left\{ W_{m_1}^R (\Theta_{\ell} + \omega_{k \ell}) W_{m_2}^{R*} (\Theta_{\ell}^{R*} + \omega_{k \ell}^R) \right\}$$

$$\times E \left\{ W_{n_1}^T (\Theta_{\ell}^T + \omega_{k \ell}^T) W_{n_2}^{T*} (\Theta_{\ell}^{T*} + \omega_{k \ell}^{T*}) \right\}. \quad (8.20)$$

Now, since the ray statistics ($\omega_{k \ell}^T$ and $\omega_{k \ell}^R$) are identically distributed (not a function of the indices $k$ or $\ell$), we may write

$$E \left\{ W_{m_1}^R (\Theta_{\ell}^R + \omega_{k \ell}^R) W_{m_2}^{R*} (\Theta_{\ell}^{R*} + \omega_{k \ell}^R) \right\} = E \left\{ W_{m_1}^R (\Theta_{\ell}^R + \omega) W_{m_2}^{R*} (\Theta_{\ell}^{R*} + \omega) \right\}$$

$$= L_{m_1m_2}^R (\Theta_{\ell}^R) \quad (8.21)$$

and

$$E \left\{ W_{n_1}^T (\Theta_{\ell}^T + \omega_{k \ell}^T) W_{n_2}^{T*} (\Theta_{\ell}^{T*} + \omega_{k \ell}^{T*}) \right\} = E \left\{ W_{n_1}^T (\Theta_{\ell}^T + \omega) W_{n_2}^{T*} (\Theta_{\ell}^{T*} + \omega) \right\}$$

$$= L_{m_1m_2}^T (\Theta_{\ell}^T). \quad (8.22)$$
The $L$ functions may be expressed explicitly as
\[
L_{q_1q_2}^P(\theta^P_\ell) = \int_{-\infty}^{\infty} d\omega \, f^P(\omega)g^P_{q_1}(\Theta^P_\ell + \omega)\theta^P_{q_2}(\Theta^P_\ell + \omega)e^{j[\psi^P_{q_1}(\Theta^P_\ell + \omega) - \psi^P_{q_2}(\Theta^P_\ell + \omega)]}. \tag{8.23}
\]

The resulting average covariance matrix is
\[
E\{R_{m_1n_1,m_2n_2}\} = \frac{1}{K} \sum_{\ell} E\{|\beta^R_{\ell}|^2\} \sum_k L^R_{m_1m_2}(\theta^R_{\ell})L^{T^*}_{n_1n_2}(\theta^T_{\ell})
= \sum_{\ell} E\{|\beta^R_{\ell}|^2\} L^R_{m_1m_2}(\theta^R_{\ell})L^{T^*}_{n_1n_2}(\theta^T_{\ell}). \tag{8.24}
\]

From trigonometry, the difference of the phase functions ($\psi[\cdot]$) may be represented in terms of the radial distance and azimuthal angle between the elements, or
\[
\psi^P_{q_1q_2}(\theta) = k_0 r^P_{q_1q_2} \cos(\theta - \phi^P_{q_1q_2}), \tag{8.25}
\]
where
\[
r^P_{q_1q_2} = \left[ (x^P_{q_1} - x^P_{q_2})^2 + (y^P_{q_1} - y^P_{q_2})^2 \right]^{\frac{1}{2}} \tag{8.26}
\]
and
\[
\phi^P_{q_1q_2} = \tan^{-1} \left[ \frac{y^P_{q_1} - y^P_{q_2}}{x^P_{q_1} - x^P_{q_2}} \right]. \tag{8.27}
\]

For certain special cases, closed-form expressions for (8.23) exist. For arbitrary antenna gain and angular ray distributions, however, (8.23) is computed numerically.

The channel matrices may be computed as follows:

1. Generate a fixed set of cluster statistics: $\Theta^T_\ell$, $\Theta^R_\ell$, and $E\{|\beta^R_{\ell}|^2\}$.
2. Compute the covariance matrix from (8.24).
3. Generate one or more multivariate complex normal channel matrices for this set of cluster statistics using methods outlined in Appendix G.

Another benefit of this derivation is the obvious relationship of the simplified SVA model with the multivariate complex normal distribution. This idea will be explored in Section 8.2.6.
8.2.4 Shift-Invariance and Separability

Appendix G discusses the multivariate complex normal distribution and two simplifying channel assumptions: separability and shift-invariance. Equation 8.24 shows explicitly that for a fixed set of cluster statistics, the SVA model is not strictly separable, but rather consists of a weighted sum of separable functions. However, if an average covariance is computed over all cluster realizations, and the path gains, receive cluster angles, and transmit cluster angles are independent of each other, the average covariance will be separable.

Shift-invariance is satisfied by the SVA model as long as the radial distance \( r_{q_1,q_2} \) and angular distance \( \phi_{q_1,q_2} \) are equal for logically adjacent elements \( q_1 - q_2 = 1 \) and the gain patterns of all elements are identical. Obvious structures that satisfy these requirements are linear and circular dipole arrays with low mutual coupling.

8.2.5 Comparison of Measured Data and SVA Model Predictions

This subsection shows the ability of the SVA model to match measured capacity PDFs for realistic model parameters. In [61], high resolution AOA measurements were performed on the same floor of the BYU engineering building as in this study. Although the measurements were at a much higher frequency \( \approx 7\text{GHz} \), the extracted parameters serve as a logical starting point for modeling. The key parameters are \( \sigma_{\{T,R\}} = 26^\circ \), \( \Gamma = 2 \), \( \Lambda = 1 \). For simulation, transmit and receive cluster arrival angles are assumed to be uniform on \([0, 2\pi]\).

For comparison, capacity PDFs are also presented for the multivariate complex normal model with covariance specified by the complex correlation method. In this case, the sample complex covariance is computed over the complete data set and \( 10^5 \) synthetic channel matrices are computed using the methods in Appendix G. Due to the problem of artificial decorrelation (see Section 8.2.6), the complex normal model with complex correlation tends to overpredict capacity.
First, capacity PDFs and pairwise PDFs from the model are compared with measured 4×4 data from collection 4×4(a). Here, the gain patterns for the antennas were the isolated element vertically polarized patch antenna patterns obtained through MOM simulation. This gain pattern is required to compute (8.23).

Figure 8.15 compares PDFs of measured data and Monte Carlo simulations of the SVA model. Pairwise amplitude and phase PDFs are discussed in Appendix G. Here the pairwise amplitude and phase PDFs for all adjacent elements are averaged to obtain a single plot. The use of pairwise PDFs for comparison is also discussed in Section 8.2.7. In this section, each comparison is based on $10^5$ channel realizations (100 cluster configurations with 1000 channels each). Apparent in the figure is the good fit of both the capacity PDFs and pairwise amplitude PDFs. The discrepancy in phase is probably due to the fact that the uniform cluster AOA/AOD assumption is not strictly valid over the limited data set.

Next, capacity PDFs and pairwise PDFs from the model are compared with measured 10×10 data from collection 10×10(a). This data set employed monopole antennas separated by $\lambda/4$, and an ideal uniform radiation pattern in azimuth was assumed. Figure 8.16 compares the PDFs for the measured and simulated 10×10 channels. While the parameters from [61] did not yield the desired fit for capacity, the figure shows that adjustment in either the cluster decay rate or angular ray spread improves the agreement. Detailed AOA/AOD measurements at the 2.4 GHz carrier are required to further study the discrepancy. Agreement in the amplitude and phase PDFs is comparable to the 4×4 data and does not change significantly with the parameter adjustments.

8.2.6 Comparison of the SVA and Multivariate Complex Normal Models

Since the channel matrix is distributed according to a complex normal distribution for a fixed set of cluster statistics, one might be tempted to assume that
Figure 8.15: Comparison of capacity, average adjacent pairwise magnitude, and average adjacent pairwise phase difference PDFs of data collection 4×4(a) and SVA model predictions
Figure 8.16: Comparison of capacity, average adjacent pairwise magnitude, and average adjacent pairwise phase difference PDFs of data collection $10 \times 10(a)$ and SVA model predictions
the channel matrix may be closely modeled with the complex normal distribution for
random cluster statistics as well. The basic flaw in this reasoning may be seen by
comparing the joint PDFs for the SVA model and the multivariate complex normal
model. The joint PDF on the channel matrix elements for the SVA model can be found
using the Monte Carlo method. The \( n \)th set of cluster statistics \((\Omega_n)\) is generated
according to some distribution, producing the closed-form conditional multivariate
complex normal distribution \( f(\overline{H}|\Omega_n) \). The unconditional distribution is

\[
f(\overline{H}) = \int d\Omega \ f(\overline{H}|\Omega) f(\Omega) \\
\approx \frac{1}{N} \sum_n f(\overline{H}|\Omega_n). \tag{8.28}
\]

On the other hand, if we believe the random channel matrix is multivariate complex
normal, the joint PDF is characterized by the average covariance matrix. Again, we
may compute the average covariance in Monte Carlo fashion as

\[
\overline{R} = \int d\Omega \ \overline{R}(\Omega) f(\Omega) \\
\approx \frac{1}{N} \sum_n \overline{R}(\Omega_n). \tag{8.29}
\]

Obviously, the distributions described by (8.28) and (8.29) can be quite different.
For example, in the case of the SVA model, the channel matrix elements may be
highly correlated for each set of \( \Omega_n \). However, as long as the phases of these complex
correlations are random, the covariance given by (8.29) will become small for the
off-diagonal elements over the ensemble. This problem of artificial decorrelation may
possibly be avoided using a power correlation model \[62\], since power correlation is
insensitive to random phase variation. The flip side of such an approach is that any
correlation in element phases is lost, which may impact statistics such as capacity.

Another interesting observation regards the marginal statistics of the channel
matrix elements. Measured data in Chapter 7 demonstrated marginal element
statistics which fit the complex normal distribution very well. The marginal PDFs of
the channel matrix elements may be obtained from the conditional method as before.
In this case the PDF for the $mn$th element of the channel matrix is found as

$$f(h_{mn}) = \int d\Omega \ f(h_{mn}|\Omega) f(\Omega),$$

(8.30)

where $f(h_{mn}|\Omega)$ is the PDF for a zero-mean complex normal random variable with variance $\sigma^2(\Omega)$. As long as this variance is fairly constant, the average PDF given by (8.30) will be very close to a complex normal distribution. Since the normalization which is usually applied ensures a fairly constant variance on the channel matrix elements, it is not surprising that the marginal element statistics look complex normal.

The remainder of this section solidifies the differences between the SVA model and the complex normal model through simulation. The complex correlation method and root power correlation method for specifying the channel covariance matrix (see Appendix G) are investigated.

### 8.2.7 Simulation Results

This section explores the differences between the following models through numerical simulation:

1. The simplified SVA model outlined in this section

2. The multivariate complex normal model with the covariance specified by the average complex covariance (the complex correlation method)

3. The multivariate complex normal model with the covariance specified by the root of the average power covariance (the power correlation method)

Table 8.6 lists the simulation parameters for the SVA model simulations. Simulation parameters were identical for transmit and receive. Mean cluster arrival and departure angles were assumed to be independent and uniformly distributed on $[0, 2\pi]$. 1000 sets of cluster statistics were computed, and the average covariance matrix was computed for each case according to equation (8.24). The average covariance matrix for each cluster realization was then used to compute 1000 channel matrices with the multivariate complex normal distribution, yielding a total of $10^6$ channel matrices.
Table 8.6: Parameters for the simulations to compare SVA and complex normal models

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Λ</td>
<td>Cluster arrival rate</td>
<td>1</td>
</tr>
<tr>
<td>Γ</td>
<td>Cluster decay constant</td>
<td>2</td>
</tr>
<tr>
<td>σ</td>
<td>Ray AOA/AOD standard deviation</td>
<td>26°</td>
</tr>
<tr>
<td></td>
<td>Array Type</td>
<td>Uniform Linear</td>
</tr>
<tr>
<td>Nₜ, Nᵣ</td>
<td>Number of transmit/receive antennas</td>
<td>4, 8</td>
</tr>
<tr>
<td>d</td>
<td>Inter-element antenna spacing</td>
<td>λ/2, λ/4</td>
</tr>
<tr>
<td>N</td>
<td>Number of cluster realizations</td>
<td>1000</td>
</tr>
<tr>
<td>M</td>
<td>Channel realizations per cluster realization</td>
<td>1000</td>
</tr>
</tbody>
</table>

The appropriate complex covariance ($\overline{R}^{c}$) and power covariance ($\overline{R}^{p}$) were computed as

$$\overline{R}^{c} = \frac{1}{N} \sum_{n=1}^{N} \text{E}\{\overline{R}_n\}$$

$$\overline{R}^{p} = \frac{1}{N} \sum_{n=1}^{N} \left| \text{E}\{\overline{R}_n\} \right|^2,$$

where $n$ is the $n$th realization of cluster parameters, and $|·|^2$ is an element-wise squaring operation. $10^5$ channel matrices were also computed using the multivariate complex normal model with both the complex correlation method (using $\overline{R}^{c}$) and the power correlation method (using $\overline{R}^{p}$). The SVA model and multivariate complex normal models were compared in two ways: (1) capacity PDFs, and (2) pairwise magnitude and phase PDFs.

Capacity is computed for each channel matrix with the water-filling solution assuming an average SISO SNR of 20 dB. The PDFs are then computed by properly normalizing a histogram taken over the computed capacities.

For a random vector consisting of complex normal elements, the joint amplitude and phase difference PDFs may be computed in closed form for any pair of elements (see Appendix G). Thus, for the complex normal channel models, the joint amplitude and phase difference PDFs of any pair of H matrix elements can be computed directly given the covariance matrix. For the SVA model, these PDFs may be
computed with the Monte Carlo method by averaging the PDFs obtained for each realization of cluster parameters. Care should be exercised when interpreting these results, however, since matching of pairwise marginal statistics will not guarantee matching of the complete joint PDFs.

To avoid the complexity associated with comparing all possible pairs of H matrix elements, only two basic cases are considered: (1) elements corresponding to adjacent receive antennas for a single transmit antenna, and (2) elements corresponding to adjacent transmit antennas for a single receive antenna. Adjacent antennas are often more interesting than more separated antennas, because the statistical dependence will tend to be higher. Since the transmit and receive statistics are identical, the transmit and receive PDFs are averaged to obtain a single plot. Also, since the mean cluster arrival angles are independent and uniformly distributed, all of the adjacent element pairwise PDFs should be identical and are therefore averaged as well.

The following subsections show that the complex normal models have difficulty matching the statistics of the SVA model, suggesting that the channels generated by the SVA model are not strictly multivariate complex normal. The non-normality of the data may be proven by showing that both the complex covariance and power covariance are random variables for varying cluster statistics. If the variances of these matrices are small, the SVA model channels are approximately complex normal, and the complex normal models should work well. However, if the variance is high, the SVA model channels will not be complex normal. To demonstrate this principle, the mean and variance of the amplitude and phase of the covariance matrix elements are plotted for the cases that follow.

4×4 Channel with λ/2 Spacing

This first case looks at the performance of the models for fairly uncorrelated antenna elements with a moderate number of elements. Figure 8.17 plots the capacity, pairwise magnitude, and pairwise phase difference PDFs for the simulated 4×4 channel matrices. Note that for all phase plots of the power correlation model, the peak response has been shifted to match the peak of the SVA phase curve. This shift
is easily accommodated by the model, since the phases of the root power covariance elements are arbitrary (see Appendix G).

For the capacity PDFs, the power correlation model results match the SVA results very well, while the complex correlation model generates capacities that are too high. The pairwise PDFs on magnitude are nearly all the same, with the power correlation model providing a better fit. The statistical dependence predicted by both models is lower than that suggested by the SVA model, which translates logically into overprediction of capacity. Statistical dependence of the element magnitudes manifests itself as conformation of contours to the diagonal line $x_1 = x_2$. In terms of the phase PDFs, the complex correlation model fits better than the power correlation model. This fact is not surprising since the power correlation model ignores phase.

Figure 8.18 partially explains the performance of the simple models for this case. The variance of the element magnitude is small ($\sigma^2 < 0.04$, $\sigma < 0.2$) and the variance of the element phases is moderate ($\approx 1$ rad) to large ($\approx 2$ rad). The low variance of the amplitude covariance shows that the power correlation method will be very successful at matching the power PDFs of the elements. The large variation in non-adjacent element phase accounts for the overprediction of capacity by the complex correlation model.

8×8 Channel with $\lambda/2$ Spacing

This next case looks at the effect of a large number of channel matrix elements on the performance of the models. Figure 8.19 plots the capacity, pairwise magnitude, and pairwise phase difference PDFs for the simulated 8×8 channel matrices.

The power correlation model still predicts the capacity of the SVA model better than the complex correlation model. However, in the low capacity tail at the left, neither model is adequate. Increasing the number of elements apparently amplifies the small error present in the complex normal models. In terms of the pairwise PDFs, the performance of the complex models is very similar to that of the 4×4 case. Figure 8.20 plots the mean and variance of the channel matrix elements.
Figure 8.17: PDFs for joint adjacent element magnitude and adjacent element phase difference for 4×4 channels with λ/2 spacing

Figure 8.18: Mean and variance of the magnitude and phase of the covariance matrix elements for the 4×4 SVA channels with λ/2 spacing
Figure 8.19: PDFs for joint adjacent element magnitude and adjacent element phase difference for $8 \times 8$ channels with $\lambda/2$ inter-element spacing.

Figure 8.20: Mean and variance of the magnitude and phase of the covariance matrix elements for the $8 \times 8$ SVA channels with $\lambda/2$ spacing
The results are much like those of the 4×4 case, which is not surprising since the antenna spacings are the same.

**8×8 Channel with λ/4 Spacing**

This final case explores the effect of close antenna spacings. Figure 8.21 plots the capacity, pairwise magnitude, and pairwise phase difference PDFs for the simulated 8×8 channel matrices.

In this case, both complex normal models overpredict capacity. The complex correlation model performs similar to the 8×8 case with λ/2 spacing. However, the power correlation model has suffered a large degradation.

The more diagonal shape of the magnitude PDF contours corresponds to the higher element dependence arising from smaller antenna separation. Again, the power correlation method matches the shape better than the complex correlation model. However, even the power correlation method begins to deviate in the high probability density region. The pairwise phase PDFs show that the power correlation method prefers a much more constant phase difference than the other two models. The complex correlation method performs similar to the λ/2 case in terms of the phase PDF.

The variance plots in Figure 8.22 illustrate the difficulty encountered by the power correlation model. The variance in element magnitude is higher for this case than the cases with λ/2 separation, especially for the non-adjacent elements, resulting in different element power PDFs for the SVA model and the power correlation model. The variance in the element phases has dropped, suggesting that the complex correlation model will not suffer as badly from artificial decorrelation as in the case with λ/2 separation.

**8.3 Dual-Polarization Model**

Antenna elements employing multiple polarizations often require less space per transmit/receive channel than spatially separated single-polarization elements. The capacity performance of multi-polarization elements is a function of the average
Figure 8.21: PDFs for joint adjacent element magnitude and adjacent element phase difference for 8×8 channels with λ/4 inter-element spacing.

Figure 8.22: Mean and variance of the magnitude and phase of the covariance matrix elements for the 8×8 SVA channels with λ/4 spacing
depolarization ratio due to scattering in the transmission environment. Environments with low depolarization lead to nearly orthogonal channels at the expense of reduced average receiver SNR, whereas environments with high depolarization behave similarly to spatially separated elements \[63\].

A more detailed analysis of capacity for multi-polarization versus single-polarization elements is treated in Section \[8.4\]. In this section, a simple method for including polarization into existing single-polarization models is presented. The capacity statistics for measured 4×4 channels is matched using this method and the SVA model.

8.3.1 Independent Subchannel Method

The data in 4×4(b) may be divided into a number of different SISO sub-channels. The basic subchannel types are represented by \(h_{RP}\) where \(R\) is the receive polarization and \(P\) is the transmit polarization. \(R\) and \(P\) may be either H or V for horizontal or vertical polarization, yielding four subchannel types. Since there are two dual-polarized antennas on each array, we have four elements in \(\overline{H}\) of each subchannel type in 4×4(b).

In order to see if there is any statistical dependence among these various types of subchannels, pairwise joint magnitude and phase difference PDFs may be plotted as before. In this case however, the elements are two subchannels with the same transmit and receive location, but distinct polarizations. There are 10 unique pairs of subchannel types, which may be divided into the categories listed in Table \[8.7\]. The like polarization pairs need not be analyzed, since they can be characterized with a single polarization type. For each of the remaining categories, the pairwise PDFs are computed by averaging the PDFs of the specific pairs that belong to that category.

Figure \[8.23\] plots the PDFs for the three categories. The plots are somewhat irregular due to the limited amount of data. However, the three subchannel types appear to have no strong dependence in magnitude or phase. Dependence in magnitude would correspond to most of the probability mass lying near a line, whereas dependence in phase would show up as a non-uniform phase difference PDF.
Table 8.7: Categories for subchannel pair types

<table>
<thead>
<tr>
<th>Category</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Like Co-pol</td>
<td>((h_{VV}, h_{VV})) ((h_{HH}, h_{HH}))</td>
</tr>
<tr>
<td>Like Cross-pol</td>
<td>((h_{VH}, h_{VH})) ((h_{HV}, h_{HV}))</td>
</tr>
<tr>
<td>Opposite Co-pol</td>
<td>((h_{VV}, h_{HH}))</td>
</tr>
<tr>
<td>Cross-pol, Co-pol</td>
<td>((h_{VH}, h_{HH})) ((h_{HV}, h_{HH})) ((h_{VV}, h_{HV})) ((h_{HV}, h_{VV}))</td>
</tr>
<tr>
<td>Cross-pol, Cross-pol</td>
<td>((h_{VH}, h_{HV}))</td>
</tr>
</tbody>
</table>

These results suggest that as a first approximation, the subchannels may be treated as being statistically independent.

In the independent subchannel method the VV, HH, VH, and HV subchannels are characterized in isolation, and the corresponding synthetic \(\overline{H}\) matrices are generated: \(\overline{H}_{VV}, \overline{H}_{HH}, \overline{H}_{VH},\) and \(\overline{H}_{HV}\). The complete channel is then formed as

\[
\overline{H} = \begin{bmatrix}
\overline{H}_{VV} & \alpha \overline{H}_{VH} \\
\alpha \overline{H}_{HV} & \overline{H}_{HH}
\end{bmatrix}. 
\]  

(8.32)

The constant \(\alpha\) is chosen to ensure that the average depolarization ratio of the synthetic channel matrices matches that of the measured data.

In the following subsections, the independent subchannel method is coupled with the SVA model to match the capacity statistics of data collection 4×4(b). A number of different methods could be used to compute the independent subchannels with the SVA model. Two possible modeling extremes are

1. The subchannels for a single channel realization could share the same cluster parameters and ray realizations, and only the phases of the complex ray gains vary for the different subchannels.

