INTEGRAL EQUATION AND DISCONTINUOUS GALERKIN METHODS
FOR THE ANALYSIS OF LIGHT-MATTER INTERACTION

By

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ABSTRACT

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Light-matter interaction is among the most enduring interests in the physical sciences. As a result, the understanding and control of this physics is of paramount importance to the design of myriad technologies ranging from stained glass, to molecular sensing and characterization techniques, to quantum computers. The development of complex engineered systems that exploit this physics is predicated at least partially upon in silico design and optimization that properly capture the light-matter coupling. In this thesis, details of computational frameworks that enable this type of analysis, based upon both Integral Equation and Discontinuous Galerkin formulations, will be explored. The primary focus will be on the development of efficient and accurate software, with results corroborating both. The secondary focus will be on the use of these tools in the analysis of a number of exemplary systems.
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This thesis is dedicated to my dear friend, Carl Coppola, whom I met on my first day as a Freshman in 2003. Over our undergraduate years we studied, lived, and laughed together, with both of us continuing on at Michigan State for our graduate education. Carl passed in 2010, and the halls of the Engineering Building are poorer in the absence of his wit, perseverance, and selflessness. I am truly privileged to have known him, and am honored to share his memory in these pages.
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KEY TO SYMBOLS AND ABBREVIATIONS

- ACE = Accelerated Cartesian Expansions
- CFL = Courant-Friedrichs-Levy
- CG = Continuous Galerkin
- CQED = Cavity Quantum Electrodynamics
- DG = Discontinuous Galerkin
- EFIE = Electric Field Integral Equation
- EM = Electromagnetic
- FMM = Fast Multipole Method
- FSS = Frequency Selective Surface
- IE = Integral Equation
- LHS = Left-Hand Side
- PDE = Partial Differential Equation
- PEC = Perfectly Electrically Conducting
- PMC = Perfectly Magnetically Conducting
- QED = Quantum Electrodynamics
- RHS = Right-Hand Side
Chapter 1: Introduction

The interaction of light and matter is among the most enduring interests of the physical sciences. The Lycurgus cup, a product of 4th century CE Roman glassmakers, is exemplary of the longevity of this subject. The cup itself is made of conventional Roman glass (i.e., silica, soda, and lime) doped with silver and gold nanoparticles that give rise to optical dichroism, its most distinct feature [1]. The cup is illustrated in Figure 1.1. Subsequent artisans have used metal nanoparticles in glass coloring as evidenced by the deep reds of the windows of the Notre Dame de Paris cathedral [2].

These aesthetic effects are a consequence of surface plasmon resonance, a phenomena in which the electromagnetic field couples strongly to the conduction electrons near the surface of the nanoparticles mixed into the glass. What makes this effect remarkable is that it is geometry-dependent, in so far as the color of the light that is most strongly scattered is a function of the size and shape of the nanoparticles [3]. What is even more remarkable is that these structures are typically smaller than the wavelength of the visible light exciting them, which places them severely outside of the realm of simple physical intuition. To this end, one of the goals of nanoscience has been to construct effective theories from which new intuition can be derived - in this case, for the manner in which light interacts with material systems that are at or below its wavelength.

The study of light in nanoscopic systems has generated tremendous advances both in terms of our fundamental understanding of the interaction between light and matter, (i.e., QED) and an astonishing range of novel technologies that exploit effects ranging from surface plasmon resonance [3] and the formation of photonic bandgaps [4], to the Purcell effect [5] and resonant energy transfer [6, 7]. The applications that rely upon this physics cover a
diverse array of fields, ranging from sensing and characterization techniques that utilize quantum dot emission in biology [8], to single photon sources [9] and systems that generate and preserve entanglement [10] in quantum information science.

Broadly speaking, the focus of this Dissertation is on the development of fast and accurate computational methods for the in silico analysis of light-matter interaction in the broad range of applications discussed above. This physics typically presents a number of challenges in terms of numerical modeling. Given the highly dispersive materials attendant to many of these systems, and the importance of resolving subwavelength geometric features, these systems present discretizations that have a high electrical density (i.e., there are many unknowns per free space wavelength). To this end, fast methods for studying scattering from these densely discretized subwavelength structures are of great relevance and will be explored in Chapter 2.4. In some cases, the light-matter interaction cannot be modeled using a simple set of constitutive relations, and often quantum equations of motion must be resolved in concert with the EM fields to reach a full understanding of the system. This is the case in cavity-mediated energy transfer physics, which will be the focus of Chapter 4.3. The remaining Chapters are more germane to numerical modeling in and of itself, and will contain important implementation details for those seeking to reproduce or extend the work in this Dissertation. Throughout, the primary focus will remain on establishing accurate and efficient methods for the solution of PDEs and IEs that arise in the modeling of light-matter physics. Specific applications will be left to future work, particularly the problem of using the developed tools for optimization, the natural next step for a mature piece of scientific code.