2. The subchannels could be generated from completely different realizations of the SVA model.

For simplicity and complete independence, case 2 was chosen. However, physical reality would probably dictate an approach somewhere between these two extremes.
Figure 8.23: Joint magnitude and phase PDFs for the three subchannel pair categories. The plots show little dependence of the subchannel pairs for either magnitude or phase.
Table 8.8: Simulations parameters for the SVA model and independent subchannel method example

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma$</td>
<td>Cluster decay constant</td>
<td>2.0</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>AOA/AOD standard deviation</td>
<td>$10^\circ$ (VV/HH subchannels)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$20^\circ$ (VH/HV subchannels)</td>
</tr>
<tr>
<td>$D$</td>
<td>Average depolarization ratio</td>
<td>-6.8 dB</td>
</tr>
<tr>
<td>$g$</td>
<td>Antenna gain patterns</td>
<td>Vertical/horizontal patch antenna gains for isolated elements</td>
</tr>
</tbody>
</table>

8.3.2 SVA Model Parameters

Due to the strong line-of-sight (LOS) nature of the scenario for collection $4 \times 4(b)$, a fairly narrow angular spread of arrivals within a cluster is expected, especially for the cluster corresponding to LOS. Also, transmit and receive patch antenna arrays were always facing each other, leading to a fixed mean cluster arrival angle for the LOS cluster. Table 8.8 lists the simulation parameters. The required increase in angular spread of the cross-polarized subchannels is reasonable due to stronger multiple reflections. The depolarization parameter $\alpha$ was chosen to match the average measured depolarization of $-6.8 \text{dB}$. The average depolarization ratio for a single $H$ matrix is computed as

$$D = \frac{\langle |h_{VH}|^2 \rangle + \langle |h_{HV}|^2 \rangle}{\langle |h_{HH}|^2 \rangle + \langle |h_{VV}|^2 \rangle},$$

where $D$ is the power depolarization, and $\langle | \cdot |^2 \rangle$ represents an average of the magnitude squares of all elements having the specified polarization type.

Figure 8.24 plots the capacity for the different simulated subchannels in isolation compared with the corresponding subchannels extracted from measured data. The sharp peak at the left of each capacity plot occurs where the water-filling solution uses only a single orthogonal subchannel, which happens frequently for these $2 \times 2$ channels exhibiting strong LOS. The sharpness of the peak results from the narrow bin size and the nearly constant gain of the strongest orthogonal subchannel taken from normalized $\overline{H}$. These plots reveal the good statistical agreement between
measured and modeled channels for the selected model parameters. This agreement suggests that the proposed mechanism for including polarization within the SVA model captures the channel behavior important for determining channel capacity.

### 8.3.3 Simulation Results

The SVA model was used to generate 100 cluster configurations with 1000 sets of $2 \times 2$ subchannel matrices each. The subchannel matrices were then formed into complete $4 \times 4$ channel matrices. Figures 8.25 shows the depolarization PDFs and capacity PDFs for measured and simulated channel matrices. The fit in depolarization and capacity is good considering the simplicity of the model.

### 8.4 SVA Model Simulations

This final section couples the electromagnetic antenna simulations from Section 8.1 with the simplified SVA model developed in Section 8.2. Model simulations are used to illustrate the impact of the following important system design issues:
Figure 8.25: Comparison of the depolarization ratio PDFs and capacity PDFs for measured data and the SVA model with the independent subchannel method

1. Closely spaced antennas and mutual coupling

2. Directive antennas

3. Dual-polarization antenna elements

Information provided by these types of simulations would be invaluable to engineers making key design choices in wireless communications systems.

An important contribution of this section is proof that channel normalization often leads to conclusions which are inconsistent with reality. Channel normalization forces the average received power to be constant for all cases considered, which will favor systems that generate and receive rich multipath interference. However, the average receive power will be highly affected by factors such as mutual coupling, the directivity of antennas, and dual polarization. Any reduction in the average receive power for a fixed amount of multipath will translate into reduced capacity in a real communications system.

Non-normalized channels are simulated by fixing receiver noise and computing the channel normalization required for a given SISO SNR for a control case. The channels for the test cases are then normalized using the same normalization factor as the control case. In this way, the test case channels may have a higher or lower
SISO SNR than the control case, and the drop or increase will reflect a change in the average receive power due to the specific antenna type or propagation environment.

### 8.4.1 Mutual Coupling

For many systems, available space for antenna placement is small, and multiple antennas will experience mutual coupling. The 10-element monopole arrays in this research consist of elements which are closely spaced ($\lambda/4$). This study assesses the impact of mutual coupling on spatial correlation and capacity statistics.

The simulation parameters for studying mutual coupling are listed in Table 8.9. Two basic antenna types are considered:

1. Monopole antennas with no mutual coupling and ideal uniform radiation patterns.

2. Monopole elements with mutual coupling and antenna gain obtained from the FDTD simulations of the complete 10-element monopole array in Section 8.1.

The antennas are studied in the presence of two levels of multipath: *rich* and *weak*. The multipath richness is controlled by the parameter $\Gamma$. Once $\Gamma$ is fixed, the expected number of clusters above a threshold may be computed. For a power threshold of

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Lambda$</td>
<td>Cluster arrival rate</td>
<td>1</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>Cluster decay constant (multipath richness)</td>
<td>2.0 (<em>rich</em>), 0.25 (<em>weak</em>)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Ray AOA/AOD standard deviation</td>
<td>$26^\circ$</td>
</tr>
<tr>
<td>$N_T, N_R$</td>
<td>Number of transmit/receive antennas</td>
<td>10</td>
</tr>
<tr>
<td>$d$</td>
<td>Inter-element antenna spacing</td>
<td>$\lambda/4$</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of cluster realizations</td>
<td>1000</td>
</tr>
<tr>
<td>$M$</td>
<td>Channel realizations per cluster realization</td>
<td>10,000</td>
</tr>
<tr>
<td>SNR</td>
<td>SISO SNR for the ideal (control) case</td>
<td>20 dB</td>
</tr>
</tbody>
</table>
Correlation Functions

Studies have appeared which demonstrate a reduction in correlation due to mutual coupling of closely spaced antennas [64]. Figure 8.12 in Section 8.1 illustrates the alteration in radiation patterns due to mutual coupling. Since the overlap in radiation patterns is reduced for the case of mutual coupling, we could expect the signals on the antennas to experience less correlation than ideal elements with the same spacing.

Figure 8.26 plots the average correlation coefficient for transmit and receive for the rich and weak multipath cases. Clear from the plot is a reduction in the correlation for small separations. Also there is no notable difference between the rich and weak multipath cases.
Mutual Coupling and Antenna Transmit/Receive Power

At first glance, we would expect the reduction in correlation experienced by the antennas with mutual coupling to translate into a capacity increase. However, we must also take into account the reduction in average received power caused by the mutual coupling. The antenna patterns in Figure 8.12 show that power radiated by the true array is much smaller than that of the ideal array, mainly due to power coupled and absorbed in adjacent elements. At the transmitter, we can apply two possible techniques to overcome the lost transmit power:

1. A sophisticated adaptive matching network could possibly be designed that matches the transmit RF hardware to the antenna array for every possible combination of transmit excitations.

2. The total power supplied to each port could be increased, such that the total power radiated from each antenna is equal to the ideal case.

For simplicity of modeling, the second case, or power boost case is considered.

By invoking reciprocity, the receive capability of the antennas is the same as the radiation patterns depicted in Figure 8.12. One may logically ask: If matching can be performed at the transmitter to ensure total radiation of available power, can a similar operation be performed at the receiver to collect as much power as the uncoupled case? Recovery of some of the lost receive power is likely to be possible with a very sophisticated matching network that adapts to a specific angular receive power distribution. However, for current systems, such an implementation is probably unrealistic. For simplicity, this study assumes that only a simple self-impedance match is performed at each port, to avoid self reflection. Without more sophisticated matching, nonzero mutual coupling translates into a receive power loss. Thus, the receive capability of each antenna is defined by reciprocity to be the patterns in Figure 8.12.
Capacity PDFs

Simulations were run for weak and rich multipath for the following basic cases:

1. An ideal monopole array with no mutual coupling,
2. The actual monopole array with normalized channel matrices,
3. The actual array with non-normalized channel matrices, and
4. The actual array with non-normalized channel matrices and power boosted at the transmitter.

Figure 8.27 plots the resulting capacity PDFs for these simulations. For both the rich and weak multipath cases, the relative order of the PDFs is the same. The array with mutual coupling exhibits slightly higher capacity than the ideal array when normalization is performed, which is likely due to the small reduction in element correlation. The actual array without channel normalization suffers a large drop in capacity due to the drop in transmit power and receiver sensitivity. For the power boost case, about half of this loss is recaptured.

![Figure 8.27: Capacity PDFs for arrays with and without mutual coupling](image)
In LOS communications systems, highly directive antennas are often desirable to avoid wasting transmit power in directions other than the LOS. On the other hand, most analyses of MIMO systems emphasize the need for multipath richness and ignore SNR. Omnidirectional antennas maximize multipath by transmitting and collecting power in all directions, while directive antennas maximize SNR by focusing power in a single direction. Since capacity depends on both the multipath richness and the average receive SNR, some optimum directivity exists for a given environment. This study demonstrates the tradeoff between multipath richness and SNR by comparing directive, single-polarized patch antennas to omnidirectional monopole antennas. Table 8.10 lists the important parameters for the directivity simulations. In many situations, alignment of the transmit and receive array is possible so that

Table 8.10: Parameters for the simulations to directive V-polarized patches to ideal unidirectional monopoles

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma$</td>
<td>Cluster decay constant</td>
<td>2 (rich), 0.25 (weak)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>First cluster arrival/departure angle</td>
<td>Aligned/Random</td>
</tr>
<tr>
<td></td>
<td>Ray AOA/AOD standard deviation</td>
<td>26°</td>
</tr>
<tr>
<td></td>
<td>Array Type</td>
<td>V-pol Patches,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ideal Monopoles</td>
</tr>
<tr>
<td>$N_T, N_R$</td>
<td>Number of transmit/receive antennas</td>
<td>4</td>
</tr>
<tr>
<td>$d$</td>
<td>Inter-element antenna spacing</td>
<td>$\lambda/2$</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of cluster realizations</td>
<td>1000</td>
</tr>
<tr>
<td>$M$</td>
<td>Channel realizations per cluster realization</td>
<td>10,000</td>
</tr>
</tbody>
</table>

the dominant cluster (often corresponding to LOS) is sent/received in the main lobe of the directional antennas. For the monopole array, the ideal alignment angle corresponds to the broadside of the array. This study looks at the effect of assuming a first cluster that is aligned with the main transmit/receive lobe versus a random first cluster angle. For both cases, however, clusters other than the first are distributed
Figure 8.28: Comparison of the correlation coefficient magnitude for uniformly radiating monopole arrays and directive patch arrays. Performance of the antennas was simulated for rich and weak multipath, and for array orientation that is either random or aligned with the dominant cluster.

Correlation Functions

Figure 8.28 plots the correlation functions for the four cases considered. For unaligned arrays, the AOA/AOD statistics of the clusters are uniform i.i.d., and the number of clusters only affects average power and not correlation statistics. As expected, the correlation of the ideal array follows Jakes’ model. The correlation of the patch array shows decreased correlation for all of the antenna spacings. This
lower correlation for spacing $\geq \lambda/2$ likely arises due to the distinct shape of the radiation patterns of the different patches (see Figure 8.3) and the limitation of the reception/radiation to a half-space.

For the case of arrays aligned with the first cluster, the amount of multipath determines the impact of alignment on the correlation statistics. For the rich multipath case, the deviation of the monopole antenna correlation is fairly small. Although the correlation has dropped for the monopoles, it is likely the result of shifted zeros rather than a reduction of the overall envelope. The correlation of the patch elements has increased since the LOS cluster looks nearly identical to all receivers and there are fewer non-LOS clusters. The effects are much more pronounced in the weak multipath case, since there are only two clusters on average and the LOS cluster dominates. Interestingly, the correlation functions look nearly identical for patches and monopoles in the weak multipath case with alignment.

**Capacity PDFs**

Figure 8.29 plots the capacity PDFs of the monopole and patch arrays for the various cases. Also, since normalization unfairly penalizes the directive patches for certain scenarios, capacity PDFs for un-normalized patch array channels are also plotted.

For the unaligned case with rich multipath, the monopole and patch arrays have almost the same average capacity. However, the monopole array can perform slightly better at times due to its ability to capture more multipath. For un-normalized patch array channels, much of the PDF shifts to a lower capacity, since half of the power comes from behind the array (on average) and is lost. However, the patch array does outperform the monopole array for cases when, by chance, clusters mainly arrive (or depart) from the front of the array. In the case of weak multipath, only two clusters are expected, and the effects of patch array misalignment are amplified.

For the aligned case with rich multipath, the average capacity of the patch array for normalized channels is again about the same as that of the monopole array.
Figure 8.29: Comparison of the capacity PDFs for uniformly radiating monopole arrays and directive patch arrays. Performance of the antennas was simulated for rich and weak multipath, and for array orientation that is either random or aligned with the dominant cluster.
On the other hand, when the channel is left un-normalized, a large increase in capacity is seen due to the superior ability of the patch array to direct and receive power in the direction of the dominant cluster. When only one or two clusters exist (the weak multipath case), the capacity increase is even more apparent.

The simulations in this section show that the limitation in multipath transmission and reception experienced by directional antennas can be outweighed by average receive power when alignment of transmit and receive is possible. The benefit is especially apparent when multipath interference is weak.

8.4.3 Dual Polarization

Systems employing dual polarization can often place twice as many antenna elements in the same aperture as single-polarization systems. In environments with low depolarization, the two orthogonal polarizations present nearly parallel, non-interfering channels. As described in Chapter 7, although parallel channels outperform interfering channels for the normalized case, the relationship is not clear for the un-normalized case.

This study assesses the capacity gains for dual-polarization antennas relative to single-polarization antennas. For simplicity, antennas in this study are elements that radiate uniformly in the horizontal plane and experience no mutual coupling. The SVA model was used to generate 100 cluster configurations with 1000 channel matrices per configuration. Every combination of the parameters listed in Table 8.11 was simulated. Pairs of dual-polarized elements were assumed to be co-located so that the spacing is actually 2d. Due to the large number of independent simulations, the metric for comparison is average capacity (bits/use) which may be tabulated.

Table 8.12 lists the percent increase in capacity of the dual-polarized configuration over the single-polarized configuration for normalized channels over all combinations of the parameters. As expected for normalized channels, the dual-polarized antennas are always superior. The most suitable use for dual-polarization is in systems with close antenna spacings (d = 0.1) and large numbers of elements (N = 8).
Table 8.11: Parameters for the mutual coupling study

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>SNR</td>
<td>Average SISO SNR for the single-pol (control) case</td>
<td>10 dB, 20 dB, 30 dB</td>
</tr>
<tr>
<td>$d$</td>
<td>Inter-element single-pol antenna spacing</td>
<td>0.5λ, 0.25λ, 0.1λ</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of transmit and receive antennas</td>
<td>2, 4, 8</td>
</tr>
<tr>
<td>$D$</td>
<td>Average power depolarization ratio</td>
<td>0 dB, -3 dB, -10 dB</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>Cluster decay constant (multipath richness)</td>
<td>2.0 (rich), 0.25 (weak)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Ray AOA/AOD standard deviation</td>
<td>26°</td>
</tr>
</tbody>
</table>

The gains are fairly insensitive to the other parameters. The gains come from the dual-polarization system allowing double antenna spacing due to co-located elements and the statistical independence of the various polarization subchannels (VV, HH, HV, VH). The gains are fairly insensitive to the power depolarization ratio, since the amount of power lost due to parallel channels is restored by the normalization. Note that for $N = 2$ and low depolarization ($D = -10$ dB) the parallel channels provide a 20% increase for the 20 dB SNR case, which was similar to data presented in Chapter 7.

Table 8.13 lists the percent increase in capacity of the dual-polarized configuration over the single-polarized configuration for un-normalized channels. The biggest difference between the normalized and un-normalized cases is the role of the power depolarization ratio. For systems employing a few elements at wide spacings, the dual-polarization configuration actually degrades system performance by lowering the receive power without substantially increasing channel independence. For narrower spacings, the power loss incurred by low depolarization is not enough to outweigh the gains from increased channel independence. Unsurprisingly, SNR controls the impact of the power loss on channel capacity.

These results show that dual-polarization is advantageous for many realistic propagation scenarios. The only place where dual-polarization fails to increase
Table 8.12: Percent increase in capacity (bits/use) for a dual-polarization system compared to a single-polarization system. All channel matrices were normalized to obtain the specified SISO SNR.

<table>
<thead>
<tr>
<th>( \Gamma )</th>
<th>( D )</th>
<th>( d = 0.50\lambda )</th>
<th>( d = 0.25\lambda )</th>
<th>( d = 0.10\lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta )</td>
<td>( N=2 )</td>
<td>( N=4 )</td>
<td>( N=8 )</td>
<td>( N=2 )</td>
</tr>
<tr>
<td>0.25</td>
<td>0 dB</td>
<td>10.6</td>
<td>18.3</td>
<td>20.8</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>11.0</td>
<td>18.2</td>
<td>20.3</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>12.9</td>
<td>15.6</td>
<td>17.7</td>
</tr>
<tr>
<td>2.00</td>
<td>0 dB</td>
<td>5.4</td>
<td>8.4</td>
<td>9.8</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>5.9</td>
<td>7.1</td>
<td>10.3</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>7.4</td>
<td>8.4</td>
<td>9.6</td>
</tr>
</tbody>
</table>

(a) SNR=10 dB

<table>
<thead>
<tr>
<th>( \Gamma )</th>
<th>( D )</th>
<th>( d = 0.50\lambda )</th>
<th>( d = 0.25\lambda )</th>
<th>( d = 0.10\lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta )</td>
<td>( N=2 )</td>
<td>( N=4 )</td>
<td>( N=8 )</td>
<td>( N=2 )</td>
</tr>
<tr>
<td>0.25</td>
<td>0 dB</td>
<td>15.6</td>
<td>21.6</td>
<td>22.3</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>14.4</td>
<td>19.7</td>
<td>22.5</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>17.6</td>
<td>18.6</td>
<td>19.4</td>
</tr>
<tr>
<td>2.00</td>
<td>0 dB</td>
<td>5.4</td>
<td>7.2</td>
<td>10.4</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>7.3</td>
<td>8.3</td>
<td>9.7</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>7.8</td>
<td>8.5</td>
<td>9.1</td>
</tr>
</tbody>
</table>

(b) SNR=20 dB

<table>
<thead>
<tr>
<th>( \Gamma )</th>
<th>( D )</th>
<th>( d = 0.50\lambda )</th>
<th>( d = 0.25\lambda )</th>
<th>( d = 0.10\lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta )</td>
<td>( N=2 )</td>
<td>( N=4 )</td>
<td>( N=8 )</td>
<td>( N=2 )</td>
</tr>
<tr>
<td>0.25</td>
<td>0 dB</td>
<td>11.6</td>
<td>17.9</td>
<td>20.8</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>12.0</td>
<td>15.7</td>
<td>17.9</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>13.8</td>
<td>18.3</td>
<td>18.1</td>
</tr>
<tr>
<td>2.00</td>
<td>0 dB</td>
<td>4.0</td>
<td>5.8</td>
<td>7.1</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>4.8</td>
<td>7.1</td>
<td>7.8</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>6.0</td>
<td>6.2</td>
<td>5.8</td>
</tr>
</tbody>
</table>

(c) SNR=30 dB
Table 8.13: Percent increase in capacity (bits/use) for a dual-polarization system compared to a single-polarization system. Channel matrices for the two cases were normalized by the same factor to avoid favoring the low depolarization case. Negative increases are shown in italics.

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$D$</th>
<th>$d = 0.50\lambda$</th>
<th>$d = 0.25\lambda$</th>
<th>$d = 0.10\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$N=2$ $N=4$ $N=8$</td>
<td>$N=2$ $N=4$ $N=8$</td>
<td>$N=2$ $N=4$ $N=8$</td>
</tr>
<tr>
<td>0.25</td>
<td>0 dB</td>
<td>10.9 18.4 21.9</td>
<td>14.4 27.8 36.1</td>
<td>21.0 40.1 51.4</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>-1.5  5.5  9.2</td>
<td>3.8  15.0  20.7</td>
<td>9.7  29.4  44.3</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>-9.9 -6.6 -4.6</td>
<td>-6.6  1.9  7.3</td>
<td>-1.9  17.0  21.2</td>
</tr>
<tr>
<td>2.00</td>
<td>0 dB</td>
<td>4.8  9.2  9.0</td>
<td>10.1 15.9 22.1</td>
<td>18.5 36.1 38.5</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>-5.2 -4.4 -0.2</td>
<td>-1.1  7.7  10.7</td>
<td>7.2  20.7  24.8</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>-13.1 -11.1 -9.8</td>
<td>-12.2 -8.2 -5.1</td>
<td>-0.5  8.5  12.8</td>
</tr>
</tbody>
</table>

(a) SNR=10 dB

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$D$</th>
<th>$d = 0.50\lambda$</th>
<th>$d = 0.25\lambda$</th>
<th>$d = 0.10\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$N=2$ $N=4$ $N=8$</td>
<td>$N=2$ $N=4$ $N=8$</td>
<td>$N=2$ $N=4$ $N=8$</td>
</tr>
<tr>
<td>0.25</td>
<td>0 dB</td>
<td>15.0 22.1 22.2</td>
<td>22.7 36.1 47.9</td>
<td>42.2 60.5 67.4</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>6.4  13.8 12.7</td>
<td>17.2 25.8 34.9</td>
<td>29.8 48.9 54.4</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>1.3   2.6  4.2</td>
<td>10.7 13.9 15.3</td>
<td>23.5 33.9 42.1</td>
</tr>
<tr>
<td>2.00</td>
<td>0 dB</td>
<td>5.7   7.2 10.8</td>
<td>10.4 22.0 29.6</td>
<td>38.1 45.7 53.1</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>2.2   3.7  2.1</td>
<td>3.2 13.0 23.8</td>
<td>27.5 36.0 41.5</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>-8.4 -6.8 -5.8</td>
<td>-3.1  4.3 10.6</td>
<td>21.8 25.0 31.9</td>
</tr>
</tbody>
</table>

(b) SNR=20 dB

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$D$</th>
<th>$d = 0.50\lambda$</th>
<th>$d = 0.25\lambda$</th>
<th>$d = 0.10\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$N=2$ $N=4$ $N=8$</td>
<td>$N=2$ $N=4$ $N=8$</td>
<td>$N=2$ $N=4$ $N=8$</td>
</tr>
<tr>
<td>0.25</td>
<td>0 dB</td>
<td>11.6 17.5 20.7</td>
<td>22.2 35.9 43.7</td>
<td>49.9 66.8 75.0</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>6.9  10.2 11.4</td>
<td>13.9 31.2 36.6</td>
<td>42.4 59.7 69.9</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>2.8   7.1  6.7</td>
<td>10.6 17.9 26.1</td>
<td>37.1 46.5 49.2</td>
</tr>
<tr>
<td>2.00</td>
<td>0 dB</td>
<td>3.2   4.1  6.9</td>
<td>9.2 21.0 32.7</td>
<td>39.0 55.7 63.5</td>
</tr>
<tr>
<td></td>
<td>-3 dB</td>
<td>1.0   2.9  2.9</td>
<td>3.2 17.3 27.2</td>
<td>32.1 47.8 57.8</td>
</tr>
<tr>
<td></td>
<td>-10 dB</td>
<td>-3.9 -4.4 -5.6</td>
<td>1.3 10.3 15.1</td>
<td>27.3 40.1 45.3</td>
</tr>
</tbody>
</table>

(c) SNR=30 dB
capacity is for systems with few elements \((N = 2)\) where wide antenna spacing (and therefore spatial independence) is possible.

### 8.5 Chapter Summary

This chapter has explored statistical modeling of the indoor wireless MIMO channel. Accurate physically based simulations are possible by analyzing antenna elements with either FDTD or MOM (to compute network characteristics and radiation patterns) and coupling these results with the SVA model. The resulting simulations provide key system performance information such as spatial correlation of antenna elements and capacity PDFs.

The chapter first presented MOM simulations of the 4-element patch array and detailed FDTD simulations of the 10-element monopole array. Although the radiation patterns of the patch antennas were perturbed by adjacent elements, the mutual coupling effects were fairly small. On the other hand, the monopole array experienced large mutual coupling and dramatic changes in the antenna radiation patterns.

Next, the chapter outlined the SVA model and a simplified version suitable for the narrowband case. Comparisons of the SVA model with simpler complex normal models showed the inability of the simple models to capture key statistics important for capacity predictions. Simulations demonstrated the highly random nature of the covariance matrix with respect to cluster statistics, proving that the channel matrices cannot be described by a stationary multivariate complex normal distribution.

Finally, the chapter provided simulations that assess the impact of key system design parameters (antenna spacing, directivity, dual-polarization) on capacity, leading to a number of important conclusions. Although closely-spaced antennas exhibited higher capacity for normalized channels, capacity was actually degraded for realistic un-normalized channels. Directive antennas provided higher capacity than omnidirectional antennas when alignment of transmit and receive was possible. Dual-polarization elements were advantageous for many propagation environments,
especially for arrays with many elements and close spacings. These discussions underlined the fact that blind application of channel normalization may lead to unwarranted conclusions about channel capacity, and that both average receive SNR and multipath richness are important.
Chapter 9

Conclusion

This work has demonstrated the use of hybrid modeling techniques to overcome certain limitations of conventional unified electromagnetic methods. Division of a problem into appropriate layers, and propagating only the needed information from one layer to another can introduce large savings in problem computation and complexity. The fundamental method was demonstrated by application in the areas of remote sensing of snow, analysis of an optical Bragg resonator, and MIMO wireless channel modeling. The results for each of these areas are summarized below.

9.1 Remote Sensing of Snow

Chapter 4 outlined application of the method to passive and active remote sensing of snow. The snow area illuminated by satellite instruments can have dimensions on the order of thousands of wavelengths, precluding the use of numerical electromagnetic solvers over the entire area. The random nature of the medium suggested, however, that a much simpler statistical representation was possible. Radiative transfer has long been used for such media, but the use of approximate radiative transfer parameters (phase matrices, extinction coefficients) leads to models which are also approximate. The proposed hybrid scheme for this method was twofold: (1) use of FDTD to compute the radiative transfer parameters exactly, and (2) numerically solving the radiative transfer equations to compute remote-sensing quantities of the random medium.

The method was tested by first analyzing a medium that has a closed-form solution—a sparse random distribution of spherical particles. FDTD coupled with
the Monte Carlo technique was used to compute the phase matrices and extinction coefficients. A convergence study demonstrated that good accuracy could be achieved as long as the FDTD simulation volume size and number of Monte Carlo realizations was above some lower threshold. Failure to meet this threshold could lead to large aberrations in the radiative transfer quantities.

Next, the method was applied to a medium with an approximate analytical solution—a random distribution of densely-packed, non-penetrating spheres. In this case QCA and QCA-CP (low frequency) provide an approximate theory for computing the extinction of a wave propagating through the particles. Computation of extinction with FDTD exhibited slightly higher scattering than the approximate theories. These dense theories in their basic form make no predictions about the shape of the phase matrix. The results of the FDTD analysis, however, showed not only a change in the extinction, but also an apparent change to the shape of the phase matrix functions.

The power of the hybrid FDTD/radiative transfer method was proven by analyzing a case with no closed-form solution—penetrating spheres. Often, when snow undergoes melt and refreeze, the particles can clump together in configurations that look like penetrating spheres. The results of the FDTD simulations demonstrated a three-fold increase in scattering over the conventional dense-medium theories that are often employed. Application of a numerical radiative transfer solver indicated the large difference in brightness temperature and backscatter coefficient as predicted by this new penetrating sphere model compared to existing dense-medium theories.

The result of this study was a powerful tool for exact analysis (within the framework of radiative transfer) of random media of large dimensions. As long as the structure of the medium can be adequately characterized, the FDTD method can compute the radiative transfer parameters exactly. Combining these exact parameters with the numerical radiative transfer solver should yield very accurate predictions of remote-sensing quantities.
9.2 Analysis of an Optical Bragg Resonator

Chapter 5 presented a general method for the analysis of large optical-guiding structures. Many optical structures may be very large compared to the excitation wavelength ($\geq 1000\lambda$). In such cases, memory and computation required for a unified numerical electromagnetic analysis are prohibitive. In many structures, however, the entire device need not be analyzed: (1) structures consisting of basic building blocks that are reused, and (2) structures consisting mainly of longitudinally homogeneous sections. Computational savings may be achieved for these structures by analyzing propagating modes, rather than fields throughout the entire structure. The hybrid scheme for solving such problems is three fold: (1) FD analysis to compute modal propagation constants and field profiles, (2) FDTD analysis to compute modal transmission and reflection in the presence of waveguide transitions and discontinuities, and (3) network analysis to combine the elements that make up the structure.

The chapter demonstrated the method by analyzing a very large ($10^4$ sections) Bragg resonator with a surface relief grating. This device was divided into $10^4$ sections that were all alike, requiring simulation of only a single section. Modes were computed for input and output of the section, and modal propagation through the section was simulated with FDTD. The resulting reflection and transmission coefficients were combined using S-parameter analysis to obtain the response of the complete Bragg resonator.

The sensitivity of the Bragg resonator required a careful analysis of the impact of numerical approximations and modeling error on the overall Bragg response. The effect of the absorbing boundary conditions and finite-difference approximations on the problem solution was studied. Even for this numerically sensitive problem, the error was small for realistic FD and FDTD simulation parameters, suggesting the applicability of the method to a broad class of optical modeling problems.
9.3 MIMO Wireless Channel Modeling

Chapters 6 and 8 developed a hybrid modeling scheme for the multiple-input multiple-output (MIMO) wireless channel. Chapter 6 presented a MIMO measurement platform capable of probing narrowband MIMO wireless channels consisting of up to 16 transmit and receive antennas. Signal-processing algorithms were presented for obtaining channel matrix elements from the raw data. Simulation results were provided to demonstrate the validity of the channel probing method. The development of this platform was considered essential for determining the validity of later MIMO models.

Chapter 7 presented data collected with the measurement platform. Data was collected for three basic scenarios: (1) a centralized server for a floor, (2) a server in a hallway with clients in rooms connected to the hallway, and (3) peer-to-peer communications without a server. Also, the antenna arrays were chosen to allow assessment of antenna spacing, directivity, and polarization on system performance. The data was analyzed in terms of marginal PDFs, spatial and temporal correlation functions, and capacity. The marginal channel PDFs fit very close to those for ideal Rayleigh fading. Spatial correlation functions compared favorably with Jakes’ model. The temporal correlation of the channel was very high over measurement times of 5-seconds, suggesting very high stationarity of the channel. Capacity of the channel was found to change with array parameters: the coupling of closely spaced antennas led to reduced capacity gains, directive antennas exhibited similar capacity to omnidirectional antennas for normalized channels, and dual-polarized elements led to nearly parallel non-interfering channels with high normalized capacity.

Chapter 8 presented a hybrid model consisting of FDTD or MOM analysis coupled with the SVA model. This model matched capacity PDFs of measured data for realistic model parameters. A comparison of the SVA model and simpler complex normal models indicated the inability of simple models to capture key channel behavior. A study of the effect of antenna spacing, directivity, and polarization on capacity demonstrated the value of the model for system performance analysis.

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9.4 Ideas for Future Research

The most obvious extension of this research is application of the presented methods to more complex electromagnetic modeling problems:

1. *Remote Sensing.* The snow modeling was only an example application of the FDTD/radiative transfer method. Other types of media could be analyzed (sea ice, foliage, etc.) for remote sensing. Further, the method could be extended to include the effects of rough surfaces. Exact surface transmission and reflection characteristics could be computed with the Monte Carlo technique coupled with method-of-moments or other surface-based numerical solutions. The rough surface models are then easily accommodated into the radiative transfer framework.

2. *Device Modeling.* The hybrid FD/FDTD/network analysis technique could be used unaltered to analyze many passive optical and microwave devices. Active devices, such as DFB lasers, could be modeled by adding gain to the FDTD simulations. Analysis of devices with multiple propagating modes and two or three-dimensional structure could also be accommodated by simply adding ports to the basic analysis blocks. Other devices, such as a Bragg resonator with a non-uniform grating, could not be modeled efficiently with this method. However, non-trivial extensions may exist which can estimate the response of all sections in a device by analyzing a few representative cases. In this case, computational savings are still possible.

3. *Wireless Modeling.* The modeling effort had a number of basic limitations: (1) only a few antenna types were studied, (2) only two-dimensions were considered in the model, (3) AOA/AOD information was not available at the 2.4 GHz carrier, and (4) lack of suitable comparison metrics. The wireless modeling could easily be extended to accommodate more complex antennas by performing the appropriate data collection or simulations. The addition of a second angle for elevation would allow assessment of the nature of multipath in the vertical plane. Vertical arrays and extension of the SVA model for a third dimension
are fairly trivial. To truly justify use of the SVA model at the 2.4 GHz band, a measurement platform capable of AOA/AOD measurements at this carrier is required. Also, there may exist efficient ways to extract AOA/AOD information from measured array data to determine the accuracy of the SVA model. Finally, although capacity was a sensitive indicator of model accuracy, other metrics are needed that have more physical or intuitive meaning.

Each of these former items represents a fairly natural extension of the current work. The work on the MIMO modeling, however, introduced a number of important questions for MIMO wireless channels:

1. Capacity in MIMO systems is dependent on the array configuration and antenna gain. Is there a way to define capacity which is independent of the particular transmit elements, receive sensors, and array configuration? In a world where new antenna geometries are constantly being proposed, a metric on the ultimate upper bound of capacity for a given transmit/receive volume would be very useful.

2. Closely spaced antennas with mutual coupling exhibited a strong reduction in capacity due to reduced receiver sensitivity. Whether this loss is due to the specifics of the analyzed array or some fundamental physical limit is uncertain. A detailed electromagnetic analysis is required to understand fundamental limits of power collection and emission capabilities for arbitrary antenna arrays. A simpler, but also interesting approach, could analyze a given channel as a single network described by S-parameters and determine whether increasing cooperation in transmit and receive could provide a better match for channel power throughput.

3. Ultimate exploitation of the MIMO channel requires transmitter and receiver to know the channel matrix. Such systems must estimate the channel and track the channel’s time evolution. Also, large amounts of feedback are required to inform the transmitter of the channel. A simplified version of the SVA model
could possibly allow both transmitter and receiver to know the channel without the need for feedback. Also, tracking the parameters of the SVA model may be simpler than tracking change in the channel matrix.

As a final note, a very non-trivial extension of this research regards an information-theoretic approach to electromagnetic modeling. Generally, numerical electromagnetic analyses attempt to model a given problem as exactly as possible, with the only error arising from discretization and finite-precision arithmetic. However, in any given analysis, not all of the modeling information has equal impact on the problem solution. This very principle was exploited in this research by dividing problems into logical layers and only propagating the most significant information from one layer to the next. Information theory could determine the required complexity of a problem to obtain a given level of solution accuracy. Such a formulation would be very powerful, since it could answer fundamental questions about the lower limit on computer resources required to solve a problem, regardless of the type of algorithm employed. Also, the efficiency of any given algorithm could be measured against an information-theoretic upper bound, determining whether or not new research is required to find a better solution.
Appendix A

Exact Mode Solutions For Cylindrical Dielectric Waveguides

This appendix provides the exact mode solutions for an infinite dielectric waveguide with a cylindrical core as depicted in Figure A.1.

Figure A.1: Cross section of the cylindrical dielectric waveguide geometry. $a$ is the radius of the core, $\epsilon$ and $\mu$ are the permittivity and permeability of the core and $\epsilon_1$ and $\mu_1$ are the permittivity and permeability of the cladding.

A.1 Field Equations

This approach begins by noticing that fields inside and outside the core may be written in terms of the $E_z$ and $H_z$ components only. Assuming $\exp(-j\omega t)$ time variation and $\exp(jk_z z)$ spatial variation of the propagating mode, Maxwell’s
equations in cylindrical coordinates may be manipulated to obtain
\[
\begin{align*}
\mathcal{E}_T &= \frac{1}{\omega^2 \mu \epsilon - k_z^2} \left[ \nabla_T \frac{\partial E_z}{\partial z} + j \omega \mu \nabla_T \times (H_z \hat{z}) \right] \quad (A.1) \\
\mathcal{H}_T &= \frac{1}{\omega^2 \mu \epsilon - k_z^2} \left[ \nabla_T \frac{\partial H_z}{\partial z} - j \omega \epsilon \nabla_T \times (E_z \hat{z}) \right], \quad (A.2)
\end{align*}
\]
where \( \mathcal{E}_T \) and \( \mathcal{H}_T \) contain only the transverse \( \hat{x} \) and \( \hat{y} \) components and
\[
\nabla_T = \hat{\rho} \frac{\partial}{\partial \rho} + \hat{\phi} \frac{\partial}{\partial \phi}.
\]

Inside the fiber, solutions to the wave equation are of the form
\[
\begin{align*}
E_z &= AJ_m(k_\rho \rho) \cos(m\phi) e^{jk_z z} \quad (A.4) \\
H_z &= BJ_m(k_\rho \rho) \sin(m\phi) e^{jk_z z} \quad (A.5)
\end{align*}
\]
with the dispersion relation \( k_z^2 + k_\rho^2 = \omega^2 \mu \epsilon = k^2 \). Substituting these expressions into (A.1) and (A.2) yields
\[
\begin{align*}
\mathcal{E}_T &= \frac{je^{jk_z z}}{k^2 - k_z^2} \left\{ \hat{\rho} \left[ Ak_z k_\rho J'_m(k_\rho \rho) + B \omega m \mu J_m(k_\rho \rho) \right] \cos(m\phi) \\
&\quad - \hat{\phi} \left[ Ak_z m J_m(k_\rho \rho) + B \omega \mu k_\rho J'_m(k_\rho \rho) \right] \sin(m\phi) \right\} \quad (A.6) \\
\mathcal{H}_T &= \frac{je^{jk_z z}}{k^2 - k_z^2} \left\{ \hat{\rho} \left[ Bk_z k_\rho J'_m(k_\rho \rho) + A \omega \epsilon m \mu J_m(k_\rho \rho) \right] \sin(m\phi) \\
&\quad + \hat{\phi} \left[ Bk_z m J_m(k_\rho \rho) + A \omega \epsilon k_\rho J'_m(k_\rho \rho) \right] \cos(m\phi) \right\}, \quad (A.7)
\end{align*}
\]
where \( \{ \cdot \}' \) denotes the first derivative. Outside the fiber, we expect radially evanescent modes and write the field solutions of the form
\[
\begin{align*}
E_z &= CH^{(1)}_{\rho m}(j\alpha_1 \rho) \cos(m\phi) e^{jk_z z} \quad (A.8) \\
H_z &= DH^{(1)}_{\rho m}(j\alpha_1 \rho) \sin(m\phi) e^{jk_z z} \quad (A.9)
\end{align*}
\]
with the dispersion relation $k_z^2 - \alpha_{1\rho}^2 = \omega^2 \mu_1 \epsilon_1 = k^2_1$. The transverse fields outside the core are found to be

$$
E_T = \frac{j e^{j k z}}{k_1^2 - k_2^2} \left\{ \hat{\rho} \left[ C_{k_z} j \alpha_{1\rho} H_m^{(1)'}(j \alpha_{1\rho}) + \frac{D \omega \mu_1 a}{J_1} H_m^{(1)}(j \alpha_{1\rho}) \right] \cos(m \phi) \\
- \hat{\varphi} \left[ \frac{C_{k_z} m}{J_1} H_m^{(1)}(j \alpha_{1\rho}) + D \omega \mu_1 J_1 H_m^{(1)'}(j \alpha_{1\rho}) \right] \sin(m \phi) \right\} \quad (A.10)
$$

$$
H_T = \frac{j e^{j k z}}{k_1^2 - k_2^2} \left\{ \hat{\rho} \left[ D_{k_z} j \alpha_{1\rho} H_m^{(1)'}(j \alpha_{1\rho}) + \frac{C \omega_1 a}{J_1} H_m^{(1)}(j \alpha_{1\rho}) \right] \sin(m \phi) \\
+ \hat{\varphi} \left[ \frac{D_{k_z} m}{J_1} H_m^{(1)}(j \alpha_{1\rho}) + C \omega_1 j \alpha_{1\rho} H_m^{(1)'}(j \alpha_{1\rho}) \right] \cos(m \phi) \right\} . \quad (A.11)
$$

### A.2 Transcendental Mode Relationship

The transcendental equation giving the discrete guided mode solutions is obtained by equating tangential field components at the interface between the core and cladding. Matching $E_z$ and $H_z$ on the $\rho = a$ interface gives

$$
A J_m(k_\rho a) = CH_m^{(1)}(j \alpha_{1\rho} a) \quad (A.12)
$$

$$
B J_m(k_\rho a) = DH_m^{(1)}(j \alpha_{1\rho} a). \quad (A.13)
$$

Matching $E_\phi$ and $H_\phi$ on the interface gives

$$
\frac{A m k_z}{k_\rho^2 a} J_m(k_\rho a) + \frac{B \omega \mu}{k_\rho} J'_m(k_\rho a) = - \frac{C m k_z}{\alpha_{1\rho}^2 a} H_m^{(1)}(j \alpha_{1\rho} a) - \frac{j D \omega \mu_1}{\alpha_{1\rho}} H_m^{(1)'}(j \alpha_{1\rho} a) \quad (A.14)
$$

$$
\frac{A \omega_1}{k_\rho} J'_m(k_\rho a) + \frac{B m k_z}{k_\rho^2 a} J_m(k_\rho a) = - \frac{j C \omega_1}{\alpha_{1\rho}} H_m^{(1)'}(j \alpha_{1\rho} a) - \frac{D m k_z}{\alpha_{1\rho}^2 a} H_m^{(1)}(j \alpha_{1\rho} a). \quad (A.15)
$$

Combining relations (A.12) and (A.13) gives

$$
A = \frac{CH}{J} \quad B = \frac{DH}{J}, \quad (A.16)
$$

where $H$ and $J$ are shorthand for $H_m^{(1)}(j \alpha_{1\rho} a)$ and $J_m(k_\rho a)$, respectively. Substitution of (A.16) into relations (A.14) and (A.15) gives

$$
CH \frac{m k_z}{k_\rho^2 a} + \frac{D H \omega \mu J'}{J k_\rho} = - \frac{C m k_z}{\alpha_{1\rho}^2 a} H - j D \frac{\omega \mu_1}{\alpha_{1\rho}} H' \quad (A.17)
$$

$$
CH \frac{\omega_1}{J} J' + D H \frac{m k_z}{k_\rho^2 a} = - j C \frac{\omega_1}{\alpha_{1\rho}} H' - D \frac{m k_z}{\alpha_{1\rho}^2 a} H. \quad (A.18)
$$
Collecting terms yields
\[ C \left( \frac{mk_z}{k_p^2a} + \frac{mk_z}{\alpha_{1_p}a} \right) H = -D \left( \frac{H \omega \mu}{J k_p} J' + \frac{j \omega \mu_1}{\alpha_{1_p}} H' \right) \] \hspace{1cm} (A.19)

\[ C \left( \frac{H \omega e}{J k_p} J' + \frac{j \omega e}{\alpha_{1_p}} H' \right) = -D \left( \frac{mk_z}{k_p^2a} + \frac{mk_z}{\alpha_{1_p}a} \right) H. \] \hspace{1cm} (A.20)

After dividing (A.19) by (A.20) and cross-multiplying, a quadratic in \((J'/J)\) is obtained, or
\[
\left( \frac{J'}{J} \right)^2 + \left( \frac{J'}{J} \right) \left[ \frac{j}{\alpha_{1_p}k_p} \left( \frac{\epsilon_1}{\epsilon} + \frac{\mu_1}{\mu} \right) \frac{H'}{H} \right] - \left\{ \left[ \frac{mk_z}{ka} \left( \frac{1}{k_p^2} + \frac{1}{\alpha_{1_p}^2} \right) \right]^2 + \frac{\epsilon_1 \mu_1}{\epsilon \mu_{1_p}^2} \left( \frac{H'}{H} \right)^2 \right\} = 0. \] \hspace{1cm} (A.21)

Applying the quadratic equation on \((J'/J)\) and manipulating yields the equation
\[
\frac{J'_m(k_p a)}{J_m(k_p a)} = -\frac{j k_p}{2 \alpha_{1_p}} \left( \frac{\epsilon_1}{\epsilon} + \frac{\mu_1}{\mu} \right) \frac{H_m^{(1)'y}(j \alpha_{1_p} a)}{H_m^{(1)y}(j \alpha_{1_p} a)} \] \hspace{1cm} (A.22)

\[ \pm \sqrt{\frac{m^2 k_p^2}{k_p^2 k^2 a^2} \left( 1 + \frac{k_p^2}{\alpha_{1_p}^2} \right)^2 - \frac{k_p^2}{4 \alpha_{1_p}^2} \left( \frac{\epsilon_1}{\epsilon} - \frac{\mu_1}{\mu} \right)^2 \left( \frac{H_m^{(1)'y}(j \alpha_{1_p} a)}{H_m^{(1)y}(j \alpha_{1_p} a)} \right)^2} \]

which is the transcendental equation for the EH\(_{mn}\) and HE\(_{mn}\) modes for the positive and negative signs on the radical, respectively. Note that \(n\) refers to the \(n\)th root of the transcendental equation for a fixed value of \(m\). Applying the identity
\[
\frac{dC_n}{dx} = \frac{1}{2} \left[ C_{n-1} - C_{n+1} \right], \] \hspace{1cm} (A.23)

where \(C_n\) is any Bessel function of the \(n\)th order yields the relationship
\[
\frac{J_{m+1}(k_p a)}{J_m(k_p a)} = \frac{m}{k_p a} + \frac{j}{2} \left( \frac{\mu_1}{\mu} + \frac{\epsilon_1}{\epsilon} \right) \frac{k_p}{\alpha_{1_p}} \frac{H_m^{(1)'y}(j \alpha_{1_p} a)}{H_m^{(1)y}(j \alpha_{1_p} a)} \] \hspace{1cm} (A.24)

\[ - \sqrt{\frac{m^2 k_p^2}{k_p^2 \omega^2 \mu \epsilon a^2} \left( 1 + \frac{k_p^2}{\alpha_{1_p}^2} \right)^2 - \frac{1}{4} \left( \frac{\mu_1}{\mu} - \frac{\epsilon_1}{\epsilon} \right)^2 \frac{k_p^2 H_m^{(1)'y}(j \alpha_{1_p} a)}{\alpha_{1_p}^2 H_m^{(1)y}(j \alpha_{1_p} a)}}, \]

where the positive and negative signs refer to the EH and HE modes, respectively.