The remainder of this Chapter will consist of an overview of some of the relevant physics
and applications that may be modeled using the techniques presented herein (Section 1.1), a brief introduction to the numerical methods that will be explored for IEs and PDEs (Section 1.2), and a brief outline of the contents of this Dissertation (Section 1.3).

1.1 Physics of Interest and Technological Relevance

In this Section, an overview of light-matter phenomenology is presented, with some indication of its associated technological relevance. This is by no means comprehensive, but should serve as inspiration for the wide range of applications that can be further enabled by the development of computational tools for analysis, and eventually design and optimization.

1.1.1 Periodic Structures: FSS, ‘Metamaterials’, and Photonic Crystals

Periodic structures will be of interest in Chapter 3, wherein fast methods for studying scattering of electromagnetic waves from these systems will be explored. Periodicity has long been used as a tool in microwave engineering, with Frequency Selective Surfaces (FSS), being one example [11]. Here, periodic arrays of subwavelength metallic patterns are distributed across a surface to achieve some sort of resonant scattering response, wherein fields are filtered based upon spectral content, polarization, or both. More recently, this resonant scattering physics has been exploited in the context of ‘metamaterials’, wherein the gross scattering response of a periodic distribution of subwavelength resonant structures is mapped onto some effective medium with exotic properties that are either not found in nature, e.g., negative or near-zero index of refraction [12], or not often found in nature, e.g. spatially dispersive constitutive parameters [13]. While the theoretical utility of this approach to engineered media has been questioned [14], the response of these systems remains interesting regardless
of the framework that one uses to rationalize phenomenology. In Chapter 3, scattering from a number of exemplary FSS and metamaterial structures will be analyzed in the context of demonstrating the utility of the ACE algorithm. One of these exemplary structures will mix periodicity with plasmon resonance in the context of achieving negative index behavior at optical frequencies, and will serve as a an indicator of the high electrical densities that arise in modeling technologically interesting light-matter systems.

Photonic crystals represent another area in which periodicity is used as a means of achieving an interesting light-matter effect. Rather than periodic metallization, photonic crystal systems consist of a periodic variation in the refractive index of some dielectric medium. A careful engineering of the scattering resonance of the unit cell, and the Bragg scattering resonance of the entire periodic system can lead to the formation of a photonic bandgap in which the existence of propagating modes of the EM field is either strongly restricted in terms of direction, or altogether forbidden [4]. This type of physics is responsible for what is known as structural color, wherein the visible color of an object is determined by the formation of photonic bandgaps that strongly reflect certain colors of light, rather than chemical mechanisms in which it is determined by selective electronic absorption of light (i.e., pigmentation) or fluorescence [15]. Photonic bandgaps arise due to naturally occurring periodic nanostructures in the coverings of numerous animals [16], and an example in which this is demonstrated for a butterfly’s wing [17, 18] is presented in Chapter 3.

1.1.2 Energy Transfer, CQED, and Quantum Information

Another form of light-matter interaction that will be discussed in Chapter 5 is the interaction of spatially separated systems through their mutual coupling to the EM field [6, 7].
The vacuum fluctuation induced dipole-dipole interaction has been of fundamental interest in molecular physics for many years, wherein this coupling gives rise to the hierarchy of Casimir-Polder, London, and Dispersion forces [19]. For many years, this interaction was studied in the context of energy transfer in polymers, dyes, and biological entities [20]. More recently, it has been studied between quantum dots [21], and quantum dots and biological macromolecules [8], yielding a number of putative technological applications. For example, energy transfer processes have been proposed as a means of realizing quantum logic gates [22], and have been successfully applied to the measurement of distances in proteins [23].

While the theory for this type of interaction is well-understood in free space or disordered environments, it becomes considerably more interesting and challenging when it occurs in the presence of some structured matter that alters the local density of photonic modes. This is a fundamental problem of CQED, the quantum field theory that governs the interaction of confined light with matter [24]. Rather than considering a pure Maxwell problem with some phenomenological treatment of matter, as will be the case in Chapter 3, the Maxwell Equations will have to be self-consistently coupled to some other model that ‘generates’ the constitutive relations that link light and matter. This presents new modeling challenges, in so far as solutions to the classical Maxwell Equations must be used to inform a material model that couples to quantum fields. A number of theoretical frameworks exist for describing cavity-mediated interactions [25, 26, 27], but only recently have some have been employed in a computational setting on non-canonical systems using commercial software [28, 29].

Quantum information applications provide ample motivation for studying light-matter interaction at this level of detail. Qubits, the fundamental unit of information in quantum computing, can be realized in terms of a number of systems that can be controlled optically,
ranging from excitons [30], to spins [31], to the polarization states of single photons [32].