### A.3 Solution Method

Guided modes for the cylindrical dielectric waveguide may be found by applying the following steps:
1. Specify physical constants and solve (A.22) or (A.24) with a root-search method to obtain $k_\rho$ and $\alpha_1\rho$.

2. Divide equations (A.12) through (A.15) by $A$ to obtain a $3 \times 3$ matrix equation. Solve for $B/A$, $C/A$, and $D/A$.

3. Plug the resulting constants into (A.4), (A.5), (A.8), and (A.9) to obtain $\hat{z}$-directed fields.

4. Plug $E_z$ and $H_z$ into (A.6), (A.7), (A.10), and (A.11) to obtain the transverse fields.
Appendix B

Plane Wave Scattering from an Infinite Dielectric Cylinder

Consider the plane-wave illumination of a dielectric cylinder as depicted in Figure B.1. Formulae for scattered far fields given the incident polarization are taken directly from [65]. The two orthogonal polarizations are considered separately below.

![Diagram of plane wave scattering](image)

Figure B.1: Plane-wave scattering from an infinite dielectric cylinder. Two possible polarizations (case I and case II) are considered for the incident plane wave. $m$ is the index of refraction of the cylinder suspended in free space.

B.1 Case I: On-Axis Polarization

In this case, the incident field is defined to be

$$E^{\text{inc}}(x, y, z, t) = E_0 e^{-jkx}e^{j\omega t} \hat{z},$$

(B.1)
where $E_0$ is the amplitude, $k$ is the wavenumber, and $\omega$ is the circular frequency of the incident wave. The field basis coefficients are

$$b_n = \frac{m J_n'(y) J_n(x) - J_n(y) J_n'(x)}{m J_n'(y) H_n(x) - J_n(y) H_n'(x)}, \quad (B.2)$$

where $x = ka$, $y = mka$, and $H_n(\cdot)$ is the $n$th order Hankel function of the second kind, or

$$H_n(z) = H_n^{(2)}(z) = J_n(z) - jN_n(z). \quad (B.3)$$

Far fields are given by the expressions

$$E_z(\theta) = \sqrt{\frac{2}{\pi kr}} T_1(\theta) E_0 \quad (B.4)$$

$$E_\theta(\theta) = 0, \quad (B.5)$$

where $r$ is radial distance from the origin, and

$$T_1(\theta) = b_0 + 2 \sum_{n=1}^{n=\infty} b_n \cos(n\theta). \quad (B.6)$$

**B.2 Case II: Off-Axis Polarization**

In this case, the incident field is defined to be

$$\mathbf{E}^{\text{inc}}(x, y, z, t) = E_0 e^{-jkx} e^{j\omega t} \hat{y}. \quad (B.7)$$

The field basis coefficients are

$$a_n = \frac{J_n'(y) J_n(x) - m J_n(y) J_n'(x)}{J_n'(y) H_n(x) - m J_n(y) H_n'(x)}, \quad (B.8)$$

Far fields are given by the expressions

$$E_\theta(\theta) = \sqrt{\frac{2}{\pi kr}} T_2(\theta) E_0 \quad (B.9)$$

$$E_z(\theta) = 0, \quad (B.10)$$

where $r$ is radial distance from the origin, and

$$T_2(\theta) = a_0 + 2 \sum_{n=1}^{n=\infty} a_n \cos(n\theta). \quad (B.11)$$
Appendix C

Plane Wave Scattering from a Dielectric Sphere
(Mie Solution)

Consider the plane-wave illumination of a dielectric sphere as depicted in Figure C.1. Formulae for scattered far fields are taken directly from [65]. The far

![Diagram of plane-wave scattering from a dielectric sphere](image_url)

Figure C.1: Plane-wave scattering from a dielectric sphere with index of refraction $m$ and radius $a$ surrounded by free space. The incident plane wave is polarized with $E$ in the $\hat{x}$ direction and propagation is in the $\hat{z}$ direction.
fields are given by the functions

\[ E_\theta = H_\phi = - \frac{j}{kr} e^{-jkr} \cos \phi \, S_2(\theta) \]  
\[ E_\phi = -H_\theta = \frac{j}{kr} e^{-jkr} \sin \phi \, S_1(\theta). \]  

The scattering functions \( S_1 \) and \( S_2 \) are given by

\[ S_1(\theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left\{ a_n \pi_n(\cos \theta) + b_n \tau_n(\cos \theta) \right\} \]  
\[ S_2(\theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left\{ b_n \pi_n(\cos \theta) + a_n \tau_n(\cos \theta) \right\}, \]

where

\[ \pi_n(\cos \theta) = \frac{1}{\sin \theta} P_n^1(\cos \theta) \]  
\[ \tau_n(\cos \theta) = \frac{d}{d\theta} P_n^1(\cos \theta) \]

and

\[ a_n = \frac{\psi_n'(y) \psi_n(x) - m \psi_n(y) \psi_n'(x)}{\psi_n(y) \zeta_n(x) - m \psi_n(y) \zeta_n'(x)} \]  
\[ b_n = \frac{m \psi_n'(y) \psi_n(x) - \psi_n(y) \psi_n'(x)}{m \psi_n(y) \zeta_n(x) - \psi_n(y) \zeta_n'(x)}, \]

with the arguments given as

\[ x = ka = \frac{2\pi a}{\lambda}, \quad y = mka. \]

The auxiliary functions \( \psi_n(z) \) and \( \zeta_n(z) \) are defined in terms of spherical Bessel functions, or

\[ \psi_n(z) = z j_{n/2}(z) = \sqrt{\frac{\pi z}{2}} J_{n+1/2}(z) \]  
\[ \zeta_n(z) = z h_{n}^{(2)}(z) = \sqrt{\frac{\pi z}{2}} H_{n+1/2}^{(2)}(z). \]

### C.1 Scatter for Horizontal and Vertical Polarization

The far field scattering for \( E \) polarized parallel to the plane of incidence (vertical) or perpendicular to the plane of incidence (horizontal) may be found as
follows. For vertical polarization, we let

\[ \phi_s = 0, \quad \theta_s = [0, 2\pi] \]

\[ E_{vs} = E_{\theta s}. \quad (C.12) \]

For horizontal polarization, we let

\[ \phi_s = \frac{\pi}{2}, \quad \theta_s = [0, 2\pi] \]

\[ E_{hs} = -E_{\phi s}. \quad (C.13) \]

C.2 Numerical Computation

The functions \( S_1(\theta) \) and \( S_2(\theta) \) may be computed using the widely available MIEV Fortran code written by Dr. Warren J. Wiscombe [66]. The MIEV0 function takes the following parameters as inputs:

**XX**

Size parameter equal to \( \chi = 2\pi a/\lambda \), where \( a \) is the radius of the sphere and \( \lambda \) is the illumination wavelength in the background.

**CREFIN**

Complex index of refraction of the sphere relative to the background.

**PERFCT**

Set to TRUE to specify a perfectly-conducting sphere. Was set to FALSE in this research.

**MIMCUT**

Value below which the imaginary refractive index is considered to be zero. Was set to \( 1 \times 10^{-8} \) for this research.

**ANYANG**

If TRUE, any angles may be specified in XMU without any special order. Was set to TRUE in this research.
NUMANG
The number of angles at which to compute $S_1$ and $S_2$.

XMU
Vector containing the cosines of the angles at which to compute $S_1$ and $S_2$.

NMOM
Highest Legendre moment to compute. Set to 1 in this research.

ISPOLZN
Specifies type of Legendre moments to compute. Set to 0 in this research, which specifies computation of the unpolarized unnormalized phase function.

MOMDIM
First dimension of PMOM. Set to 2 in this research.

PRT
Vector specifying whether or not to print information. Set to FALSE in this research.

The following output arguments are returned from the MIEV0 function:

QEXT
Returns the extinction efficiency, which is the ratio of the extinction cross-section to the physical cross-section, or $q_e = \sigma_e/(\pi a^2)$.

QSCA
Returns the scattering efficiency, which is the ratio of the scattering cross-section to the physical cross-section, or $q_s = \sigma_s/(\pi a^2)$.

GQSC
Asymmetry factor. Not used in this research.

$S_1$
Vector of complex values for the $S_1$ function.
Vector of complex values for the $S_2$ function.

The rest of the output parameters were not necessary for this research and were ignored.
Appendix D

Numerical Solutions to Radiative Transfer

This appendix describes the numerical approach which was used to solve the radiative transfer equations. The method accommodates layered media with phase matrices and boundary conditions that have azimuthal symmetry. Both the active and passive cases are considered.

D.1 Discrete Formulation

Figure D.1 depicts the basic configuration for the scattering media. The medium to be modeled is divided into $L$ scattering layers. The $\ell = 0$ and $\ell = L + 1$ layers are homogeneous and semi-infinite. Propagation in the layers $\ell \in [1, L]$ is governed by the equation of transfer. To obtain the discrete form of the equation of transfer, we begin with equation (3.4), or

$$
\frac{dI(r, \hat{s})}{ds} = -k_e(r, \hat{s})I(r, \hat{s}) + J(r) + \int_{4\pi} d\Omega' \overline{P}(\hat{r}, \hat{s}, \hat{s}')I(\hat{r}, \hat{s}'),
$$

(D.1)

where $k_e$, $J$, and $\overline{P}$ will vary from layer to layer. Assuming a homogeneous, isotropic medium, the equation simplifies to

$$
\frac{dI(\overline{r}, \hat{s})}{ds} = -\overline{k}_e(\overline{r}, \hat{s})I(\overline{r}, \hat{s}) + \overline{J}(\overline{r}) + \int_{4\pi} d\Omega' \overline{P}(\hat{s}, \hat{s}')I(\overline{r}, \hat{s}').
$$

(D.2)

If the media has azimuthal symmetry and the illumination is uniform,

$$
\frac{dI}{dx} = \frac{dI}{dy} = 0.
$$

(D.3)
Figure D.1: Multi-layer configuration for numerical radiative transfer solution

Since variation only occurs in the $\hat{z}$ direction, we perform a change of variables to express position in terms of $z$ only. Also, for convenience, we replace $\cos \theta$ with $\mu$:

$$z = s \cos \theta = s \mu \quad \text{and} \quad -d\mu = \sin \theta d\theta$$

$$\frac{dz}{\mu} = ds \quad \text{and} \quad d\Omega' = \sin \theta' d\theta' d\phi' = -d\mu' d\phi'.$$  \hspace{1cm} (D.4)

Substitution of the appropriate expressions from (D.4) into (D.2) leads to

$$\mu \frac{d\bar{T}(z; \mu, \phi)}{dz} = -k_e \bar{T}(z; \mu, \phi) + \mathcal{T}(z) + \int_{-1}^{1} d\mu' \int_{0}^{2\pi} d\phi' \bar{P}(\mu, \phi; \mu', \phi') \bar{T}(z; \mu', \phi').$$  \hspace{1cm} (D.5)

Next, the functions are sampled in azimuth and elevation angle, or

$$\bar{T}(z)[n, m] = \bar{T}(z; \mu_n, \phi_m)$$

$$\bar{P}[n, n'; m, m'] = \bar{P}(\mu_n, \phi_m; \mu_{n'}, \phi_{m'}).$$  \hspace{1cm} (D.6)

where the samples assume the orders

$$-1 < \mu_0 < \mu_1 < \ldots < \mu_{N-1} < 1$$

$$0 = \phi_0 < \phi_1 < \ldots < \phi_{M-1} < 2\pi.$$  \hspace{1cm} (D.7)
For later reference, upward directions are associated with $\mu > 0$ and downward directions are associated with $\mu < 0$. The integral in (D.5) may be approximated as

$$
\int_{-1}^{1} d\mu' \int_{0}^{2\pi} d\phi \overline{P}(\mu, \phi; \mu', \phi') I(z; \mu', \phi') \approx \sum_{n'=0}^{N-1} \sum_{m'=0}^{M-1} w_{n'} w_{m'} \overline{P}[n, m; n', m'] I[z][n', m'],
$$

(D.8)

where $w_{n'}$ and $w_{m'}$ are summation weights chosen to approximate the integral. For problems with azimuthal symmetry, $w_{m'} = (2\pi)/M$ is a good choice, which corresponds to the midpoint integration rule. The $w_{n'}$ may also use the midpoint rule $w_{n'} = 2/N$ or use more sophisticated methods such as Gaussian quadrature. From (D.8), the equation of transfer becomes

$$
\mu_n \frac{d\overline{I}[n, m]}{dz} = -k_e I[n, m] + J + \sum_{n'} \sum_{m'} w_{n'} w_{m'} \overline{P}[n, m; n', m'] I[n', m'],
$$

(D.9)

where the $z$ dependence is now implicit. The interdependence of the azimuthal samples may be removed by transforming the equations to the Fourier domain. Expanding $\overline{I}$ and $\overline{P}$ as discrete-time Fourier series in $m$ and $m - m'$, respectively, yields

$$
\overline{I}[n, m] = \sum_{k=0}^{M-1} \overline{I}^k[n] e^{j\Omega m}
$$

(D.10)

and

$$
\overline{P}[n, m; n', m'] = \sum_{k=0}^{M-1} \overline{P}^k[n, n'] e^{j\Omega (m - m')},
$$

(D.11)

where $\Omega = (2\pi/M)$, and the superscript $k$ on $\overline{I}$ and $\overline{P}$ is an index, as opposed to a power. The summation term in (D.9) becomes

$$
\sum_{n'} \sum_{m'} \sum_{k_1} w_{n'} \left(\frac{2\pi}{M}\right) \overline{P}^{k_1}[n, n'] e^{j\Omega (m - m') \sum_{k_2} \overline{T}^{k_2}[n', n'] e^{j\Omega m'}
$$

$$
= \frac{2\pi}{M} \sum_{n'} w_{n'} \sum_{k_1} \sum_{k_2} \overline{P}^{k_1}[n, n'] \overline{T}^{k_2}[n'] e^{j\Omega m'} \sum_{m'} e^{j\Omega m'(k_2 - k_1)} S(k_2 - k_1).
$$

(D.12)

From Fourier analysis, the summation $S(k_2 - k_1)$ is

$$
S(k_2 - k_1) = M \delta[k_2 - k_1]
$$

(D.13)
and (D.12) becomes
\[ 2\pi \sum_{n'} w_{n'} \sum_k \bar{T}^k[n, n']T^k[n']e^{jk\Omega m}. \] (D.14)

Substitution of the Fourier series representations into the discrete equation of transfer yields
\[
\mu_n \sum_k \frac{d\bar{T}^k[n]}{dz} e^{jk\Omega m} = -k_e \sum_k \bar{T}[n] e^{jk\Omega m} + J \sum_k \delta_k e^{jk\Omega m} \\
+ 2\pi \sum_{n'} w_{n'} \sum_k \bar{T}^k[n, n']T^k[n']e^{jk\Omega m}. \] (D.15)

Since this equation must hold for all \( m \), we can equate the independent frequency components to give
\[
\mu_n \frac{d\bar{T}^m[n]}{dz} = -k_e \bar{T}^m[n] + J \delta_m + 2\pi \sum_{n'} w_{n'} \bar{T}^m[n, n']T^m[n']. \] (D.16)

At this point, use of block matrix notation is convenient. Since each component in (D.16) may be unique from layer to layer, a subscript will be added to denote the layer number. To simplify the block notation, we define the following operations
\[
\mathbb{F} = \text{col}_n \left\{ \bar{F}[n] \right\} \\
\text{Stacks the matrix (or vector) argument to form a block column vector} \\
\left[ \bar{F}[1]; \bar{F}[2]; \ldots; \bar{F}[N] \right].
\]
\[
\mathbb{F} = \text{block}_{m,n} \left\{ \bar{F}[m, n] \right\} \\
\text{Creates a block matrix out of elements of } \bar{F}[m, n] \text{ as} \\
\begin{bmatrix}
\bar{F}[1,1] & \bar{F}[1,2] & \cdots & \bar{F}[1,N] \\
\bar{F}[2,1] & \bar{F}[2,2] & \cdots & \bar{F}[2,N] \\
\vdots & \vdots & \ddots & \vdots \\
\bar{F}[M,1] & \bar{F}[M,2] & \cdots & \bar{F}[M,N]
\end{bmatrix} \] (D.17)
\[ \mathbb{F} = \text{diag} \left\{ \mathbb{F}[n] \right\} \]

Forms a diagonal block matrix with the diagonal blocks taken from \( \mathbb{F}[n] \) or

\[
\begin{bmatrix}
\mathbb{F}[1] & 0 & \cdots & 0 \\
0 & \mathbb{F}[2] & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \mathbb{F}[N]
\end{bmatrix}
\]

(D.18)

The limits of the indexing on the block commands are to be understood from context.

The block vector quantities in layer \( \ell \) are

\[
\begin{align*}
\mathbb{I}^m_\ell &= \text{col}_n \left\{ \mathbb{I}^m_\ell[n] \right\} \quad \text{(D.19)} \\
\mathbb{P}^m_\ell &= \text{block}_{n,n'} \left\{ w_{n'} \mathbb{P}^m_\ell[n,n'] \right\} \quad \text{(D.20)} \\
\mathbb{S}_\ell &= \text{diag}_n \left\{ \bar{I} \frac{1}{\mu_n} \right\} \quad \text{(D.21)} \\
\mathbb{K}_{e,\ell} &= -\text{diag}_n \left\{ \mathbb{K}_{e,\ell} \right\} \quad \text{(D.22)} \\
\mathbb{J}_\ell &= \text{col}_n \left\{ \mathbb{J}_\ell \right\} \quad \text{(D.23)}
\end{align*}
\]

In block notation, the equation of transfer for each layer becomes

\[
\frac{d \mathbb{I}^m_\ell}{dz} = \mathbb{S}_\ell \left\{ \left[ \mathbb{K}_{e,\ell} + 2\pi \mathbb{P}^m_\ell \right] \mathbb{I}^m_\ell + \mathbb{J}_\ell \delta_m \right\} = \mathbb{S}^m_\ell \mathbb{I}^m_\ell + \mathbb{S}^m_\ell \mathbb{J}_\ell \delta_m. \quad \text{(D.24)}
\]

D.2 Active Remote Sensing Solution

For active remote sensing, thermal emission may usually be neglected and we set \( \mathbb{J}_\ell = 0 \). Equation (D.24) becomes a system of homogeneous first-order differential equations, which may be solved using standard eigenanalysis techniques [67]. The general solution is

\[
\mathbb{I}^m_\ell = \left[ \mathbb{V}^m_\ell \text{diag} \left\{ e^{\bar{\lambda}^m_\ell z} \right\} \right] \bar{v}^m_\ell \equiv \bar{Q}^m_\ell \bar{v}^m_\ell, \quad \text{(D.25)}
\]

where \( \text{diag} \{ \cdot \} \) without a subscript generates a diagonal matrix out of the vector argument, and \( e^{()} \) is an element-by-element exponent, \( \bar{\lambda}^m_\ell \) is the vector of eigenvalues.
of $\overline{R}_m^\ell$, and $\overline{V}_m^\ell$ is the matrix of eigenvectors of $\overline{R}_m^\ell$. The last remaining task involves finding the unknown constants $\overline{c}_m^\ell$, which is done by enforcing boundary conditions at each interface. Solving for $\overline{Q}$ at the top and bottom interfaces of each layer yields

$$
\overline{Q}_m^T = \overline{V}_m^\ell \text{diag} \left\{ e^{\lambda_m^\ell z} \right\} \bigg|_{z=0} = \overline{V}_m^\ell \quad \text{(D.26)}
$$

$$
\overline{Q}_m^B = \overline{V}_m^\ell \text{diag} \left\{ e^{\lambda_m^\ell z} \right\} \bigg|_{z=-d_\ell} = \overline{V}_m^\ell \text{diag} \left\{ e^{-\lambda_m^\ell d_\ell} \right\}. \quad \text{(D.27)}
$$

### D.2.1 Boundary Conditions

To impose the boundary conditions, we divide quantities into upward and downward intensities, or

$$
\begin{align*}
\mathbb{I}_m^\ell &= \begin{bmatrix}
\mathbb{I}_m^D & \mathbb{I}_m^U
\end{bmatrix}
\quad \overline{Q}_m^B = \begin{bmatrix}
\overline{Q}_m^D & \overline{Q}_m^U
\end{bmatrix}
\quad \overline{Q}_m^T = \begin{bmatrix}
\overline{Q}_m^T & \overline{Q}_m^U
\end{bmatrix}
\end{align*}
\quad \text{(D.28)}
$$

with the relations

$$
\begin{align*}
\mathbb{I}_U^m &= \mathbb{Q}_U^m \overline{c}_m^\ell \\
\mathbb{I}_D^m &= \mathbb{Q}_D^m \overline{c}_m^\ell
\end{align*} \quad \text{(D.29)}
$$

$$
\begin{align*}
\mathbb{Q}_U^m &= \mathbb{Q}_U^m \overline{c}_m^\ell \\
\mathbb{Q}_D^m &= \mathbb{Q}_D^m \overline{c}_m^\ell
\end{align*} \quad \text{(D.30)}
$$

The eigenanalysis solution led to $4MNL$ unknown coefficients ($\overline{c}_m^\ell$) which are found by imposing the boundary conditions. If azimuthal symmetry is satisfied in the boundary conditions, we may solve for the $4NL$ unknowns for each Fourier coefficient separately. In this case, we will find that the top and bottom interfaces yield $2N$ equations, and intermediate interfaces yield $4N$ equations, giving a total of $4NL$ equations for each Fourier coefficient. Although this development assumes a constant number of elevation angles $N$ in each layer, a variable number of elevation angles is not precluded, and may be advantageous in certain problems. Variable numbers of angles are accommodated by forming transmission matrices that have a different number of angles for input and output, and the rest of the development remains unchanged. Figure D.2 depicts the three types of interfaces to be considered.
Figure D.2: Three types of interfaces which will aid writing of boundary conditions

**Top Interface**

At the top interface we assume some incident radiation described by $I_{inc}^m$. The boundary condition relating the downward intensity in layer 1 is

\[
T_{D1}^m = T_{D0}^m I_{inc}^m + R_{U0}^m T_{U1}^m
\]  
(D.31)

\[
\overline{Q}_{D1}^m c_1^m = T_{D0}^m I_{inc}^m + R_{U0}^m \overline{Q}_{U1}^m c_1^m
\]  
(D.32)

\[
-T_{D0}^m I_{inc}^m = \left( R_{U0}^m \overline{Q}_{U1}^m - \overline{Q}_{D1}^m \right) c_1^m.
\]  
(D.33)

The intensity leaving the top layer $I_{out}^m$ may be computed from

\[
I_{out}^m = T_{U0}^m I_{U1}^m
\]  
(D.34)

**Intermediate Interfaces**

An intermediate interface is one which has both scattering layers above and below and yields $4N$ equations. In the layer above the interface, we write

\[
\overline{I}_{U\ell}^m = \overline{T}_{U\ell}^m \overline{I}_{U,\ell+1}^m + \overline{R}_{DL}^m \overline{I}_{DL}^m
\]  
(D.35)

\[
\overline{Q}_{U\ell}^m c_\ell^m = \overline{T}_{U\ell}^m \overline{I}_{U,\ell+1}^m c_{\ell+1}^m + \overline{R}_{DL}^m \overline{Q}_{DL}^m c_\ell^m
\]  
(D.36)

\[
0 = \frac{\overline{T}_{U\ell}^m \overline{Q}_{U,\ell+1}^m c_{\ell+1}^m}{\overline{I}_{U\ell}^m} + \left( \overline{R}_{DL}^m \overline{Q}_{DL}^m c_\ell^m - \overline{Q}_{U\ell}^m \right) c_\ell^m
\]  
(D.37)
and in the layer below the interface

\[ T_{mD}^{Tm} = T_{mD}^{Bm} + R_{U\ell}^{Tm} \]

\[ Q_{D,\ell+1}^{Tm} c_{\ell+1}^m = T_{mD}^{Bm} Q_{D\ell}^{Tm} c_{\ell}^m + R_{U\ell}^{Tm} Q_{U,\ell+1}^{Tm} c_{\ell+1}^m \]

\[ 0 = T_{mD}^{Tm} Q_{D\ell}^{Bm} c_{\ell}^m + \left( R_{U\ell}^{Tm} Q_{U,\ell+1}^{Tm} - Q_{D,\ell+1}^{Tm} \right) c_{\ell+1}^m \]

for layers \( \ell \in [0, L - 1] \), yielding \( 4N(L - 1) \) equations.

**Bottom Interface**

The bottom interface yields another \( 2N \) equations. In the layer above the bottom interface, we write

\[ T_{UL}^{Bm} = R_{DL}^{mBm} \]

\[ Q_{UL}^{Bm} c_{L} = R_{DL}^{mBm} Q_{DL}^{Bm} c_{L} \]

\[ 0 = \left( R_{DL}^{mBm} Q_{DL}^{Bm} - Q_{UL}^{Bm} \right) c_{L} \]

**Half-Space Condition**

Instead of having a half-space of homogeneous dielectric, we may wish to model a half-space of scattering media. This situation is easily modeled by imposing the condition that intensity be strictly non-increasing in the downward direction in the half-space medium. Numerically, we force coefficients associated with negative eigenvalues to be 0 in the bottom layer. The \( 2N \) equations for the bottom interface are thus replaced with the equations

\[ c_{L}^m = 0, \quad \forall \lambda_{L}^m < 0. \]
D.3 Matrix Equation

The 4NL equations may now be formed into the matrix equation which has a staggered block structure

\[
\begin{pmatrix}
R_m U_0 & 0 & \cdots & 0 \\
R_m U_1 & T_m D_1 & \cdots & 0 \\
R_m U_2 & T_m D_2 & \ddots & \vdots \\
\vdots & \vdots & \ddots & \ddots \\
R_m U_L & T_m D_L & \cdots & \cdots & \cdots & 0 \\
\end{pmatrix}
\begin{pmatrix}
\vec{c}_1^m \\
\vec{c}_2^m \\
\vec{c}_3^m \\
\vdots \\
\vec{c}_L^m \\
\end{pmatrix}
= 
\begin{pmatrix}
-\bar{T}_{D0}^m \bar{m}^m_{\text{inc}} \\
0 \\
0 \\
\vdots \\
0 \\
-\bar{T}_{UL}^m \bar{m}^m_{\text{bot}} \\
\end{pmatrix},
\tag{D.45}
\]

which may be written as

\[\mathcal{A} C = F.\]  \tag{D.46}

Each block in \(\mathcal{A}\) is \(2N \times 4N\), and there are \(2L \times L\) blocks. Each block in \(\mathcal{C}\) is \(4N \times 1\) and there are \(L\) blocks. Each block in \(\mathcal{F}\) is \(2N \times 1\) and there are \(2L\) blocks. The equation is solved by matrix inversion to obtain the unknown constants in \(\mathcal{C}\).

D.3.1 Bistatic and Backscatter Coefficient Computation

Figure D.3 depicts the basic geometry considered for computing bistatic and backscatter coefficients. Bistatic scattering coefficients are computed from the expression

\[\gamma_{\beta\alpha} = \frac{4\pi r^2 |E^s_\beta|^2}{|E^i_\alpha|^2 A \cos \theta_i},\]  \tag{D.47}

where \(r\) is a distance from the scattering object, \(E^i_\alpha\) is the incident \(E\) field amplitude with polarization \(\alpha\), \(E^s_\beta\) is the scattered field amplitude with polarization \(\beta\), and \(A\) is the illumination area.

First, we assume the area \(dA\) is illuminated with a plane wave, with power density

\[S_i = \frac{|E^i_\alpha|^2}{\eta} \equiv 1,\]  \tag{D.48}
Figure D.3: Configuration for obtaining bistatic scattering coefficients

where $\eta$ is the wave impedance in the medium. Unit power density may be achieved with an incident intensity

$$I(\hat{s}) = \hat{I}_i \delta(\hat{s} - \hat{s}_i),$$

where $\delta(\hat{s})$ integrates to a total specific intensity of 1 over a sphere. $\hat{I}_i$ is a vector indicating the incident polarization. For $\alpha = V$ we have $\hat{I}_i = [1 \ 0 \ 0 \ 0]^T$, and for $\alpha = H$ we have $\hat{I}_i = [0 \ 1 \ 0 \ 0]^T$. The quantity

$$P_{\text{sphere}} = \frac{4\pi r^2 |E^s_\beta|^2}{\eta}$$

represents the power on a sphere of radius $r$, assuming uniform power density on the surface. In a neighborhood of $\hat{s}_s$, we may approximate the power per unit solid angle as

$$\frac{dP_s}{d\Omega} \approx \frac{P_{\text{sphere}}}{4\pi} = \frac{r^2 |E^s_\beta|^2}{\eta}.$$  

Differential power flowing through area $dA_s$ is

$$dP_s = I(\hat{s}_s)dA_s d\Omega$$

and power per unit solid angle in the $\beta$ polarization is

$$\frac{dP_s}{d\Omega} = I_\beta(\hat{s}_s)dA_s.$$  

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where $\beta = V$ corresponds to the first element of $\mathbf{I}(\hat{s}_s)$, and $\beta = H$ corresponds to the second element of $\mathbf{I}(\hat{s}_s)$. Performing the proper substitutions, we obtain

$$
\gamma_{\beta\alpha}(\hat{s}_s, \hat{s}_i) = \frac{4\pi I_\beta(\hat{s}_s) \cos \theta_s}{\cos \theta_i}.
$$

(D.54)

Since the intensity domain is discretized in direction, we use a pulse function that has the same area over angle as the Dirac delta function or

$$
I^i[n] = \begin{cases} 
\frac{M}{2\pi w_n}, & n = n_i \\
0, & \text{otherwise}
\end{cases}.
$$

(D.55)

where $n_i$ is the index of the discrete incident direction. The backscatter coefficient may be computed from the bistatic scattering coefficients using

$$
\sigma_{\beta\alpha}(\theta, \phi) = \gamma_{\beta\alpha}(\theta_s = \theta_i, \phi_s = \pi + \phi_i; \theta_i, \phi_i).
$$

(D.56)

### D.4 Passive Remote Sensing Solution

For the passive case, we rewrite (D.24) in terms of brightness temperature. Also, since sources only exist for the $m = 0$ term and the Fourier components are independent, only the $m = 0$ case need be considered. Also, when azimuthal symmetry is satisfied, only the first two Stokes parameters are nonzero. Recasting (D.24) for the passive case gives

$$
\frac{d\mathbb{B}_\ell(z)}{dz} = \mathbb{S}_\ell \left\{ \left[ \mathbb{K}_{e,\ell} + 2\pi \mathbb{P}_\ell \right] \mathbb{B}_\ell(z) + \mathbb{K}_{a,\ell} \mathbb{T}_\ell(z) \right\}
\equiv \mathbb{K}_{e,\ell} \mathbb{B}_\ell(z) + \mathbb{S}_\ell \mathbb{K}_{a,\ell} \mathbb{T}_\ell(z),
$$

(D.57)

with

$$
\mathbb{B}_\ell(z) = \text{col}_n \{ \mathcal{B}_\ell(z)[n] \},
$$

(D.58)

$$
\mathbb{P}_\ell = \text{block}_{n,n'} \{ w_{n'} \mathbb{P}_\ell[n,n'] \},
$$

(D.59)

$$
\mathbb{S}_\ell = \text{diag}_n \{ \frac{1}{\mu_n} \},
$$

(D.60)

$$
\mathbb{K}_{e,\ell} = -\text{diag}_n \{ \mathbb{K}_{e,\ell} \},
$$

(D.61)

$$
\mathbb{K}_{a,\ell} = \text{diag}_n \{ \mathbb{K}_{a,\ell} \},
$$

(D.62)

$$
\mathbb{T}_\ell(z) = \text{col}_n \{ T_\ell(z)[1 1]^T \},
$$

(D.63)
where \( T_\ell(z) \) is the physical temperature function in the \( \ell \)th layer, and \( \overline{B}_\ell[n] \) is a brightness temperature.

### D.4.1 Homogeneous Solution

The solution to (D.57) consists of the sum of the homogeneous and particular solutions. The homogeneous solution is found by removing the \( \overline{F} \) forcing term in (D.57), giving the same solution as the active case, or

\[
\overline{E}_\ell^h = \left[ \overline{V}_\ell \text{diag} \left\{ e^{\lambda_\ell z} \right\} \right] \overline{c}_\ell \equiv \overline{Q}_\ell \overline{c}_\ell. \tag{D.64}
\]

The \( \overline{Q} \) functions are solved at the top and bottom interfaces according to

\[
\overline{Q}_\ell^T = \left[ \overline{V}_\ell \text{diag} \left\{ e^{\lambda_\ell z} \right\} \right] \bigg|_{z=0} = \overline{V}_\ell \\
\overline{Q}_\ell^B = \left[ \overline{V}_\ell \text{diag} \left\{ e^{\lambda_\ell z} \right\} \right] \bigg|_{z=-d_\ell} = \overline{V}_\ell \text{diag} \left\{ e^{-\lambda_\ell d_\ell} \right\}, \tag{D.65}
\]

and quantities are divided into upward and downward intensities as

\[
\overline{E}_\ell^h = \begin{bmatrix} \overline{E}_{D\ell}^h \\ \overline{E}_{U\ell}^h \end{bmatrix}, \quad \overline{Q}_\ell^B = \begin{bmatrix} \overline{Q}_{D\ell}^B \\ \overline{Q}_{U\ell}^B \end{bmatrix}, \quad \overline{Q}_\ell^T = \begin{bmatrix} \overline{Q}_{D\ell}^T \\ \overline{Q}_{U\ell}^T \end{bmatrix}, \tag{D.66}
\]

with the relations

\[
\overline{E}_{U\ell}^{hT} = \overline{Q}_{U\ell}^T \overline{c}_\ell^m \quad \overline{E}_{U\ell}^{hB} = \overline{Q}_{U\ell}^B \overline{c}_\ell^m \quad \overline{E}_{D\ell}^{hT} = \overline{Q}_{D\ell}^T \overline{c}_\ell^m \quad \overline{E}_{D\ell}^{hB} = \overline{Q}_{D\ell}^B \overline{c}_\ell^m. \tag{D.67}
\]

### D.4.2 Particular Solution

The particular solution is found by including the forcing term. The form of the particular solution will depend on the functional form of the temperature profile in each layer. In general, the particular solution will be a function of \( z \) coordinate. Once found, we compute the particular solution at the top and bottom interfaces, and split into upward and downward directions to facilitate formation of the boundary
conditions, or

\[ \mathbb{E}_\ell^{TP} = \mathbb{E}_\ell^P(z = 0) \]
\[ \mathbb{E}_\ell^{BP} = \mathbb{E}_\ell^P(z = -d_\ell) \]  
(D.70)

and

\[ \mathbb{E}_\ell^{TP} = \begin{bmatrix} \mathbb{E}_{TPD_\ell}^P \\ \mathbb{E}_{TPU_\ell}^P \end{bmatrix} \]
\[ \mathbb{E}_\ell^{BP} = \begin{bmatrix} \mathbb{E}_{BPD_\ell}^P \\ \mathbb{E}_{BU_\ell}^P \end{bmatrix} \]  
(D.71)

The following temperature profiles will be considered: constant, exponential, and polynomial.

**Constant Temperature Profile**

The simplest case assumes that the temperature is constant in each layer. In a single layer we have

\[ \mathbb{\bar{\mathbb{T}}} (z) = \mathbb{\bar{\mathbb{T}}} = \text{col}_n \{ \mathbb{T}_0 \} , \quad \mathbb{T}_0 = \mathbb{T}_0 \begin{bmatrix} 1 \\ 1 \end{bmatrix} \]  
(D.72)

Substitution into [D.57] gives

\[ \mathbb{S} \left\{ \left[ \mathbb{K}_e + 2\pi \mathbb{P} \right] \mathbb{E}^P + \mathbb{K}_a \mathbb{T}_0 \right\} = 0 \]  
(D.73)

\[ \mathbb{S} \left[ \mathbb{K}_e + 2\pi \mathbb{P} \right] \mathbb{E}^P = -\mathbb{S} \mathbb{K}_a \mathbb{T}_0 . \]  
(D.74)

Since \( \mathbb{S} \) consists only of nonzero diagonal elements, we can remove \( \mathbb{S} \) from both sides to obtain

\[ \underbrace{\left[ \mathbb{K}_e + 2\pi \mathbb{P} \right]}_{\mathbb{A}} \mathbb{T}^P = -\mathbb{K}_a \mathbb{T}_0 . \]  
(D.75)

which may be solved for \( \mathbb{T}^P \) using a linear solver.

**Exponential Temperature Profile**

In the case of an exponential temperature profile, the temperature in the layer is of the form

\[ T(z) = T_1 e^{kz} \]  
(D.76)

\[ \mathbb{T}(z) = \mathbb{T}_1 e^{kz} , \quad \mathbb{T}_1 = \text{col}_n \{ T_1 [1 \ 1]^T \} . \]  
(D.77)
Specifying the temperature at depth \(d\) to be \(T_2\), we have

\[
T(z = -d) = T_1 e^{-kd} = T_2
\]

\[ k = \frac{-1}{d} \ln \left( \frac{T_2}{T_1} \right). \tag{D.78} \]

Assuming a particular solution of the form

\[
B^P(z) = \alpha e^{kz} \tag{D.79}
\]

and substituting into (D.57) gives

\[
\overline{U} \alpha k e^{kz} = \left( \overline{k_e} + 2\pi \overline{P} \right) \alpha e^{kz} + \overline{k_a} \overline{I}_{1} e^{kz}, \tag{D.80}
\]

where

\[
\overline{U} = \overline{S}^{-1} = \text{diag} \left\{ \overline{I}_{n}, \mu_n \right\}. \tag{D.81}
\]

Canceling the exponential terms and rearranging gives

\[
\begin{bmatrix}
 k \overline{U} - \overline{k_e} - 2\pi \overline{P} \\
 \overline{b}
\end{bmatrix} \alpha = \overline{k_a} \overline{T}, \tag{D.82}
\]

which again may be solved with a linear solver.

**Polynomial Temperature Profile**

Assuming a polynomial temperature profile of the form

\[
\overline{\mathbf{T}}(z) = \sum_{k=0}^{K-1} \bar{t}_k z^k, \quad \bar{t}_k = \text{col}_n \left\{ t_k \left[ \begin{array}{c} 1 \\ 1 \end{array} \right] ^T \right\}, \tag{D.83}
\]

we assume the same form for the particular solution, or

\[
\overline{B}^P(z) = \sum_{k=0}^{K-1} \bar{b}_k z^k. \tag{D.84}
\]

Substitution into (D.57) gives

\[
\overline{U} \sum_{k=1}^{K-1} k \bar{b}_k z^{k-1} = \left( \overline{k_e} + 2\pi \overline{P} \right) \sum_{k=0}^{K-1} \bar{b}_k z^k + \overline{k_a} \sum_{k=0}^{K-1} \bar{t}_k z^k. \tag{D.85}
\]
The left sum may be shifted down an index to give
\[
\mathcal{U} \sum_{k=0}^{K-2} (k + 1) \bar{b}_{k+1} z^k = \left( \overline{K_e} + 2\pi \overline{P} \right) \sum_{k=0}^{K-1} \bar{b}_k z^k + \overline{K_a} \sum_{k=0}^{K-1} \bar{t}_k z^k. \tag{D.86}
\]

Equating powers of \( z \) gives separate cases for \( k = K - 1 \) and \( k \in [0, K - 2] \). First, for \( k = K - 1 \), we have
\[
\left( \overline{K_e} + 2\pi \overline{P} \right) \bar{b}_{K-1} + \overline{K_a} \bar{t}_{K-1} = 0
\]
\[
\left( \overline{K_e} + 2\pi \overline{P} \right) \bar{b}_{K-1} = -\overline{K_a} \bar{t}_{K-1}, \tag{D.87}
\]

which is similar to the constant case. For other values of \( k \), we have
\[
\mathcal{U}(k + 1) \bar{b}_{k+1} = \left( \overline{K_e} + 2\pi \overline{P} \right) \bar{b}_k + \overline{K_a} \bar{t}_k
\]
\[
\left( \overline{K_e} + 2\pi \overline{P} \right) \bar{b}_k = \mathcal{U}(k + 1) \bar{b}_{k+1} - \overline{K_a} \bar{t}_k, \tag{D.88}
\]

which again represents a linear system from which \( \bar{b}_k \) can easily be solved. The basic strategy involves solving for \( \bar{b}_{K-1} \) using (D.87). Then, moving in backward fashion from \( K - 2 \) down to 0, we use (D.88) to obtain the rest of the \( \bar{b}_k \).

### D.4.3 Boundary Conditions

The boundary conditions for the passive remote sensing case are very similar to those for the active case. There are two important modifications, however. First, boundary conditions are enforced on the total brightness temperature (the combination of the homogeneous and particular solutions). Second, the transmission matrices assume a slightly different form due to the definition of brightness temperature.

First, we may write the total brightness temperature in each layer as the sum of the homogeneous and particular solutions or
\[
\Xi_\ell(z) = \Xi^h_\ell(z) + \Xi^P_\ell(z)
\]
\[
= \left[ \overline{\nabla_\ell} \text{diag} \left\{ e^{\overline{\lambda}_\ell z} \right\} \right] \overline{\nu}_\ell + \Xi^P_\ell(z) \equiv \overline{Q}_\ell(z) \overline{\nu}_\ell + \Xi^P_\ell(z). \tag{D.89}
\]
Second, brightness temperature in terms of specific intensity is

$$B_\ell = T_\ell \frac{\lambda_\ell^2}{K}.$$  \hfill (D.90)

Next, we consider each of the interface types as in the active case.

**Top Interface**

In terms of specific intensity, the relation in the layer just below the top interface is

$$I_{TD_1} = R_{U0} I_{TU_1},$$  \hfill (D.91)

where down welling from the atmosphere has been neglected. Transforming into brightness temperature, we have

$$K B_{TD_1} = R_{U0} K B_{TU_1},$$  \hfill (D.92)

where $K$ is Boltzmann’s constant and $\lambda_\ell$ is the wavelength in the $\ell$th layer. Expanding the brightness temperature as the sum of the homogeneous and particular parts, we have

$$[B_{TD_1} + B_{TP}] = \frac{K B_{U1}}{\lambda_1^2} \left[ B_{Tu_1} + B_{Tu_1} \right]$$

$$Q_{TD_1} T_1 + B_{TP} = R_{U0} \left[ Q_{TU_1} T_1 + B_{TP} \right]$$

$$B_{TD_1} - R_{U0} B_{U1} = \left[ R_{U0} Q_{TU_1} - Q_{TD_1} \right] \bar{e}_1,$$  \hfill (D.93)

To include the effects of down welling from layer 0, the equation becomes

$$B_{TD_1} - R_{U0} B_{U1} = \frac{\epsilon_0 R_{TD_0} T_{D0}}{\epsilon_1} \left[ R_{U0} Q_{TU_1} - Q_{TD_1} \right] \bar{e}_1,$$  \hfill (D.94)
where $T_{D_0}$ is the apparent temperature in the top homogeneous medium. The brightness temperature emerging from layer 1 may be found from

$$I_{\text{out}} = T_{U0} T_{U1}$$

$$K E_{\text{out}} = \frac{\lambda_0^2}{\lambda_1^2} T_{U0} K E_{U1}$$

$$E_{\text{out}} = T_{U0} \frac{\epsilon_1}{\epsilon_0} (E_{U1} + E_{U1}^P)$$

$$E_{\text{out}} = T_{U0} \frac{\epsilon_1}{\epsilon_0} (\overline{Q}^T_{U1} \overline{c}_1 + E_{U1}^P). \quad (D.95)$$

Top welling may be included by adding

$$\overline{R}_{D0} T_{D0} \quad (D.96)$$

to the right hand side of the expression.