The realization of practical technologies that actually control these systems requires the engineering of light at the single photon level. Reliable single photon [33] and single plasmon sources [34] have been enabled by the careful understanding of surface plasmon physics, wherein the high energy density achieved in plasmonic modes ensures a strong light-matter coupling. Somewhat more challenging is the generation of entangled pairs of photons. This is typically achieved at low efficiency by way of parametric down conversion, though recent advances have shown that the careful application of the Purcell effect can be used to engineer the coupling between biexcitons and excitons in two-cavity systems as to yield much more efficient generation of entangled photons [10]. In excitonic cubits, cavity-plasmon mediated interactions have been proposed as a means of generating entanglement between spatially separated quantum dots [35, 29].

While this is necessarily an incomplete overview of the many avenues through which light-matter interaction promises to enable quantum information technology, it should provide sufficient evidence that this is a field that will benefit greatly from the development of the computational methods being proposed in this Dissertation. Chapter 5 presents preliminary work to this end, with a focus on energy transfer applications, but with proposals for ongoing/future work that are more strongly focused on quantum computation applications.

1.2 Overview of Numerical Methods for the Maxwell Equations

The accurate discretization and numerical solution of the Maxwell Equations has been the focus of significant intellectual effort for many years. The following Sections serve to give an overview of some of the results of this effort germane to the contents of this Dissertation,
as well as to establish a common notation and framework for the diverse methods that will be discussed. Basic notations are established in Section 1.2.1. Given the breadth of methods utilized in this work, generality is maintained with respect to establishing a notation that is suitable for both IE- and PDE-based formulations. Similarly, Section 1.2.2 gives a brief overview of Galerkin’s method for discretization at a level of generality that is suitable for both formulations. In Section 1.2.3, the relative advantages and disadvantages of both IEs and PDEs will be discussed, justifying their application to the different applications presented in this thesis. Sections 1.2.4 and 1.2.5 will focus on details specific to IEs and PDEs, respectively. In the former, fast methods for the solution of IEs, which take the form of dense linear systems upon discretization, will be discussed. In the latter, differences between Discontinuous and Continuous Galerkin discretizations will be explored, with a focus on elaborating the advantages of DG.

1.2.1 Notation

Before discussing the details of various numerical methods, it is useful to develop the notations that will be used throughout. Regardless of whether IE or PDE formulations are used, much of the useful notations remain the same. To this end, the discretization and solution of some IE or PDE of interest can be decomposed into the following steps:

1. Discretizing the domain of the problem (i.e., meshing).

2. Constructing basis functions used to represent the problem solution and data.

3. Establishing a norm for measuring the ‘correctness’ of possible solutions.

4. Defining a residual that captures the physics of the problem, and projecting the residual
onto a set of test functions to form a system of equations.

5. Resolving the system of equations numerically.

Notations attendant to each step of this generic process will now be developed, while details specific to various formulations of the Maxwell problem will be discussed later.

In meshing, there will be some idealized domain $\Omega$, with boundary $\partial \Omega$, upon which the continuous problem is defined. This domain will be approximated in terms of some tessellation of non-overlapping subdomains:

$$\Omega \approx \Omega_h = \bigcup_{e=1}^{N_e} T_e$$

The subdomains, $T_e$, will also be referred to as elements. The boundary of $T_e$ is indicated by $F_e$. An exemplary tetrahedral mesh is illustrated in Figure 1.2

Upon discretizing the domain, appropriate basis functions can be defined relative to geometric primitives in $\Omega_h$. In the IE formulations that will be utilized for PEC scatterers, linear vector basis functions will be associated with interior edges of triangular meshes. For IE formulations for dielectric scatterers, linear vector basis functions will be associated with all faces of tetrahedral meshes. In the PDE formulations used in this thesis, higher order basis functions will be assigned to all tetrahedra. Both modal and nodal basis sets will be employed, i.e., occasionally it will be convenient to work with orthogonal polynomials, and occasionally it will be convenient to work with interpolating polynomials [36]. In all cases, a solution to the problem will be specified as:

$$f(\mathbf{r}) \approx f_h(\mathbf{r}) = \sum_{q=1}^{N_q} \sum_{p=1}^{N_p(q)} c_q^p f_p(\mathbf{r})$$

Here, the subscript $h$ indicates that $f_h(\mathbf{r})$ is an approximation of $f(\mathbf{r})$ relative to $\Omega_h$. The summation on $q$ is over the geometric primitives (i.e., edges, faces, volumes) to which the basis functions are tied, and the summation on $p$ is over the $N_p(q)$ basis functions on the $q$th primitive. The $p$th basis function on the $q$th primitive is $l_p^q(\mathbf{r})$, which is weighted by an unknown coefficient, $c_p^q$. Prior to resolving $c_p^q$, however, a means for establishing how ‘good’ such an approximation is, is necessary.