**D.4.4 Intermediate Interfaces**

Just above the $\ell$th interface, we have the relation

$$T_{U\ell}^B = T_{U\ell}^T T_{U,\ell+1}^T + R_{D\ell} T_{U\ell}^B$$

$$E_{U\ell}^B = \frac{\lambda_1^2}{\lambda_{\ell+1}^2} T_{U\ell} E_{U,\ell+1}^T + R_{D\ell} E_{U\ell}^B$$

$$\overline{Q}^B_{U\ell} \overline{c}_\ell + E_{U\ell}^B = \frac{\epsilon_{\ell+1}}{\epsilon_\ell} T_{U\ell} \left( \overline{Q}^T_{U,\ell+1} \overline{c}_{\ell+1} + E_{U,\ell+1}^T \right) + R_{D\ell} \left( \overline{Q}^B_{D\ell} \overline{c}_\ell + E_{D\ell}^B \right)$$

$$\overline{T}_{U\ell}^B - \frac{\epsilon_{\ell+1}}{\epsilon_\ell} T_{U\ell} \overline{T}_{U,\ell+1}^T - R_{D\ell} \overline{E}_{D\ell}^B = \frac{\epsilon_{\ell+1}}{\epsilon_\ell} T_{U\ell} \overline{Q}^T_{U,\ell+1} \overline{c}_{\ell+1} + \left( R_{D\ell} \overline{Q}^B_{D\ell} - \overline{Q}^B_{U\ell} \right) \overline{c}_\ell. \quad (D.97)$$
Below the $\ell$th interface, we have

\[
\Pi_{D,\ell+1}^T = \Pi_{D\ell+1}^B + R_{U\ell} \Pi_{U,\ell+1}^T,
\]

\[
\Xi_{D,\ell+1}^T = \frac{\lambda_{\ell+1}^2}{\lambda_\ell} \Pi_{D\ell}^B + R_{U\ell} \Xi_{U,\ell+1}^T
\]

\[
\left[ Q_{D,\ell+1}^T c_{\ell+1} + \Xi_{D,\ell+1}^T \right] = \frac{\epsilon_{\ell}}{\epsilon_{\ell+1}} \Pi_{D\ell}^B + R_{U\ell} \left[ Q_{U,\ell+1}^T c_{\ell} + \Xi_{U,\ell+1}^T \right]
\]

\[
\Xi_{D,\ell+1}^{TP} - \frac{\epsilon_{\ell}}{\epsilon_{\ell+1}} \Pi_{D\ell}^B - R_{U\ell} \Xi_{U,\ell+1}^{TP} = \frac{\epsilon_{\ell}}{\epsilon_{\ell+1}} \Pi_{D\ell}^B + R_{U\ell} \left[ Q_{U,\ell+1}^T c_{\ell} + \Xi_{U,\ell+1}^T \right] - \left[ Q_{D,\ell+1}^T c_{\ell+1} \right]
\]

(Bottom Interface)

Finally, the bottom interface is governed by the relation

\[
\Pi_{UL}^L = R_{DL} \Pi_{DL}^L + \Pi_{UL}^K \Xi_{L+1}^L,
\]

where $\Xi_{L+1}$ is an apparent brightness of the bottom homogeneous layer. Substitution yields

\[
\Xi_{UL}^L - \frac{\epsilon_{L+1}}{\epsilon_{L}} \Pi_{UL}^L + \Pi_{DL}^L \Xi_{DL}^L = \frac{\epsilon_{L}}{\epsilon_{L+1}} \Pi_{DL}^L + \left( R_{DL} Q_{DL}^L c_{L} + \Xi_{DL}^L \right)
\]

(D.100)

D.4.5 Half-Space Condition

The half-space condition for passive remote sensing is exactly the same as that for active remote sensing, as defined in Section [D.2.1]
D.5 Matrix Equation

The equations for the passive boundary conditions may now be formed into the complete matrix equation

\[
\begin{bmatrix}
\bar{R}_{U0} & \bar{T}_{U1} & 0 & \cdots & 0 \\
\bar{R}_{D1} & \bar{T}_{U1} & & & \\
\bar{T}_{D1} & \bar{R}_{U1} & \bar{T}_{U2} & & \\
& \bar{R}_{D2} & \bar{T}_{U2} & & \\
& & \ddots & \ddots & \\
& & \bar{R}_{D\ell} & \bar{T}_{U\ell} & \\
& & & \bar{T}_{D\ell} & \bar{R}_{U\ell} \\
0 & \bar{R}_{D,L-1} & \bar{T}_{U,L-1} & & \\
& \bar{T}_{D,L-1} & \bar{R}_{U,L-1} & \bar{R}_{D,L} & \\
\end{bmatrix}
\begin{bmatrix}
\bar{c}_1 \\
\bar{c}_2 \\
\bar{c}_3 \\
\vdots \\
\bar{c}_L \\
\end{bmatrix}
= 
\begin{bmatrix}
\bar{F}_D^{BP} - \bar{R}_U \bar{F}_U^{BP} \\
\bar{F}_U^{BP} - \bar{t}_U \bar{F}_U^{BP} - \bar{R}_D \bar{F}_D^{BP} \\
\bar{F}_D^{BP} - \bar{t}_D \bar{F}_D^{BP} - \bar{R}_U \bar{F}_U^{BP} \\
\vdots \\
\bar{F}_U^{BP} - \bar{t}_U \bar{F}_U^{BP} - \bar{R}_D \bar{F}_D^{BP} \\
\bar{F}_D^{BP} - \bar{t}_D \bar{F}_D^{BP} - \bar{R}_U \bar{F}_U^{BP} \\
\end{bmatrix} 
\]

(D.101)

which may be written as

\[ \mathcal{A} \mathcal{C} = \mathcal{F} \]  

(D.102)

and solved with a linear solver.
Appendix E

Computation of Phase Matrices

This appendix outlines methods for the computation of phase matrices as related to this research. Section E.1 describes a method for obtaining a complete phase matrix function from the phase matrix in the plane of incidence for isotropic media. Section E.2 provides expressions for the Rayleigh phase matrix, which is appropriate for spheres that are small compared to the illumination wavelength. Section E.3 provides more complex expressions for the Mie phase matrix, appropriate for spheres of any size. Section E.4 provides a simple method for scaling the phase matrix to account for the effects of dense media.

E.1 Complete Phase Matrix Computation

For isotropic media, the phase matrix is only a function of the angular separation between the incident and scattered intensity in the plane of incidence (POI). Computation of the full phase matrix $\overline{P}(\hat{s}, \hat{s}')$ from the phase matrix in the POI $\overline{P}_{\text{poi}}$ requires computation of the angle between the incident and scattered directions ($\theta$) and the rotation angles ($\phi_1$ and $\phi_2$) that align the global (incident/scattered) and local (POI) coordinate systems. Figure E.1 depicts the global and local (POI) coordinate systems.
Figure E.1: Global and local plane-of-incidence coordinate systems. The figure shows the case for $\phi_s = 0$.

The global coordinate systems for the incident and scattered intensity consist of the vectors $(\hat{v}, \hat{h}, \hat{k})$ and are defined as

\[
\begin{align*}
\hat{k}_i &= \sin \theta_i \hat{x} + \cos \theta_i \hat{z} \\
\hat{v}_i &= \cos \theta_i \hat{x} - \sin \theta_i \hat{z} \\
\hat{h}_i &= \hat{y} 
\end{align*}
\]  
\tag{E.1}

and

\[
\begin{align*}
\hat{k}_s &= \sin \theta_s \cos \phi_s \hat{x} + \sin \theta_s \sin \phi_s \hat{y} + \cos \theta_s \hat{z} \\
\hat{v}_s &= \cos \theta_s \cos \phi_s \hat{x} + \cos \theta_s \sin \phi_s \hat{y} - \sin \theta_s \hat{z} \\
\hat{h}_s &= -\sin \phi_s \hat{x} + \cos \phi_s \hat{y}, 
\end{align*}
\]  
\tag{E.2}
where \( \phi_i \) has been chosen to be 0 for simplicity. The plane of incidence is defined by the normal vector \( \hat{n} \) which is given by

\[
\hat{n} = \frac{1}{\alpha} [\hat{k}_i \times \hat{k}_s], \tag{E.3}
\]

and the angular separation of incident and scattered vectors in the plane of incidence is obtained from \( \cos \theta = \hat{k}_i \cdot \hat{k}_s \). \( \alpha \) is the scalar required to make \( \hat{n} \) a unit vector, or \( \alpha = |\sin \theta| \).

First, we consider the case where \( |\sin \theta| \) is nonzero, and therefore \( \hat{n} \) is uniquely defined. Figure [E.2] depicts how the angle \( \phi \) must be computed to align the vertical and horizontal components of the global and local coordinate systems.

![Figure E.2: Rotation of coordinate systems for phase matrix](image)

The Stokes rotation matrix \( \overline{L}(\phi) \) rotates a Stokes vector \( \vec{I} \) by the prescribed angle and is given by \[37\]

\[
\overline{L} = \begin{bmatrix}
\cos^2 \phi & \sin^2 \phi & \frac{1}{2} \sin 2\phi & 0 \\
\sin^2 \phi & \cos^2 \phi & -\frac{1}{2} \sin 2\phi & 0 \\
-\sin 2\phi & \sin 2\phi & \cos 2\phi & 0 \\
0 & 0 & 0 & 1
\end{bmatrix} \tag{E.4}
\]
The global phase matrix for each angle of separation is given by

\[ \mathbf{\overline{P}} = \mathbf{L}(\phi_2)\mathbf{\overline{P}}_{\text{poi}} \mathbf{L}(\phi_1), \]  

(E.5)

where \( \phi_1 \) is the angle required to rotate the global incident coordinate system to the local POI coordinate system and \( \phi_2 \) is the angle required to rotate the local POI coordinate system to the global scattered coordinate system. Sometimes, this expression is written with a \(-\phi_2\), but here the sign has been taken into account in the definition of \( \phi_2 \). The angle \( \phi_1 \) is defined by recognizing the fact that

\[ \cos \phi_1 = \hat{h}_i \cdot \hat{h}_\ell \]  

(E.6)

\[ \sin \phi_1 = -\hat{v}_i \cdot \hat{h}_\ell, \]  

(E.7)

and by applying the definitions of the local coordinate vectors, we can write these in terms of global unit vectors only:

\[ \cos \phi_1 = \hat{h}_i \cdot \hat{h}_\ell = -\hat{h}_i \cdot \hat{n} 
\]

\[ = -(\hat{k}_i \times \hat{v}_i) \cdot \hat{n} \]

\[ = -\frac{(\hat{k}_i \times \hat{v}_i) \cdot (\hat{k}_i \times \hat{k}_s)}{|\sin \theta|} \]

\[ = -\frac{(\hat{k}_i \cdot \hat{k}_s)(\hat{v}_i \cdot \hat{k}_s) - (\hat{k}_i \cdot \hat{k}_s)(\hat{v}_i \cdot \hat{k}_i)}{|\sin \theta|} \]

\[ = -\frac{\hat{v}_i \cdot \hat{k}_s}{|\sin \theta|} \]  

(E.8)

\[ \sin \phi_1 = -\hat{v}_i \cdot \hat{h}_\ell = \hat{v}_i \cdot \hat{n} \]

\[ = \frac{\hat{v}_i \cdot (\hat{k}_i \times \hat{k}_s)}{|\sin \theta|} \]

\[ = \frac{(\hat{h}_i \times \hat{k}_i) \cdot (\hat{k}_i \times \hat{k}_s)}{|\sin \theta|} \]

\[ = \frac{(\hat{h}_i \cdot \hat{k}_i)(\hat{k}_i \cdot \hat{k}_s) - (\hat{h}_i \cdot \hat{k}_s)(\hat{k}_i \cdot \hat{k}_i)}{|\sin \theta|} \]

\[ = -\frac{\hat{h}_i \cdot \hat{k}_s}{|\sin \theta|}. \]  

(E.9)
The angle $\phi_2$ is defined in a similar manner. However, in this case the sign of the angle is opposite since we are transforming in the reverse direction:

$$\cos \phi_2 = \hat{h}_s \cdot \hat{h}_\ell = -\hat{h}_s \cdot \hat{n}$$

$$= -\frac{(\hat{k}_s \times \hat{v}_s) \cdot (\hat{k}_i \times \hat{k}_s)}{|\sin \theta|}$$

$$= -\frac{(\hat{k}_s \cdot \hat{k}_i) (\hat{v}_s \cdot \hat{k}_s) - (\hat{k}_s \cdot \hat{s}_s)(\hat{v}_s \cdot \hat{k}_i)}{|\sin \theta|}$$

$$= \frac{\hat{v}_s \cdot \hat{k}_i}{|\sin \theta|}$$

$$\sin \phi_2 = \hat{v}_s \cdot \hat{h}_\ell = -\hat{v}_s \cdot \hat{n}$$

$$= -\frac{(\hat{h}_s \times \hat{k}_s) \cdot (\hat{k}_i \times \hat{k}_s)}{|\sin \theta|}$$

$$= -\frac{(\hat{h}_s \cdot \hat{k}_i)(\hat{k}_s \cdot \hat{k}_s) - (\hat{h}_s \cdot \hat{s}_s)(\hat{k}_s \cdot \hat{k}_i)}{|\sin \theta|}$$

$$= -\frac{\hat{h}_s \cdot \hat{k}_i}{|\sin \theta|}.$$  \hspace{1cm} (E.10)

Finally, we consider the case where $|\sin \theta| = 0$, which corresponds to the incident and scattered directions being parallel or antiparallel. In this case, the plane of incidence is arbitrary. For simplicity, we choose the plane of incidence so that $\hat{v}_\ell = \hat{v}_i$ and $\hat{h}_\ell = \hat{h}_i$, requiring no rotation of the incident Stokes parameters. In this case:

$$\cos \phi_1 = 1$$ \hspace{1cm} (E.12)

$$\sin \phi_1 = 0$$ \hspace{1cm} (E.13)

$$\cos \phi_2 = \hat{h}_i \cdot \hat{h}_s = \cos \phi_s$$ \hspace{1cm} (E.14)

$$\sin \phi_2 = \hat{v}_s \cdot \hat{h}_\ell = \hat{v}_s \cdot \hat{h}_i = \cos \theta_s \sin \phi_s.$$ \hspace{1cm} (E.15)
E.2 Rayleigh Phase Matrix

The Rayleigh model is appropriate for dielectric spheres which are small compared to the illumination wavelength. In this case the phase matrix is given by

\[
\overline{P}(\theta, \phi; \theta', \phi') = \begin{bmatrix}
P_{11} & P_{12} & P_{13} & 0 \\
P_{21} & P_{22} & P_{23} & 0 \\
P_{31} & P_{32} & P_{33} & 0 \\
0 & 0 & 0 & P_{44}
\end{bmatrix}
\]  

(E.16)

with

\[
P_{11} = w [\sin^2 \theta \sin^2 \theta' + 2 \sin \theta \sin \theta' \cos \theta \cos \theta' \cos(\phi - \phi') \\
+ \cos^2 \theta \cos^2 \theta' \cos^2(\phi - \phi')]
\]

\[
P_{12} = w \cos^2 \theta \sin \theta(\phi - \phi')
\]

\[
P_{13} = w [\cos \theta \sin \theta \sin \theta' \sin(\phi - \phi') \\
+ \cos^2 \theta \cos \theta' \sin(\phi - \phi') \cos(\phi - \phi')] 
\]

\[
P_{21} = w \cos^2 \theta' \sin^2(\phi - \phi')
\]

\[
P_{22} = w \cos^2(\phi - \phi')
\]

\[
P_{23} = -w \cos \theta' \sin(\phi - \phi') \cos(\phi - \phi')
\]

\[
P_{31} = w [-2 \sin \theta \sin \theta' \cos \theta' \sin(\phi - \phi') \\
- 2 \cos \theta \cos^2 \theta' \cos(\phi - \phi') \sin(\phi - \phi')] 
\]

\[
P_{32} = 2w \cos \theta \sin(\phi - \phi') \cos(\phi - \phi')
\]

\[
P_{33} = w [\sin \theta \sin \theta' \cos(\phi - \phi') \\
+ \cos \theta \cos \theta' [\cos^2(\phi - \phi') - \sin^2(\phi - \phi')]] 
\]

\[
P_{44} = w [\sin \theta \sin \theta' \cos(\phi - \phi') + \cos \theta \cos \theta'],
\]  

(E.17)

where

\[
w = \frac{3}{8\pi} k_s.
\]  

(E.18)
The scattering and absorption coefficients are given by

\[ k_s = \frac{8\pi}{3} n_0 k^4 a^6 |y|^2 \]
\[ = 2 f k^4 a^3 |y|^2 \tag{E.19} \]
\[ k_a = f k \frac{\epsilon''_s}{\epsilon} \frac{3\epsilon}{\epsilon_s + 2\epsilon}^2, \tag{E.20} \]

where

\[ y = \frac{\epsilon_s - \epsilon}{\epsilon_s + 2\epsilon}, \tag{E.21} \]

and \( a \) is the radius of the scatterers, \( n_0 \) is the number of scatters per unit volume, \( f \) is the fractional volume of scatterers, \( \epsilon \) is the background permittivity, \( \epsilon_s \) is the scatterer permittivity, \( \epsilon''_s \) is the imaginary part of the scatterer permittivity, and \( k \) is the wavenumber in the background. Alternatively, the phase matrix may be computed from the phase matrix in the plane of incidence, given by

\[ \overline{P}_{\text{pol}}(\theta) = w \begin{bmatrix} \cos^2 \theta & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos \theta & 0 \\ 0 & 0 & 0 & \cos \theta \end{bmatrix}. \tag{E.22} \]

### E.3 Mie Phase Matrix

The theory behind Mie scattering is given in [65], and the formulae for computing far-field scattering is given in Appendix C along with information on how to compute the \( S_1 \) and \( S_2 \) field coefficient functions with the MIEV code. Scattering and extinction coefficients are computed from the extinction and scattering efficiencies (\( q_e \) and \( q_s \)) as

\[ k_e = n_0 \pi a^2 q_e \tag{E.23} \]
\[ k_s = n_0 \pi a^2 q_s, \tag{E.24} \]

where \( n_0 = 3f/(4\pi a^3) \) is the number of scatterers per unit volume. The phase matrix in the plane of incidence is computed by consideration of Figure E.3.
Scattered far fields are related to the $S_1$ and $S_2$ functions as

\begin{align*}
E_{1s} &= -jE_{1i}e^{jkr}S_1 \\
E_{2s} &= -jE_{2i}e^{jkr}S_2,
\end{align*}

which allows the scattering matrix to be written as

\[
\overline{F} = \frac{j}{k} \begin{bmatrix} S_2 & 0 \\ 0 & S_1 \end{bmatrix}.
\]

The phase matrix for the single sphere is

\[
\overline{P}_0 = \frac{1}{k^2} \begin{bmatrix} |S_2|^2 & 0 & 0 & 0 \\ 0 & |S_1|^2 & 0 & 0 \\ 0 & 0 & \text{Re} \{S_2S_1^*\} & -\text{Im} \{S_2S_1^*\} \\ 0 & 0 & \text{Im} \{S_2S_1^*\} & \text{Re} \{S_2S_1^*\} \end{bmatrix}.
\]

Finally, the phase matrix for a random medium of dielectric spheres with $n_0$ spheres per unit volume is

\[
\overline{P}_{\text{poi}} = n_0 \overline{P}_0.
\]

### E.4 QCA/QCA-CP Scaled Phase Matrix

For a medium consisting of densely packed spheres, the level of scattering is greatly reduced due to coherent interactions. The quasi-crystalline approximation
without and with coherent potential (QCA/QCA-CP) provide effective propagation constants for propagation in a medium of densely-packed spheres. The method for computing the QCA/QCA-CP effective propagation constants and absorption and scattering coefficients is provided in Appendix F. To use the radiative transfer equations for dense media, we also require a phase matrix which reflects the reduction in scattering. Beginning with the phase matrix \( \overline{P} \) and scattering coefficient \( k_s \) for either Rayleigh or Mie spheres, we perform the scaling

\[
\overline{P}_{\text{qca}} = \frac{k_{\text{qca}}}{k_s} \overline{P}, \tag{E.30}
\]

where \( \overline{P}_{\text{qca}} \) is the new QCA/QCA-CP scaled phase matrix, \( k_{\text{qca}} \) is the QCA/QCA-CP scattering coefficient.
Appendix F

Quasicrystalline Approximation (QCA/QCA-CP)

This appendix provides detail for computing effective propagation constants and the corresponding absorption and scattering coefficients for QCA and QCA-CP. Theory concerning QCA and QCA-CP may be found in [29]. This theory is appropriate for densely-packed, non-penetrating spheres.

F.1 QCA Low-Frequency Solution

Assuming that scatterers are very small compared to the wavelength, a low-frequency solution may be found in closed form, or

$$K^2 = k^2 + \frac{3fk^2y}{1-fy} \left[ 1 + jk^3a^2y \frac{2(1-f)^4}{3(1-fy)(1+2f)^2} \right], \quad (F.1)$$

where

$$y = \frac{\epsilon_s - \epsilon}{\epsilon_s + 2\epsilon}, \quad (F.2)$$

$K$ is the effective propagation constant, $k$ is the propagation constant in the background medium, $f$ is the fractional volume, $a$ is the radius of the spheres, $\epsilon$ is the background permittivity, and $\epsilon_s$ is the scatterer permittivity.
F.2 QCA General Solution

To compute the effective propagation constant for arbitrary frequency, we must find roots ($K$) which satisfy the generalized Lorentz-Lorenz law:

$$X^{(M)}_{\nu} = -2\pi n_0 \sum_{n,p} (2n + 1) \left[ L_p(k, K|b) + M_p(k, K|b) \right]$$

$$\times \left\{ T_n^{(M)} X^{(M)}_1 a(1, n|-1, \nu|p) A(n, \nu, p) + T_n^{(N)} X^{(N)}_1 a(1, n|-1, \nu|p, p-1) B(n, \nu, p) \right\} \quad (F.3)$$

$$X^{(N)}_{\nu} = -2\pi n_0 \sum_{n,p} (2n + 1) \left[ L_p(k, K|b) + M_p(k, K|b) \right]$$

$$\times \left\{ T_n^{(M)} X^{(M)}_1 a(1, n|-1, \nu|p, p-1) B(n, \nu, p) + T_n^{(N)} X^{(N)}_1 a(1, n|-1, \nu|p) A(n, \nu, p) \right\} \quad (F.4)$$

where

$$A(n, \nu, p) = \frac{1}{n(n+1)(2\nu+1)} \left[ 2\nu(\nu+1)(2\nu+1) + (\nu+1)(n+\nu-p)(n+p-\nu+1) \right.$$

$$\left. - \nu(n+\nu+p+2)(\nu+p-n+1) \right]$$

$$B(n, \nu, p) = \frac{1}{n(n+1)} \left[ (n+\nu+p+1)(\nu+p-n)(n+p-\nu)(n+\nu-p+1) \right]^{\frac{1}{2}} \quad (F.5)$$

and $2b = a$. In these relations, the sums form an infinite series with $n \geq 1$ and $\nu \geq 1$. In practice, a finite number of equations are considered, and $\nu \in [1, N]$, yielding $2N$ equations. The basic procedure for finding the roots is

1. Begin with an initial guess for $K$. The low frequency solution is often a good choice.

2. For the fixed value of $K$, form the matrix equation $\overline{A} \mathbf{X} = \mathbf{0}$.

3. Compute the determinant of $\overline{A}$, which ideally should be zero.

4. Compute a correction to $K$ according to the optimization or root-finding technique and return to step 2.

Although conceptually simple, the theory involves many auxiliary relations and functions which are explained in the following sections.
F.2.1 T-Matrix Coefficients for Spheres

The T-matrix coefficients for spheres are given as

\[ T_n^{(M)} = \frac{j_n(k_s a)[kaj_n(ka)'][j_n(k_s a)j_n(ka)'] - j_n(k_s a)[kah_n(ka)'][h_n(ka)[k_s a]j_n(ka)']} {j_n(k_s a)[kah_n(ka)'][h_n(ka)[k_s a]j_n(ka)']} \]

\[ T_n^{(N)} = \frac{[k_s^2 a^2 j_n(k_s a)][kaj_n(ka)'][j_n(k_s a)j_n(ka)'] - [k_s^2 a^2 j_n(k_s a)][k_s a]j_n(ka)'} {[k_s^2 a^2 j_n(k_s a)][kah_n(ka)'][h_n(ka)[k_s a]j_n(ka)']} \] (F.6)

where \( k_s \) is the propagation constant in the scatterer material, and \( j_n(·) \) and \( h_n(·) \) are the spherical Bessel and Hankel functions.

F.2.2 L and M Functions

\[ L_p(k, K|\rho) = -\frac{b^2}{K^2 - k^2} \left[ kh_p'(kb)j_p(Kb) - Kh_p(kb)j_p'(Kb) \right] \] (F.7)

and

\[ M_p(k, K|\rho) = \int_b^\infty dr \frac{r^2}{2} \left[ g(r) - 1 \right] h_p(kr)j_p(Kr), \] (F.8)

where \( g(r) \) is the pairwise distribution function. Generally, the Percus-Yevick pairwise distribution function is used. \( M_p \) is evaluated using numerical integration. If we make the substitutions \( y = \rho b \) and \( 2b = a \) into (F.8), we obtain

\[ M_p(k, K|\rho) = 8a^3 \int_1^\infty dx \frac{x^2}{2} \left[ g(x) - 1 \right] h_p(2kax)j_p(2Kax). \] (F.9)

In practice, the integrand decays rapidly, and the upper infinite limit may be replaced with a finite point (5 was used in this research).

F.2.3 Percus-Yevick Pairwise Distribution Function

Pairwise distribution functions define a potential which varies with the distance between two particles. The Percus-Yevick pairwise distribution for hard spheres \([68, 69]\) is

\[ g(x) = \sum_{n=1}^\infty g_n(x) \]

\[ g_n(x) = \frac{(-1)^{n+1}}{12 \cdot 2\pi j f x} \int_{\delta-j\infty}^{\delta+j\infty} dt e^{t(x-n)} \left( \frac{L(t)}{S(t)} \right)^n. \] (F.10)
We note that \( g(x) = 0 \) for the special case of \( x < 1 \), representing penetrating particles. Also, \( g_n(x) = 0 \) for \( x < n \), meaning the summation need extend no farther than \( x \).

The integral in \((F.10)\) is an inverse Laplace transform, and is evaluated by summing the residues associated with the three roots of \( S(t) \). \( L(t) \) and \( S(t) \) are defined as

\[
L(t) = 12f \left[ \left(1 + \frac{f}{2}\right)t + (1 + 2f) \right]
\]

\[
S(t) = (1 - f)^2 t^3 + 6f(1 - f)t^2 + 18f^2 t - 12f(1 + 2f).
\] \( (F.11) \)

The roots of \( S(t) \) are found as

\[
t_1 = \frac{1}{f - 1} \left[ (2\alpha)^{1/3} - \frac{2^{2/3}f^2}{\alpha^{1/3}} + 2f \right]
\]

\[
t_2 = \frac{1}{2(f - 1)} \left[ -(2\alpha)^{1/3} + \frac{2^{2/3}f^2}{\alpha^{1/3}} + 2f + j\sqrt{3} \left\{ (2\alpha)^{1/3} + \frac{2^{2/3}f^2}{\alpha^{1/3}} \right\} \right]
\]

\[
t_3 = \frac{1}{2(f - 1)} \left[ -(2\alpha)^{1/3} + \frac{2^{2/3}f^2}{\alpha^{1/3}} + 2f - j\sqrt{3} \left\{ (2\alpha)^{1/3} + \frac{2^{2/3}f^2}{\alpha^{1/3}} \right\} \right]
\] \( (F.12) \)

with

\[
\alpha = f \left[ f^2 - 3f - 3 + \sqrt{3}\sqrt{f^4 - 2f^3 + f^2 + 6f + 3} \right],
\] \( (F.13) \)

and \( S(t) \) is expressed as

\[
S(t) = (1 - 2f + f^2)(t - t_1)(t - t_2)(t - t_3).
\] \( (F.14) \)

Next, we consider the complex integration in \((F.10)\) as depicted in Figure \( \text{F.1} \). To compute the integral, we choose \( \delta' \) to be to the right of the three roots. Next, we ensure that one of the integrals at infinity always vanishes. If \( x < n \),

\[
e^{i(x-n)} \to 0 \quad \text{as} \quad t \to \infty.
\] \( (F.15) \)

Also, since the contour integration \((C_1,C_{R1})\) encloses no roots, the complex integration must be zero and we have

\[
\int_{C_1} + \int_{C_{R1}} = 0
\]

\[
\int_{C_1} = 0
\] \( (F.16) \)
Figure F.1: Complex integration for the Percus-Yevick pair distribution function

For the case where $x \geq n$, we let 
\[ t = Re^{j\phi} \quad dt = jRe^{j\phi}d\phi \quad c = x - n. \] (F.17)

The integration on contour $C_{R2}$ is
\[
\int_{C_{R2}} = \lim_{R \to \infty} \int_{\phi = \frac{\pi}{2}}^{\frac{3\pi}{2}} d\phi \ jRe^{j\phi}Re^{j\phi}e^{Re^{j\phi}c} \left[ \frac{L(t)}{S(t)} \right]^n
\]
\[
= \lim_{R \to \infty} \int_{\phi = \frac{\pi}{2}}^{\frac{3\pi}{2}} d\phi \ jR^2e^{j2\phi}e^{Re^{j\phi}c} \left[ \frac{L(t)}{S(t)} \right]^n \] (F.18)

\[
A = jR^2[\cos(2\phi) + j \sin(2\phi)] \exp \left\{ Rc[\cos \phi + j \sin \phi] \right\}
\]
\[
= jR^2 \left\{ \cos(2\phi) + j \sin(2\phi) \right\} \exp \left\{ Rc[\cos \phi] \right\} [\cos(Rc \sin \phi) + j \sin(Rc \sin \phi)] .
\]

\[
\text{bounded} \quad \text{bounded}
\]
\[
\to 0 \quad \text{for} \quad \frac{\pi}{2} \leq \phi \leq \frac{3\pi}{2}
\]

Thus, in this case, the integral on $C_{R2}$ is 0, which implies that
\[
\int_{C_1} = g_n(x) = 2\pi j \sum_{i=1}^{3} \text{res}(t_i). \] (F.20)

The residues are found according to the equation
\[
\text{res}(t_i) = \frac{1}{(n - 1)!} \lim_{t \to t_i} \left\{ \frac{d^{n-1}}{dt^{n-1}} (t-t_i)^n f(t) \right\} , \] (F.21)
where
\[ f(t) = \frac{(-1)^{n+1}}{12 \cdot 2\pi j f x} \left\{ t e^{t(x-n)} \left[ \frac{L(t)}{S(t)} \right]^n \right\}. \]  
\( \text{(F.22)} \)

Therefore, we need to be able to symbolically find the \( n \)th order derivative of
\[ \frac{d^{n-1}}{dt^{n-1}} \left\{ t e^{t(x-n)} \left[ \frac{L(t)}{S(t)} \right]^n (t - t_i)^n \right\}. \]  
\( \text{(F.23)} \)

Symbolic differentiation is accomplished by defining operators for the extended product rule, differentiation of the \( t \exp(ct) \) term, and polynomial differentiation. The extended product rule operator gives the \( n \)th derivative of the product of \( fg \) in terms of derivatives of \( f \) and \( g \) alone, or
\[
[f g]^{(0)} = f g \\
[f g]^{(1)} = f' g + f g' \\
[f g]^{(2)} = f'' g + 2 f' g' + f g'' \\
[f g]^{(n)} = \sum_{k=0}^{n} \binom{n}{k} f^{(n-k)} g^{(k)}. \]  
\( \text{(F.24)} \)

We also require the \( n \)th derivative of the function \( f = t \exp(ct) \), or
\[
f^{(0)} = t e^{ct} \\
f^{(1)} = e^{ct} [tc + 1] \\
f^{(2)} = e^{ct} [tc^2 + 2c] \\
f^{(3)} = e^{ct} [tc^3 + 3c^2] \\
f^{(n)} = e^{ct} [tc^n + nc^{n-1}], \quad n > 0. \]  
\( \text{(F.25)} \)

Symbolic polynomial differentiation is trivial. With these basic operations in hand, the derivative may be evaluated using the following steps:

1. For each root, the polynomial \( F(t) = S(t)/(t - t_i) \) is formed from \( \text{[F.14]} \) by just removing the appropriate root from the expression.

2. Compute the 0 to \((n - 1)\)th derivatives of \([L(t)/F(t)]^n\) as follows:

   A. Let \( N(t) = [L(t)]^n \) and \( D(t) = [F(t)]^n \) where the \((\cdot)^n\) is performed by applying symbolic polynomial multiplication \( n \) times.
B. Compute the $n$th derivative of $N(t)/D(t)$ by applying the quotient rule $n$ times. This is accomplished by beginning with
\[
N(t) = N(t), \quad \text{and} \quad D(t) = D(t).
\] (F.26)

For each application of the product rule, we have
\[
N(t) \Leftarrow D(t)N'(t) - N(t)D'(t)
\]
\[
D(t) \Leftarrow [D(t)]^2.
\]

C. Evaluate the resulting expression at the given root.

3. Compute the $0$ to $(n - 1)$th derivatives of $t \exp(\ct)$ according to (F.25) and evaluate at the given root.

4. Combine the results from steps 2 and 3 using the expression for the extended product rule in (F.24). Note that this step only requires manipulating the numerical (not symbolic) results of 2 and 3.

F.2.4 Multiple Scattering Equations

The multiple scattering equations are given by
\[
a(m, n|\mu, \nu|p) = (-1)^{m+\mu}(2p + 1) \left[ \frac{(n + m)!\nu!(p - m - \mu)!}{(n - m)!\nu!(p + m + \mu)!} \right]^{\frac{1}{2}} \times \binom{n \nu p}{m \mu -(m + \mu)} \binom{n \nu p}{0 \ 0 \ 0},
\] (F.27)

where the function is nonzero only for
\[
n \geq |m| \quad \nu \geq |\mu| \quad |n - \nu| \leq p \leq n + \nu.
\] (F.28)

Also, we have
\[
a(m, n|\mu, \nu|p, q) = (-1)^{m+\mu}(2p + 1) \left[ \frac{(n + m)!\nu!(p - m - \mu)!}{(n - m)!\nu!(p + m + \mu)!} \right]^{\frac{1}{2}} \times \binom{n \nu p}{m \mu -(m + \mu)} \binom{n \nu q}{0 \ 0 \ 0},
\] (F.29)
where the function is nonzero only for

\[ n \geq |m| \quad \nu \geq |\mu| \quad |n - \nu| \leq q \leq n + \nu. \] (F.30)

Note that the constraints (F.28) and (F.30) set the limits on the summation indices in the original system of equations given in (F.3), which are

\[ n \geq 1 \quad \nu \geq 1 \quad |n - \nu| + 1 \leq p \leq n + \nu. \] (F.31)

The functions

\[
\begin{pmatrix}
    j_1 & j_2 & j_3 \\
    m_1 & m_2 & m_3
\end{pmatrix}
\] (F.32)

are the Wigner 3j symbols [70] tables of which appear in [71]. In this research, the DRC3JM function written by R. G. Gordon and K. Schulten was used to compute the Wigner 3j symbols [72]. Note that the Wigner 3j symbols are only nonzero for

\[ |m_i| \leq j_i, \quad i = 1, 2, 3 \]
\[ |j_1 - j_2| \leq j_3 \leq j_1 + j_2. \] (F.33)

### F.3 QCA-CP Low Frequency Solution

The quasicrystalline approximation with coherent potential (QCA-CP) only has a general solution in the low frequency limit, which is given by

\[
K^2 = k^2 + \frac{f(k_s^2 - k^2)}{1 + \frac{k_s^2 - k^2}{3K^2}(1 - f)} \left\{ 1 + j \frac{2(k_s^2 - k^2)Ka^3(1 - f)^4}{9 \left[ 1 + \frac{k_s^2 - k^2}{3K^2}(1 - f) \right] (1 + 2f)^2} \right\}, \] (F.34)

where \( k \) is the propagation constant in the background, \( k_s \) is the propagation constant in the scatterer, \( f \) is the fractional volume of scatterers, \( a \) is the radius of the scatterers, and \( K \) is the effective propagation constant. Note that (F.34) has \( K \) on both sides of the equation and can be manipulated into an expression of the form

\[ a_6K^6 + a_5K^5 + a_4K^4 + a_2K^2 + a_0 = 0 \] (F.35)

whose roots may be found numerically. The root with the positive nonzero real part gives the desired effective propagation constant in the scattering medium.
F.4 Computation of Extinction Coefficients and Effective Permittivity

This section explains how to convert effective propagation constants into quantities required by the radiative transfer code: absorption coefficient, scattering coefficient, and effective permittivity.

Assuming possibly lossy spheres with relative permittivity

$$\epsilon_r = \epsilon'_r + j\epsilon''_r$$  \hspace{1cm} (F.36)

suspended in free space, we compute the effective propagation in the presence of absorption and scattering as

$$K_1 = \text{eff}_\text{prop}(\epsilon'_r + j\epsilon''_r)$$ \hspace{1cm} (F.37)

and the effective propagation in the presence of scattering only as

$$K_2 = \text{eff}_\text{prop}(\epsilon'_r),$$ \hspace{1cm} (F.38)

where $\text{eff}_\text{prop}(\epsilon_r)$ returns an effective propagation constant (either QCA or QCA-CP) given a scatterer relative permittivity of $\epsilon_r$. The imaginary part of the effective propagation constants $K_1$ and $K_2$ represents loss. For $K_1$ the loss is due to both absorption and scattering, and for $K_2$ the loss is due to scattering only. Thus, we can compute the extinction and scattering coefficients as

$$k_e = 2\text{Im}\{K_1\}$$ \hspace{1cm} (F.39)

$$k_s = 2\text{Im}\{K_2\}$$ \hspace{1cm} (F.40)

and the absorption coefficient as

$$k_a = k_e - k_s.$$ \hspace{1cm} (F.41)

The effective permittivity of the medium can be defined as

$$\epsilon_{eff} = \frac{K_1^2}{\omega \mu}.$$ \hspace{1cm} (F.42)
Appendix G

The Multivariate Complex Normal Distribution

The multivariate complex normal distribution describes the statistics of a random vector containing complex normal elements with the proper covariance relationship. This distribution is fundamental to the study of many MIMO channel analyses, since the elements of a stacked channel matrix may be represented as a complex normal random vector. Section G.1 provides a convenient definition of the distribution. Section G.2 gives closed-form expressions of the marginal PDFs for joint pairwise magnitude and differential phase. Section G.3 defines the covariance matrix appropriate for channel modeling and defines separability and shift-invariance. Section G.4 provides details for generating multivariate complex normal vectors on a computer. Finally, section G.5 describes two methods for specifying the covariance matrix appropriate for channel modeling.

G.1 Definition

The joint multivariate complex normal distribution may be defined as

\[
f(\mathbf{x}) = \frac{1}{\pi^N |\mathbf{R}|} \exp\left[-(\mathbf{x} - \mathbf{\mu})^H \mathbf{R}^{-1} (\mathbf{x} - \mathbf{\mu})\right],
\]

(G.1)

where \( \mathbf{R} \) is the covariance matrix, \( N \) is the dimensionality of \( \mathbf{R} \), and \( \mathbf{\mu} \) is the mean of \( \mathbf{x} \). The pairwise joint PDF \( f(x_m, x_n) \) is given as (G.1) with \( \mathbf{R} \) replaced by the covariance submatrix \( \mathbf{\overline{R}} \), or

\[
\mathbf{\overline{R}} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{R}_{21} & \mathbf{R}_{22} \end{bmatrix} = \begin{bmatrix} R_{mm} & R_{mn} \\ R_{nm}^* & R_{nn} \end{bmatrix},
\]

(G.2)
where identical marginal distributions have been assumed for the two elements \((R_{mm} = R_{nn})\).

**G.2 Pairwise PDFs**

For a zero-mean bivariate complex normal distribution \((\mu = 0)\) with covariation matrix \(\bar{R}\) and identically distributed elements, the joint PDF is

\[
f(x_1, x_2) = \frac{1}{\pi^2 \Delta} \exp \left[ -\frac{(|x_1|^2 + |x_2|^2)R_{11} - 2\Re \{x_1^* x_2 R_{12}\}}{\Delta} \right],
\]

where

\[
\Delta = R_{11}^2 - |R_{12}|^2.
\]

We are interested in obtaining the marginal joint magnitude \(f(|x_1|, |x_2|)\) and differential phase \(f(\arg[x_2/x_1])\) distributions to allow easier visualization of the PDFs. The complex variables \(x_1\) and \(x_2\) may be written as

\[
x_1 = r_1 \exp(j\phi_1)
\]
\[
x_2 = r_2 \exp(j\phi_2).
\]

Noting the differential relationship

\[
dx_{iR} dx_{iI} = r_i \, dr_i \, d\phi_i,
\]

where \(R\) and \(I\) represent real and imaginary parts, the joint PDF may be expressed as

\[
f(r_1, r_2, \phi_1, \phi_2) = \frac{r_1 r_2}{\pi^2 \Delta} \exp \left\{ \frac{1}{\Delta} \left[ -R_{11}(r_1^2 + r_2^2) + 2|R_{12}|r_1 r_2 \cos(\phi_2 - \phi_1 + \theta_{12}) \right] \right\},
\]

where \(\theta_{12} = \arg(R_{12})\). We note that this PDF is only a function of the phase difference \((\phi_1 - \phi_2)\) and not absolute phase. The joint magnitude PDF (similar to the Rayleigh distribution for the univariate case) is obtained by integrating \((G.7)\) over the complete
ranges of \( \phi_1 \) and \( \phi_2 \), or

\[
f(r_1, r_2) = \int_{2\pi} \int_{2\pi} d\phi_1 \, d\phi_2 \, f(r_1, r_2, \phi_1, \phi_2)
\]

\[
= \int_{2\pi} d\phi_1 \, \frac{2r_1r_2}{\pi \Delta} \exp \left[ - \frac{R_{11} (r_1^2 + r_2^2)}{\Delta} \right] J_0 \left( -2j \frac{|R_{12}| r_1 r_2}{\Delta} \right)
\]

\[
= \frac{4r_1r_2}{\Delta} \exp \left[ - \frac{R_{11} (r_1^2 + r_2^2)}{\Delta} \right] J_0 \left( -2j \frac{|R_{12}| r_1 r_2}{\Delta} \right). \quad (G.8)
\]

For large \( r_1 \) and \( r_2 \), the Bessel function with imaginary argument in (G.8) becomes numerically large. In this case, we require an asymptotic form of the integral. To this end, we write

\[
J_0(-j\rho) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dx \, e^{\rho \cos x}, \quad \rho \to \infty. \quad (G.9)
\]

The major contribution to this integral comes from the maximum of \( \cos x \), which occurs at \( x = 0 \). Approximating \( \cos x \) about \( x = 0 \) in a Taylor series gives

\[
\cos x \approx 1 - \frac{1}{2} x^2. \quad (G.10)
\]

Substitution into (G.9) and extending integration limits to \([-\infty, \infty]\) yields

\[
J_0(-j\rho) \approx \frac{\exp(\rho)}{\sqrt{2\pi} \rho}. \quad (G.11)
\]

Thus, the asymptotic form of (G.8) for large \( r_1 r_2 \) is

\[
f(r_1, r_2) = \frac{4r_1r_2}{\Delta} \exp \left[ \frac{1}{\Delta} \left( - \frac{R_{11} (r_1^2 + r_2^2)}{\Delta} + 2 \frac{|R_{12}| r_1 r_2}{\Delta} \right) \right]
\]

\[
\frac{\sqrt{4\pi |R_{12}| r_1 r_2 / \Delta}}, \quad (G.12)
\]

which is valid for

\[
\frac{2|R_{12}| r_1 r_2}{\Delta} > 12. \quad (G.13)
\]

The PDF for pairwise phase difference is found by making the substitution \( \phi_2 = \Delta \phi + \phi_1 \), and integrating over the variables \( r_1, r_2 \), and \( \phi_1 \). The joint phase difference PDF is computed as

\[
f(\Delta \phi) = \int_{0}^{\infty} \int_{0}^{\infty} \int_{2\pi} d\phi_1 dr_1 dr_2 f(r_1, r_2, \phi_1, \Delta \phi), \quad (G.14)
\]

which belongs to a class of integrals of the form

\[
f = \int_{0}^{\infty} \int_{0}^{\infty} dx \, dy \, x \, y \, e^{a(x^2+y^2)+bxy}. \quad (G.15)
\]
Transforming (G.15) to polar coordinates, or

\[ x = r \cos \theta \]  \hspace{1cm} (G.16)

\[ y = r \sin \theta \]  \hspace{1cm} (G.17)

\[ dx \, dy = r \, dr \, d\theta, \]  \hspace{1cm} (G.18)

we can manipulate the integral as

\[
\begin{align*}
 f &= \int_0^\infty r \, dr \int_0^{\pi/2} d\theta \, r^2 \cos \theta \sin \theta \, e^{ar^2 + br^2 \sin \theta \cos \theta} \\
 &= \int_0^{\pi/2} d\theta \, \cos \theta \sin \theta \int_0^\infty dr \, r^3 \, e^{r^2(a+b\sin \theta \cos \theta)}. \tag{G.19}
\end{align*}
\]

A convenient substitution is

\[
\begin{align*}
 -u &= r^2(a + b \sin \theta \cos \theta) \\
 r^2 &= \frac{-u}{a + b \sin \theta \cos \theta} \\
 r \, dr &= \frac{-du}{2(a + b \sin \theta \cos \theta)}, \tag{G.20}
\end{align*}
\]

which transforms the integral (G.19) to

\[
\begin{align*}
 f &= \int_0^{\pi/2} d\theta \, \cos \theta \sin \theta \left( \int_0^\infty du \, \frac{ue^{-u}}{2(a + b \sin \theta \cos \theta)^2} \right) \\
 &= \int_0^{\pi/2} d\theta \, \cos \theta \sin \theta \left( \int_0^\infty du \, \frac{ue^{-u}}{2(a + b \sin \theta \cos \theta)^2} \right) \\
 &= 1, \tag{G.21}
\end{align*}
\]

where we require that \((a + b \sin \theta \cos \theta) < 0\). The remaining integral over \(\theta\) is even symmetric about \(\pi/4\) and may be rewritten as

\[
\int_0^{\pi/2} d\theta \, \frac{\cos \theta \sin \theta}{(a + b \sin \theta \cos \theta)^2} = \chi^{-1} + \frac{2b}{\chi^2} \left[ \tan^{-1} \left( \frac{b}{\chi} \right) - \tan^{-1} \left( \frac{2a + b}{\chi^2} \right) \right], \tag{G.22}
\]

where

\[ \chi = 4a^2 - b^2. \tag{G.23} \]

In terms of equation (G.14), we have

\[ f(\Delta \phi, \phi_1) = \frac{1}{\pi^2 \Delta} f, \tag{G.24} \]
where
\[ \chi = 4a^2 - b^2 \]
\[ a = -R_{11}/\Delta \]
\[ b = (2|R_{12}|/\Delta) \cos(\Delta \phi + \text{arg}\{R_{12}\}). \] (G.25)

Integrating over the uniformly-distributed variable \( \phi_1 \) gives
\[ f(\Delta \phi) = \frac{\chi^{1/2} + 2b \left[ \tan^{-1} \left( \frac{b}{\chi^{1/2}} \right) - \tan^{-1} \left( \frac{2a+b}{\chi^{1/2}} \right) \right]}{\left( \pi \Delta / 2 \right) \chi^{3/2}}. \] (G.26)

G.3 Covariance Matrices and Simplifying Assumptions

The zero mean multivariate complex normal distribution is completely characterized by the covariance matrix \( \overline{R} \). For the purpose of modeling the channel matrix \( \overline{H} \), the \((N_T N_R) \times (N_T N_R)\) covariance matrix is defined as
\[ R_{ij,k\ell} = \mathbb{E} \{ H_{ij} H_{k\ell}^* \}, \] (G.27)
where \(i\) and \(j\) combine to form a row index of \( \overline{R} \) and \(k\) and \(\ell\) combine to form a column index of \( \overline{R} \).

A number of assumptions are convenient when working with the covariance matrix. Separability assumes that the full covariance matrix may be written as a product of transmit covariance \((\overline{R}_T)\) and receive covariance \((\overline{R}_R)\) or
\[ R_{ij,k\ell} = R_{R,ik} R_{T,j\ell}. \] (G.28)

For such channels, the transmit and receive covariance matrices can be computed from the full covariance matrix as
\[ R_{T,ij} = \frac{1}{\alpha} \sum_{k=1}^{N_R} R_{ki,kj}, \] (G.29)
\[ R_{R,ij} = \frac{1}{\beta} \sum_{k=1}^{N_T} R_{ik,jk}, \] (G.30)
where \(\alpha\) and \(\beta\) are chosen such that
\[ \alpha \beta = \sum_{k_1=1}^{N_R} \sum_{k_2=1}^{N_T} R_{k_1,k_2,k_1k_2}. \] (G.31)
In the case where $\overline{R}$ is a correlation coefficient matrix, we may choose $\alpha = N_R$ and $\beta = N_T$. Separability makes implications about the statistical independence of multipath fading due to transmit location and receive position and orientation.