A global inner product, and norm must be defined to establish the quality of an approximation. For functions defined on $\Omega_h$, $f(\mathbf{r})$ and $g(\mathbf{r})$, the global inner product is defined as:

$$\langle f, g \rangle_{\Omega_h} = \int_{\Omega_h} d\mathbf{r} f(\mathbf{r}) g(\mathbf{r})$$  \hspace{1cm} (1.3)

For complex-valued functions, the complex conjugate of $f(\mathbf{r})$ is typically used on the RHS of Equation 1.3. For vector-valued functions, the vector inner product of the two arguments is taken, in addition to integration. Such an inner product is useful for defining a global norm, which is defined as:

$$\| f \|_{L^2(\Omega)} = \langle f, f \rangle_{\Omega_h}$$  \hspace{1cm} (1.4)

Similarly, it may be useful to work with an $L^\infty(\Omega)$ norm:

$$\| f \|_{L^\infty(\Omega_h)} = \sup_{\mathbf{r} \in \Omega_h} |f(\mathbf{r})|$$  \hspace{1cm} (1.5)
Using these norms, error metrics for approximation can be constructed:

\[
\begin{align*}
\epsilon_{L^2}^2 &= \|f - f_h\|_{L^2(\Omega_h)} \quad (1.6a) \\
\epsilon_{L^\infty} &= \|f - f_h\|_{L^\infty(\Omega_h)} \quad (1.6b)
\end{align*}
\]

Similarly, the convergence of solutions will be validated in a discrete \(L^2\) norm.

The solution to our unspecified problem can be formulated in terms of defining a residual, a functional that measures the degree to which a solution fails to satisfy the IE or PDE of interest, and forcing it to vanish in some sense. The Galerkin projection of the residual will be forced to vanish, a process that will be described in more detail in Section 1.2.2. This process will result in a system of \(N = \sum_{q=1}^{Nq} N_p(q)\) equations in \(N\) unknowns, rendered as a matrix equation for numerical representation. The entries of the attendant matrices will require the evaluation of a number of local inner products that will now be defined. The aforementioned concerns associated with complex- and vector-valued functions are still assumed. For IEs, the local inner product will be taken with respect to the support of the testing function:

\[
\langle f, g \rangle_{\text{supp}(f)} = \int_{\text{supp}(f)} d\bar{r} f(\bar{r}) g(\bar{r}) \quad (1.7)
\]

In the DG framework that will be used for PDEs, a local inner product will be defined on each element:

\[
\langle f, g \rangle_{T_e} = \int_{T_e} d\bar{r} f(\bar{r}) g(\bar{r}) \quad (1.8)
\]

In so far as the support of \(f\) and \(g\) will typically be \(T_e\), this isn’t necessarily distinct from Equation 1.7; however, the notation will be more convenient in context. Additionally a local
inner product on the trace (boundary) of $T_e$, $F_e$, will be essential:

$$\langle f, g \rangle_{F_e} = \oint_{F_e} d\mathbf{r} f(\mathbf{r}) g(\mathbf{r})$$

(1.9)

In the DG framework, it is essential to consider inner products with multi-valued functions on some exemplary $F_e$. Values are defined on both the positive and negative traces, $f^+$ and $f^-$, where convention dictates that the positive trace is defined on the outside of $T_e$, and the negative trace is defined on the inside of $T_e$. To quantify the behavior of multi-valued functions at boundaries, the average and jump operators are defined. The average is indicated:

$$\{\{ f \} \} = \frac{f^- + f^+}{2}$$

(1.10)

Here, $f^+$ and $f^-$ refer to the value of $f$ on the positive and negative traces of a particular element. The jump operator is defined as:

$$[ f ] = f^+ - f^-$$

(1.11)

Upon evaluating the necessary inner products, the discrete problem will be rendered in terms of a finite linear system of equations, which takes following well-known form:

$$\mathbf{A} \mathbf{x} = \mathbf{b}$$

(1.12)

Here, $\mathbf{A}$ is an $N \times N$ matrix, the entries of which are generated using the inner products defined above, $\mathbf{x}$ is an $N$ vector of unknown coefficients, and $\mathbf{b}$ is a $N$ vector the entries of which are inner products with the problem data. The mapping of both IE and PDE
formulations of the EM field equations onto problems of this form will be the focus of the numerical aspects of this Dissertation.

1.2.2 Galerkin Methods

Among the most prevalent means of discretizing continuous linear problems are Galerkin methods. These exist among the broader class of weighted residual methods, which includes collocation and least squares methods, among others [37]. The essence of these methods is the construction of an approximate solution in terms of basis functions that span some space in which the regularity/physics of the problem is well-represented. A residual with respect to the exact solution is then defined, and forced to vanish in some method-dependent manner. In collocation methods, the residual is forced to vanish at a discrete set of points, whereas in Galerkin methods the residual is forced to be orthogonal to the span of the basis functions used in representing the approximate solution. It is this constraint equation on the residual that is used to generate a linear system of equations that can be solved using matrix methods. To give an overview of the Galerkin method that is sufficiently general to cover both IE and PDE-based problem, an abstract problem is presented first. It is relevant to note that the sense in which Galerkin method is being used here, is not as rigorous as would be employed by many applied mathematicians. For example, the Method of Moments, that will be applied to the discretization of IEs is not generally a Galerkin method. It can, however, be realized as one, and there is little practical consequence to this distinction germane to the heuristic discussion presented in this Section.