*Shift-invariance* assumes that the covariance matrix is only a function of antenna separation and not absolute antenna location. The relationship between the full covariance and shift-invariant covariance ($R^S$) is

$$R_{ij,k\ell} = R^S_{i-k,j-l}.$$  \hspace{1cm} (G.32)

The combination of separability and shift-invariance allows full covariance matrices to be generated from existing correlation functions, which relate correlation to receive element displacement. For example, we may use Jakes’ model to obtain

$$R_{ij,k\ell} = J_0 \left[ 2\pi \| \overline{x}_i^R - \overline{x}_k^R \| \right] J_0 \left[ 2\pi \| \overline{x}_j^T - \overline{x}_\ell^T \| \right],$$  \hspace{1cm} (G.33)

where $\overline{x}_i^{(T,R)}$ is the vectorial location of the $i$th transmit or receive antenna in wavelengths, and $\| \cdot \|$ is the vector norm.

### G.4 Computer Generation

Computer generation of zero mean complex normal vectors for a specified covariance matrix $\overline{R}$ is performed by generating vectors of i.i.d. complex normal elements with unit variance ($\overline{\alpha}$). The transformation

$$\overline{y} = \overline{\Sigma} \overline{\Lambda}^{1/2} \overline{\alpha}$$  \hspace{1cm} (G.34)

produces a new complex normal vector with the proper covariance, where $\overline{\Sigma}$ and $\overline{\Lambda}$ are the matrix of eigenvectors and the diagonal matrix of eigenvalues of $\overline{R}$, respectively.

### G.5 Joint Complex Normal Models

The multivariate complex normal distribution can be used to model the channel matrix directly by simply specifying the channel element covariance matrix. The wealth of correlation information provided by antenna diversity studies makes
this approach particularly attractive. This section provides two methods for specifying the covariance matrix: the complex correlation method and the power correlation method.

G.5.1 Complex Correlation Method

This method assumes that the underlying distribution on $\overline{H}$ is multivariate complex normal and specifies a covariance matrix ($\overline{R}$) as

$$
\overline{R} = E \{ \overline{h} \, \overline{h}^H \}, \tag{G.35}
$$

where $\overline{h}$ is a stacked channel matrix. Once the channel covariance matrix is known, the method in Section G.4 may be used to generate channel matrices ($\overline{H}$).

G.5.2 Power Correlation Method

In this method, the covariance matrix is derived from the power covariance matrix given as

$$
R_{ij,kl}^P = E \{ |H_{ij}|^2 |H_{kl}|^2 \} - E \{ |H_{ij}|^2 \} \, E \{ |H_{kl}|^2 \}. \tag{G.36}
$$

The same power covariance behavior can be generated using a zero mean multivariate complex normal distribution with covariance matrix $\overline{R} = (\overline{R}^P)^{1/2}$, where $(\cdot)^{1/2}$ is element-wise square root. However, care is required since the root of the power covariance matrix is not necessarily positive definite. Under such circumstances, the method outlined in Section G.4 cannot be used directly. An interesting feature of this method is that the phases of the $\overline{R}$ are arbitrary. By properly phasing the rows and columns of $\overline{R}$, the mean AOA and AOD may be arbitrarily specified.
Appendix H

MIMO Channel Normalization

Obtaining a good statistical sample of MIMO channels requires collecting data in a variety of scenarios. Large movement in transmit and receive location leads to substantial change in the bulk path loss of propagating signals. Effects of path loss can easily overshadow interesting channel behavior such as spatial correlation of transmit and receive signals. One way to remove this effect from collected data is to normalize the channel matrices. There are two simple criteria for channel normalization: fixed average SISO SNR and fixed average receive SNR.

For both normalizations, the equation for the narrowband received signal vector is given as

\[ y = \overline{H} \, x + \eta, \]  

(H.1)

where \( y \) is the vector of received baseband signals, \( \overline{H} \) is the \( N_R \times N_T \) channel matrix, \( x \) is the transmit baseband vector, and \( \eta \) is additive i.i.d. white Gaussian noise with single element variance \( \sigma^2_\eta \). The following sections define the two normalization criteria.

H.1 Fixed Average SISO SNR

A simple criterion for fixing SNR, which is independent of the transmitted signals, sets an average SNR over all single-input single-output (SISO) channels, assuming for each case that all available transmit power is sent to that channel. Specifically,

\[ \text{SNR} = \frac{P_T}{\sigma^2_\eta} \frac{1}{N_T N_R} \sum_{ij} |H_{ij}|^2, \]  

(H.2)
and the receiver noise is therefore equal to

$$\sigma^2_\eta = \frac{P_T}{\text{SNR} N_T N_R} \| \mathbf{F} \|^2_F,$$

where $\| \cdot \|_F$ is the Frobenius norm. Often, it is convenient to normalize the channel matrix $\mathbf{F}$ to obtain a new channel matrix $\mathbf{F}_N$, or

$$\mathbf{F}_N = \frac{\sqrt{N_R N_T}}{\| \mathbf{F} \|_F} \mathbf{F}, \quad (H.4)$$

which forces unit average SISO gain. If the normalized channel matrix is now used, the receiver noise is simply

$$\sigma^2_\eta = \frac{P_T}{\text{SNR}}. \quad (H.5)$$

Sometimes, a more realistic analysis is possible by normalizing a whole data set, rather than the individual channel matrices which make up the set. In this case, the normalization is extended to cover a set of $K$ channel matrices, or

$$\mathbf{F}_N = \frac{\sqrt{N_R N_T K}}{\| \mathbf{F} \|_F} \mathbf{F}, \quad (H.6)$$

where

$$\mathbf{F} = \begin{bmatrix} \mathbf{F}_1 & \mathbf{F}_2 & \ldots & \mathbf{F}_K \end{bmatrix}. \quad (H.7)$$

In this case, the power relationship between the channel matrices is preserved.

**H.2 Fixed Average Receive SNR**

The average receive SNR may be written as

$$\text{SNR} = \frac{\mathbb{E}\{|y_i|^2\}}{\mathbb{E}\{|\eta_i|^2\}} = \frac{\mathbb{E}\left\{ \left| \{\mathbf{F}^H \mathbf{F} \} \right|_i \right\}^2}{\mathbb{E}\{|\eta_i|^2\}}$$

$$= \frac{1}{N_R} \sum_i \mathbb{E}\left\{ \left[ \mathbf{F}^H \mathbf{F} \right]_{ii} \right\} \frac{\sigma^2_\eta}{\sigma^2_\eta}$$

$$= \frac{1}{N_R} \sum_i \left( \mathbf{F}^H \mathbb{E}\{\mathbf{F} \mathbf{F}^H\} \mathbf{F}^H \right)_{ii} \frac{\sigma^2_\eta}{\sigma^2_\eta}. \quad (H.8)$$

For arbitrary transmit streams, the receiver noise must be fixed at

$$\sigma^2_\eta = \frac{1}{N_R \text{SNR}} \left( \mathbf{F}^H \mathbb{E}\{\mathbf{F}^H \mathbf{F} \} \mathbf{F}^H \right)_{ii}. \quad (H.9)$$
If the transmit streams are uncorrelated and power is distributed evenly across the transmitters, we have

\[ E \{ \pi \pi^H \} = \frac{\bar{T} P_T}{N_T}, \]  

(H.10)

and the noise variance becomes

\[ \sigma^2 = \frac{P_T}{\text{SNR} \ N_R N_T} \sum_i (\bar{H} \bar{H}^H)_{ii} \]

\[ = \frac{P_T}{\text{SNR} \ N_R N_T} \| \bar{H} \|^2_F, \]  

(H.11)

which is identical to the expression for fixed average SISO SNR.
Appendix I

MIMO Channel Capacity Computation

This appendix presents expressions for the Shannon capacity of the narrowband MIMO channel for two important cases:

1. Both transmitter and receiver have perfect channel knowledge (informed transmit and receive)

2. Only the receiver knows the channel (uninformed transmitter)

The relationship between the baseband receive signal vector $\mathbf{y}$ and the narrowband transmit signal vector $\mathbf{x}$ is

$$\mathbf{y} = H \mathbf{x} + \eta,$$

(I.1)

where $H$ is the $N_R \times N_T$ channel matrix and $\eta$ is additive i.i.d. white Gaussian noise with single element variance $\sigma_\eta^2$. The two types of capacity are considered in the sections that follow.

I.1 Informed Transmit and Receive

The problem of the general MIMO channel may be cast into the parallel Gaussian channel framework by applying the singular value decomposition (SVD) to the channel matrix. The SVD of the channel matrix is

$$H = UV^H,$$

(I.2)
where $\overline{U}$ and $\overline{V}$ are the unitary matrices of left and right singular vectors, and $\overline{S}$ is the diagonal matrix of singular values. We may now write (I.1) as

$$y = \overline{U} \overline{S} \overline{V}^H x + \eta$$

which may be interpreted as sending the new transmit vector $\overline{x}'$ through a set parallel non-interfering channels and receiving the new receive vector $\overline{y}'$, or

$$y'_i = \lambda_i x'_i + \eta_i, \quad \lambda_i = S_{ii},$$

where the invariance of noise to the unitary transformation was used, or

$$\mathbb{E}\{\eta' \eta'^H\} = \overline{U}^H \mathbb{E}\{\eta \eta^H\} \overline{U} = \overline{U}^H \overline{U} (\sigma^2 \eta^2 I) = \sigma^2 \eta^2 I. \quad (I.5)$$

In this hypothetical scheme, the transmitter and receiver cooperate to synthetically form the parallel channels. Specifically, the transmitter must transform the arbitrary transmit vector $\overline{x}$ to obtain $\overline{x}'$, and the receiver must transform $\overline{y}$ to obtain $\overline{y}'$. Given a total transmit power of $P_T$, capacity is attained for parallel Gaussian channels when the transmitted signals $x'_i$ (and therefore the $y'_i$ as well) are independent Gaussian and the power for $i$th channel is determined by the channel gain ($\lambda_i$) and the water-filling solution [74]:

$$C = \frac{1}{2} \sum_i \log_2 \left( 1 + \frac{P_i}{N_i} \right), \quad (I.6)$$

where

$$N_i = \frac{\sigma^2 \eta}{|\lambda_i|^2}$$

$$P_i = (\nu - N_i)^+$$

$$\sum_i P_i = P_T.$$  

Equation (I.6) is appropriate for a real Gaussian channel. For a fixed noise variance and transmit power, an additional independent dimension doubles capacity, thus the factor of 1/2 should be removed for the complex channel.
One method for determining the water-filling solution forms the matrix equation
\[
\begin{bmatrix}
-1 & 1 \\
-1 & 1 \\
\vdots & \vdots \\
-1 & 1 \\
1 & 1 & \cdots & 1 & 0
\end{bmatrix}
\begin{bmatrix}
P_1 \\
P_2 \\
\vdots \\
P_K \\
\nu
\end{bmatrix}
= 
\begin{bmatrix}
N_1 \\
N_2 \\
\vdots \\
N_K \\
PT
\end{bmatrix},
\] (I.8)
where empty matrix positions are zero, \(\vec{N}\) is the vector of channel noise given by (I.7) sorted from smallest to largest, and \(K\) is initially chosen to be the number of nonzero singular values. If the solution of (I.8) yields any negative \(P_i\), \(K\) is decremented by one (the most noisy channel is removed), and the process is repeated. A valid solution is found when all of the \(P_i\) given by (I.8) are positive. In this case, the capacity is found by substitution of \(N_i\) and \(P_i\) into equation (I.6).

### I.2 Uninformed Transmit Capacity

The transmitter cannot form parallel Gaussian channels if it has no knowledge of the channel matrix, and a different approach is required. The Shannon capacity is the maximum mutual information taken over all possible transmit vectors, or
\[
C = \max_{\vec{x}} \sum_{i} |x_i|^2 = P_T \ I(\vec{x}; \vec{y}),
\] (I.9)
where total transmit power has been fixed to \(P_T\). The expression for mutual information may be expanded in terms of differential entropy \(h(\cdot)\), or
\[
I(\vec{x}; \vec{y}) = h(\vec{y}) - h(\vec{y}|\vec{x}).
\] (I.10)
Looking at the second term, the differential entropy of the receive vector \(\vec{y}\) given that the transmit signal is known will just be the noise, or
\[
h(\vec{y}|\vec{x}) = h(\vec{y}|\vec{x}) = h(\vec{y}) = \sum_i h(\eta_i),
\] (I.11)
where the last equality results from the i.i.d. nature of the noise vector. Therefore, to maximize (I.10), we need to maximize the differential entropy of \(\vec{y}\).
For a random variable of fixed variance, the differential entropy is maximized if the variable is Gaussian distributed. For a random vector, the entropy is maximized for i.i.d. Gaussian elements. If the transmitter generates an i.i.d. Gaussian random vector $\mathbf{x}$ with single element variance $P_T/N_T$, $\mathbf{y}$ will also be joint Gaussian, but in general the elements will be correlated due to the interference in the channel. The correlation matrix $\mathbf{K}$ for the received signal vector is

$$k_{i\ell} = \mathbb{E}\{y_i^* y_{\ell}^*\}$$

$$= \mathbb{E}\left\{\left[\sum_j H_{ij}x_j + \eta_i\right]\left[\sum_k H_{\ell k}^* x_k^* + \eta_{\ell}^*\right]\right\}$$

$$= \sum_j \sum_k H_{ij} H_{\ell k}^* \mathbb{E}\{x_j x_k^*\} + N_i \delta_{i\ell}$$

$$= \sum_j H_{ij} H_{\ell j}^* \mathbb{E}\{|x_j|^2\} + N_i \delta_{i\ell}, \quad (I.12)$$

where $N_i$ is the noise variance at the $i$th receiver. Converting back to matrix notation, we have

$$\mathbf{K} = \frac{P_T}{N_T} \mathbf{H} \mathbf{H}^H + \mathbf{N}, \quad (I.13)$$

since the noise is i.i.d. with single channel noise variance $N$. Differential entropy for complex Gaussian random variables (or vectors) is given by

$$h(\mathbf{y}) = \log_2(\pi e)^{N_R}|\mathbf{K}|, \quad (I.14)$$

where $|\cdot|$ is the determinant, and $N_R$ is the dimensionality of $\mathbf{K}$, which in this case corresponds to the number of receivers. The differential entropy of the i.i.d. Gaussian noise vector is

$$h(\mathbf{\eta}) = \sum_i \log_2(\pi e) N_i$$

$$= \log_2(\pi e)^{N_R} N_i. \quad (I.15)$$
Finally, capacity may be computed from (I.10) as

\[ I(y; x) = \log_2 (\pi e)^{N_{R}} |\tilde{K}| - \log_2 (\pi e)^{N_{R} N_{R}} \]

\[ = \log_2 \left[ \frac{(\pi e)^{N_{R}} |\tilde{K}|}{(\pi e)^{N_{R} N_{R}}} \right] \]

\[ = \log_2 \left[ \frac{|\tilde{K}|}{N_{R}} \right] \]

\[ = \log_2 \left[ N^{-N_{R}} \left| \frac{P_T}{N_T} \tilde{H} \tilde{H}^H + N\tilde{I} \right| \right] \quad (I.16) \]

giving the final result

\[ C = \log_2 \left| \tilde{I} + \frac{P_T}{N_T} \tilde{H} \tilde{H}^H \right|. \quad (I.17) \]

As a final note, this solution may also be obtained by orthogonalizing the channel as in the water-filling solution, but exciting each orthogonal channel with independent Gaussian streams of equal power. This procedure is equivalent to exciting each transmit antenna with equal-power uncorrelated Gaussian streams, a procedure that does not require the transmitter to know the channel.
Appendix J

Approximating Arbitrary Metal Surfaces in FDTD

This appendix outlines an approach for simulating arbitrary metal surfaces in an FDTD simulation with a uniform grid. Generally, metal surfaces in FDTD simulations are drawn to align with the principal axes, and all tangential E-field components on these surfaces are set to zero. The monopole antenna structure analyzed in Section 8.1.2 however, required simulation of cylindrical surfaces. When a metal surface does not naturally align with the FDTD grid, all tangential E-field components which are close to the surface need to be set to zero. To this end, metal surfaces are approximated by drawing a square surface perpendicular to each E-field component in the Yee grid as depicted in Figure J.1. For each such surface intersected by metal,

![Diagram of FDTD approximation of arbitrary metal surfaces](image)

Figure J.1: FDTD approximation of arbitrary metal surfaces. Faces are drawn perpendicular to each surface. All faces cut by the metal surface are considered to lie on a metal surface.
the E-field component is set to zero to simulate a perfect conductor. The method is applied to monopole antenna from Section 8.1.2 as an example. Figure J.2 depicts a top view and side view of the antenna. Solid lines show where the metal surfaces were specified, and the arrows indicate E-field components to be set to zero in the simulation.

Figure J.2: Specified metal surfaces and forced E components for a single monopole antenna. Lines show where the metal surfaces were specified, and the arrows show which field components were considered tangential to the metal surface (and set to zero).
Appendix K

Far Field E-Field Computation with an Infinite Ground Plane

In FDTD modeling of antenna radiation problems, we may wish to model a large antenna ground plane as an infinite conducting sheet. In normal FDTD simulations, radiation is obtained by storing fields on a box enclosing the radiator, and computing the radiation due to equivalent electric and magnetic currents on this box. In the case of the infinite ground plane, a slight modification to this operation is necessary. Consider Figure K.1 which depicts a monopole antenna over an infinite ground plane. In the case of the infinite ground plane, we could replace fields on all of the faces (besides the $z = 0$ face) with equivalent currents and compute the radiated far fields according to Huygens’ principle. However, we require a Green’s function which includes the effect of ground plane. An equivalent problem is obtained by simply replacing the ground plane with image currents on box B. In this case, the

Figure K.1: Geometry for computing the far fields from a radiator over a ground plane. Surface A is a surface enclosing the radiator above the ground plane, and surface B is its mirror image.
usual free-space Green’s function may be used. The relationship between electric \( (\overrightarrow{M}) \) and magnetic \( (\overrightarrow{J}) \) currents on box A and box B is

\[
\begin{align*}
M^A_x(x, y, z) &= M^B_x(x, y, -z) & J^A_x(x, y, z) &= -J^B_x(x, y, -z) \\
M^A_y(x, y, z) &= M^B_y(x, y, -z) & J^A_y(x, y, z) &= -J^B_y(x, y, -z) \\
M^A_z(x, y, z) &= -M^B_z(x, y, -z) & J^A_z(x, y, z) &= J^B_z(x, y, -z).
\end{align*}
\]

(K.1)

The currents are computed from the fields on the box according to

\[
\begin{align*}
\overrightarrow{M} &= -\hat{n} \times \overrightarrow{E} \\
\overrightarrow{J} &= \hat{n} \times \overrightarrow{H},
\end{align*}
\]

(K.2)

where \( \hat{n} \) is the outward normal vector on the surfaces A and B. For simplicity, we first write the far fields as a product of radial and angular parts:

\[
\begin{align*}
E_\theta(r, \theta, \phi) &= -j \frac{k_0 e^{-jk_0 r}}{4\pi r} E_\theta(\theta, \phi) \\
E_\phi(r, \theta, \phi) &= j \frac{k_0 e^{-jk_0 r}}{4\pi r} E_\phi(\theta, \phi).
\end{align*}
\]

(K.3)

The angular parts may be expressed as integrals over the currents on surfaces A and B. The \( E_\theta \) component becomes

\[
E_\theta(\theta, \phi) = E^A_\theta(\theta, \phi) + E^B_\theta(\theta, \phi),
\]

(K.4)

where

\[
E^A_\theta(\theta, \phi) = \int \int_S dS' \left[ -M_x \sin \phi + M_y \cos \phi \\
+ \eta_0 (J_x \cos \theta \cos \phi + J_y \cos \theta \sin \phi - J_z \sin \theta) \right] \\
\times \exp \left[ jk_0 (x' \sin \theta \cos \phi + y' \sin \theta \sin \phi + z' \cos \theta) \right].
\]

(K.5)
The integral on the bottom surface B may instead be performed on surface A by making use of relations (K.2) and substituting \( z' \leftarrow -z' \). In this case, we have

\[
E^B_\theta (\theta, \phi) = \int_A dS' \left[ -M_x \sin \phi + M_y \cos \phi \\
+ \eta_0(-J_x \cos \theta \cos \phi - J_y \cos \theta \sin \phi - J_z \sin \theta) \right] \\
\times \exp \left[ jk_0(x' \sin \theta \cos \phi + y' \sin \theta \sin \phi - z' \cos \theta) \right]
\]

\[
= \int_A dS' \left[ -M_x \sin \phi + M_y \cos \phi \right. \\
\left. + \eta_0(J_x \cos \theta' \cos \phi + J_y \cos \theta' \sin \phi - J_z \sin \theta') \right] \\
\times \exp \left[ jk_0(x' \sin \theta' \cos \phi + y' \sin \theta' \sin \phi + z' \cos \theta') \right]
\]

\[
= E^A_\theta (\theta', \phi), \tag{K.6}
\]

where \( \theta' = \pi - \theta \), and the \( E_\theta \) component may be written as

\[
E_\theta (\theta, \phi) = E^A_\theta (\theta, \phi) + E^A_\theta (\pi - \theta, \phi). \tag{K.7}
\]

This last form is useful, since computer codes which solve for the far fields due to an enclosed radiator or scatterer need not be rewritten. Instead, the far fields are computed in the normal way on A (omitting the face at \( z = 0 \)) to obtain \( E^A_\theta (\theta, \phi) \). Substitution into (K.7) will yield the actual far fields in the top half space. The same operation may be used to obtain a similar expression for \( E_\phi (\theta, \phi) \) as follows.

\[
E_\phi (\theta, \phi) = E^A_\phi (\theta, \phi) + E^B_\phi (\theta, \phi), \tag{K.8}
\]

where

\[
E^A_\phi (\theta, \phi) = \int_S dS' \left[ M_x \cos \theta \cos \phi + M_y \cos \theta \sin \phi - M_z \sin \theta \\
- \eta_0(-J_x \sin \phi + J_y \cos \phi) \right] \\
\times \exp \left[ jk_0(x' \sin \theta \cos \phi + y' \sin \theta \sin \phi + z' \cos \theta) \right]. \tag{K.9}
\]
Again, we move the integral on surface B back to surface A using relations (K.2) and letting $z' = -z'$, or

$$E_\phi^B (\theta, \phi) = \int\int_A dS' \left[ M_x \cos \theta \cos \phi + M_y \cos \theta \sin \phi + M_z \sin \theta 
- \eta_0 (J_x \sin \phi - J_y \cos \phi) \right]$$

$$\times \exp \left[ jk_0 (x' \sin \theta \cos \phi + y' \sin \theta \sin \phi - z' \cos \theta) \right]$$

$$= -\int\int_A dS' \left[ M_x \cos \theta' \cos \phi + M_y \cos \theta' \sin \phi - M_z \sin \theta' 
- \eta_0 (-J_x \sin \phi + J_y \cos \phi) \right]$$

$$\times \exp \left[ jk_0 (x' \sin \theta' \cos \phi + y' \sin \theta' \sin \phi + z' \cos \theta') \right]$$

$$= -E_\phi^A (\pi - \theta, \phi), \quad (K.10)$$

and we obtain the expression

$$E_\phi (\theta, \phi) = E_\phi^A (\theta, \phi) - E_\phi^A (\pi - \theta, \phi). \quad (K.11)$$
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