Consider the resolution of some unknown function, $\psi$, supported by a $d-$dimensional open subset of $\mathbb{R}^d$, $\Omega$. The $(d - 1)$-dimensional boundary of $\Omega$, denoted $\partial\Omega$ is sufficiently
smooth that it admits the definition of trace operators that meaningfully restrict $\psi$ to $\partial \Omega$. $\psi$ verifies the following equations:

$$D\psi(\vec{r}) = f(\vec{r}), \quad \forall \vec{r} \in \Omega \quad (1.13a)$$

$$B\psi(\vec{r}) = g(\vec{r}), \quad \forall \vec{r} \in \partial \Omega \quad (1.13b)$$

Here, $D$ is a linear operator acting on some space of functions supported by $\Omega$, and $B$ is some trace operator that meaningfully restricts $\psi$ to $\partial \Omega$. The data, $f$ and $g$, as well as the operators, $D$ and $B$, are specified in sufficient detail to ensure that Equation 1.13 is well-posed, i.e., it has a unique solution that exists and is not pathologically sensitive to the data [38].

The first step in solving this problem with a Galerkin method is the selection of a function space that approximates the solution of Equation 1.13, $\mathcal{W}(\Omega) = \{w_i \mid \text{supp}(w_i) \subseteq \Omega, i \in 1, \ldots, N\}$, here $N$ is a finite number. The exact details of $\mathcal{W}(\Omega)$ will be contingent upon the specifics of the problem being solved. To this end, a very general list of details concerning the choice of $\mathcal{W}(\Omega)$ follows:

- Degree of regularity consistent with the solution of the continuous problem, i.e., if $D$ or $B$ require integration/differentiation, elements of $\mathcal{W}(\Omega)$ should be commensurately integrable/differentiable.

- Systematic improvability, i.e., $\mathcal{W}(\Omega)$ can be enlarged in such a way that approximation error gets better, or at the very least does not get worse.

- Existence of convenient norms for estimating approximation error.

- Easy integration/differentiation of elements of $\mathcal{W}(\Omega)$ (numerical or analytical)
Having chosen $\mathcal{W}(\Omega)$, the approximate solution of Equation 1.13, $\psi_h$, is expressed as a linear combination of functions in $\mathcal{W}(\Omega)$, as illustrated previously in Equation 1.2:

$$
\psi_h(\vec{r}) = \sum_{i=1}^{N} c_i w_i(\vec{r})
$$

(1.14)

Assuming that the form of the $w_i(\vec{r})$ are known, $\psi_h(\vec{r})$ is practically specified by the set of expansion coefficients, $\{c_i| i \in 1, \ldots, N\}$.

The next step of the Galerkin method is the resolution of these unknowns via the construction of a residual - a functional that quantifies the extent to which $\psi_h$ fails to satisfy Equation 1.13. Moving the data to the left hand side of Equation 1.13, a simple point-wise residual can be constructed by considering the extent to which the right hand side is non-zero.

$$
\mathcal{D}\psi_h(\vec{r}) - f(\vec{r}) = \mathcal{R}_h(\vec{r}), \quad \forall \vec{r} \in \Omega
$$

(1.15a)

$$
\mathcal{B}\psi_h(\vec{r}) - g(\vec{r}) = \mathcal{R}_{h,\partial}(\vec{r}), \quad \forall \vec{r} \in \partial\Omega
$$

(1.15b)

It is apparent that $\psi_h(\vec{r})$ for which $\mathcal{R}_h$ and $\mathcal{R}_{h,\partial}$ vanish almost everywhere over the closure of $\Omega$ is the solution to Equation 1.13. Knowing this, however, does little to actually solve for $\psi_h(\vec{r})$, or equivalently, the set $\{c_i| i \in 1, \ldots, N\}$. To this end, $\mathcal{R}_h$ and $\mathcal{R}_{h,\partial}$ must be driven to zero in some manner such that $\{c_i| i \in 1, \ldots, N\}$ can be practically resolved. In so far as $N$ basis functions are being used to construct $\psi_h(\vec{r})$, naively it should suffice to find $N$ unique vanishing projections of the residuals to fully determine $\{c_i| i \in 1, \ldots, N\}$. While this approach will not, in general, result in residuals that vanish almost everywhere over the closure of $\Omega$, i.e., the true solution, approximate solutions computed in this manner can
typically be made to converge to the actual solution in some meaningful way. The rigorous understanding of this convergence is a problem of functional analysis beyond the scope of the heuristic outline provided in this Dissertation.

The defining feature of Galerkin methods, over other weighted residual methods, is the specific choice of projections for which the residual vanishes. In general, the residual is forced to vanish when projected onto the problem’s dual space, \( W^*(\Omega) \). For a self-adjoint problem, this is \( W(\Omega) \), though it is not in general. In either case, the discrete problem is rendered:

\[
\langle v_i, D\psi_h \rangle_{\Omega_h} - \langle v_i, f \rangle_{\Omega_h} = \langle v_i, R_h \rangle_{\Omega_h} = 0, \quad \forall v_i \in W^*
\]

(1.16a)

\[
\langle v_i, B\psi_h \rangle_{\partial\Omega_h} - \langle v_i, g \rangle_{\partial\Omega_h} = \langle v_i, R_{h,\partial} \rangle_{\partial\Omega_h} = 0, \quad \forall v_i \in W^*
\]

(1.16b)

By the linearity of \( D \) and \( B \), this can be cast in terms of a linear system of \( N \) equations in \( N \) unknowns, of the form given in Equation 1.12. Here, the inner products in Equation 1.16 constitute elements of some matrix \( A \) some vector \( b \), with the unknown vector \( x \) consisting of the basis function coefficients. More specifically, for the IE problems presented in this Dissertation, the elements of the matrix \( A \) will be the tested IE operators, with boundary conditions implicitly enforced by the Green’s function, and the elements of the vector \( b \) will be the tested data, i.e., the incident field. The nature of the problem will be somewhat different for the DG problems, as they will be first rendered in a semi-discrete form. Here, a Galerkin residual will be formed, but discretization will proceed first in space, to render the Maxwell PDEs as a system of ODEs. Applying an explicit time marching scheme to the system of ODEs will yield an Equation of this form, but \( A \) will be a simple block-diagonal matrix, and \( b \) will be some complicated function of the data and boundary conditions. More precise details concerning both will be given in Chapters 1.4 and 3.8.
1.2.3 Comparison of IE and PDE-Based Methods

As both IE and PDE-based methods are discussed in this Dissertation, it is worth addressing the relative advantages and disadvantages of both, to make apparent the need for this diversity of methodology.

IE formulations of the Maxwell problem typically rely on equivalence theorems that replace materials with equivalent currents radiating into an environment with a response that is exactly captured by an appropriate Green’s function. Boundary conditions are implicitly satisfied by the solution fields generated by this Green’s function. This is especially important when considering scattering problems, in which asymptotic boundary condition must be satisfied by scattered fields as they propagate to infinity. However, this formulation will give rise to a dense system of equations when discretized, due to the non-local character of the associated integral operators. For a system with $N$ discrete degrees of freedom, IE discretizations will give rise to matrices with $\mathcal{O}(N^2)$ non-zero entries, and will require $\mathcal{O}(N^3)$ or $\mathcal{O}(N^2)$ operations to solve directly or iteratively, respectively.

PDE formulations of the Maxwell problem typically deal with the electromagnetic fields directly, and require the explicit treatment of fields throughout the computational domain. While boundary conditions can be satisfied exactly on finite domains, a well-known deficiency of PDE formulations is that radiation problems cannot be treated exactly, and require augmentation. Some of the methods for realizing proper asymptotic boundary conditions for PDE problems include absorbing boundary conditions [39], perfectly matched layers [40], infinite elements [41], hybridization with a boundary integral [42, 43], or pole condition/Hardy space methods [44, 45, 46]. The benefit to using PDE-based formulations of the Maxwell problem primarily lie in the sparse nature of the linear algebra problems that they spawn.
For a system with $N$ discrete degrees of freedom, PDE discretizations will give rise to matrices with $\mathcal{O}(N)$ non-zero entries that can be solved rapidly using either direct or iterative methods. Here, the cost of solution is more complex, and depends upon factors including the dimensionality of the problem, the ordering of unknowns, and the presence or absence of other sparse structure that may be exploited.

The relative computational cost of PDEs and IEs is a bit misleading as presented, as the number of degrees of freedom will change dramatically between the two methods. One of the primary benefits of IE methods is that only the scattering surfaces/volumes need be discretized. In PDE formulations, the surrounding vacuum must also be discretized, increasing the number of unknowns. Further, IEs can also be formulated in terms of equivalent surface problems for volumetric scatterers, using the PMCHWT [47] or Müller [48] formalisms, increasing the intrinsic disparity in the number of unknowns even further.

Time domain simulations provide another set of criteria for comparison. In PDE-based methods, numerical dispersion becomes a significant issue, wherein propagating waves no longer obey the proper physical dispersion relation due to the discretization process [49]. While this is not an issue in IE-based methods, there are significant issues related to stability that are much more readily addressed in PDE-based methods. It is worth noting, however, that there is a growing body of research on the stability of time domain IEs [50, 51].

For the purposes of this Dissertation, IE methods will be applied to the analysis of scattering problems in Chapter 3. In particular, scattering from doubly periodic planar structures will be of interest, wherein the use of the appropriate periodic Green’s function yields solution currents that satisfy both Bloch-periodic conditions in plane, and the proper asymptotic boundary conditions out of plane. However, the PDE-based DG framework will
be utilized for time domain simulations of cavity structures in Chapters 4 and 5. Here, the easy realization of a fast stable solver for closed domain problems is the primary motivating factor.

1.2.4 Fast Methods for IEs

In Section 1.2.3, the high computational cost of using IE methods was briefly addressed. Since the 1980s, a topic of considerable research interest has been the development of fast methods to amortize this cost. While fast direct solvers are a topic of intense current research, the majority of the work that has been done over the past 25 years has been focused on fast iterative solvers. To this end, the primary cost being reduced is that of matrix-vector multiplication between the discretized IE operator and a sequence of trial solutions that converge to the correct solution, if the problem is well-posed. Methods for accelerating the iterative solution of IEs in this manner can be broadly split into two classes: those that effect this through the use of FFTs, and others that exploit some manifest rank deficiency in the IE operator.

The flagship FFT-based method is the Adaptive Integral Method due to Bleszynski [52]. Since their development in the 60s [53], it has been established that FFTs can be used to accelerate the discrete convolution of two sequences of length $N$ from $O(N^2)$ to $O(N \log(N))$. The basis for AIM is the notion that the application of the discrete integral operator to a trial solution in an iterative solver can be reduced to such a discrete convolution. However, FFT methods can only be applied if the data lies on a uniform grid. To this end, an essential step of the AIM algorithm is to anterpolate currents from a non-uniform mesh to a uniform grid, and the subsequent interpolation of fields from the uniform grid back onto the non-
uniform mesh after the FFT is applied. Overall, AIM yields fast \( O(N \log(N)) \) iterative solutions. The AIM algorithm has seen success in a number of problems in computational electromagnetics, ranging from integration into time domain codes [54], fast FE-BI codes [55], and highly scalable parallel codes [56].

While a number of methods that exploit manifest rank deficiency exist (ACA, H-matrices, etc), one of the primary concerns of this Dissertation will be on the ACE algorithm, which is a variation on the FMM and its descendants [57, 58]. These methods are predicated upon the construction of an addition theorem that permits the separation of source and testing domains in the representation of the IE kernel. Rank deficiency arises in considering interactions between aggregate source and testing domains that are well separated in some metric, i.e., while \( N \) sources may be tested by \( N \) observers, only \( O(N \log(N)) \) or \( O(N) \) interactions need be evaluated, rather than \( O(N^2) \). Intuitively, one can think of the multipole expansion of the potential due to some charge distribution. Receding away from the distribution, progressively fewer multipoles will give appreciable contributions to the total potential. Consequently, at a sufficiently large distance, it is more economical to represent the potential in terms of the multipole moments of the distribution about some centroid, rather than the individual charges comprising the distribution. The specific details of the ACE algorithm [59], a hierarchical fast method similar to FMM, will be discussed in Chapter 3. In particular, its extension to periodic systems with long-range interactions, namely low-frequency Helmholtz, weakly-screened Yukawa, and Coulomb potentials.
1.2.5 Discontinuous Galerkin vs. Continuous Galerkin

The solver that has been developed as a component of Chapters 4 and 5 is based upon a DG framework. To this end, it is interesting to consider the relative advantages and disadvantages of DG relative to its Continuous Galerkin (CG) counterparts.

Discretization schemes based upon a CG framework are guided by the principle that the underlying function space should be ‘conforming’. This means, that given the function space in which the solution to the continuous problem exists, the discretization space should be chosen as one of its finite dimensional subspaces. Preferably, this is associated with some framework for selecting sequentially ‘better’ subspaces, that realize a solution that is in some sense closer to the continuous one, and this gives rise to the notion of $h$, $p$, and $hp$ adaptivity. This choice should also be mindful of regularity requirements, and will typically have some means of being tied to a mesh. To this end, nodal CG discretizations rely upon the definition of a set of interpolating polynomials defined in terms of nodes tied to mesh elements in some regular way [60]. Within this framework, it is possible to generate a basis set that is polynomial complete to a particular order that continuously interpolates over the entire domain. A useful consequence of this is that the approximate solution will be single-valued at all points, by construction. Other choices of CG basis functions include Nedelec/Whitney elements [61, 62], that are conformal to the appropriate space of vector-valued functions in which Maxwell fields exist.

While the basis functions in a CG framework meet many of the associated criteria, (i.e., regularity, improvability) there are a number of drawbacks. As CG basis functions are defined in terms of the global geometry, the underlying mesh is required to maintain some degree of regularity. To this end, these methods are restricted in their ability be applied to meshes
constructed from many different parts, with geometric primitives that do not necessarily overlap. These meshes are deemed ‘non-conformal’, and one is illustrated in Figure 1.3

This may arise in a number of scenarios - perhaps the physics of the problem leads to a solution with different length scales in different regions, as might be the case in an EM problem in which two domains with very different refractive indices exist. Otherwise, it may be the case that many different engineers designed various parts of the mesh of a larger structure, and it is technically challenging to force them to be conformal. Otherwise, another negative consequence of the global nature of the basis function definition arises in time-dependent problems, wherein strong restrictions are placed on the nature of the time integration scheme that can be utilized. Typically, one is restricted to implicit methods for CG discretizations, which require the solution of a sparse linear algebra problem at each time step. For higher-order methods, conditioning of the associated system worsens, and this restriction becomes increasingly burdensome. The DG framework seeks to remedy some of these problems.

In a DG framework the associated function spaces still typically consist of polynomial spaces, however they are completely local, and the global functions space is described as ‘broken’. By local, it is meant that each basis function is defined with respect to exactly one geometric primitive (typically a simplex), remaining agnostic to the global structure of the mesh. The implication of the associated function space being broken is that it no longer guarantees an approximate solution that is single-valued throughout the domain by construction. It is in fact the case that the global solution will be discontinuous across elements. To this end, these functions spaces are not conforming in the same sense as the ones used in CG methods. To guarantee the construction of solutions with minimal numerical
discontinuity the concept of a ‘numerical flux’ is introduced to DG. Here, the multi-valued nature of the solution at inter-element boundaries is introduced into the associated matrices in such a way as to either solve some locally defined Riemann problem [63], or to penalize the breaking of boundary conditions in a variational sense, i.e., interior penalty methods [64].

Here, the restrictions that were previously outlined are largely lifted. Non-conformal meshes [65], as well as non-conformal approximation order [36] are possible, thanks to the new found global agnosticism of the basis. Similarly, in time-dependent problems, the restriction on time integration methods is lifted as the relevant matrices are rendered block diagonal, and explicit methods can be applied to circumvent issues of sparse linear algebra and conditioning [66, 67]. To deal with the introduction of a CFL-like condition, DG also supports the use of local time stepping algorithms, in which different regions of a mesh can be evolved at different rates, to prevent multiscale discretizations from being dominated by their smallest scales [68]. Other advantages include the ability to construct essentially arbitrary basis sets can be constructed, particularly from non-polynomial functions that better describe the problem physics [69]. DG also becomes a natural means of realizing domain decomposition, and this has been used to realize adaptive local basis functions [70]. The benefits of DG do not come without some disadvantages, though, and the element-wise definition of basis functions means that there are more unknowns than in a CG framework [71]. However, this has been recently combatted by mapping a CG method into the DG framework for advection-diffusion problems [72].
1.3 Layout of this Dissertation

The contents of the remainder of this Dissertation are as follows:

• **Chapter 2**: A brief outline of the surface and volumetric EFIEs that will be used to study scattering from periodic structures.

• **Chapter 3**: The use of the ACE algorithm for accelerating the computation of pairwise potentials on periodic domains, and the solution of periodic EFIEs.

• **Chapter 4**: An overview of the DG framework as applied to the time domain Maxwell Equations.

• **Chapter 5**: A formalism for studying field-mediated interactions between quantum emitters using a time domain Maxwell solver, and proposals for future work.

Many of the results in Chapter 3 have been published elsewhere in [73, 74].

1.4 Figures
Figure 1.1: The Lycurgus cup, a piece of 1700 year old Roman nanotechnology exhibiting optical dichroism. © Trustees of the British Museum. For interpretation of the references to color in this and all other figures, the reader is referred to the electronic version of this dissertation.

Figure 1.2: (Left) The domain upon which some continuous problem is defined. (Right) A tetrahedral mesh of that domain, upon which the discrete problem will be solved. Each of the tetrahedra into which this geometry is decomposed, is one of the subdomains, $T_e$. 
Figure 1.3: Illustration of a non-conformal mesh comprised of two hexahedra resolved at different discretization rates.
Chapter 2: IEs for the Time-Harmonic Maxwell Problem

2.1 Overview of IEs

In IE-based formulations of the electromagnetic field equations, the unknown quantity is some equivalent source distribution, in terms of which potential integrals and, equivalently, fields can be constructed. From these integral expressions of the fields in terms of the equivalent source distribution, equations can be constructed and resolved in terms of unknowns distributed over some subset of the computational domain. Of concern in this Chapter will be two forms of the Electric Field Integral Equation (EFIE) - one in terms of unknowns defined on a surface, for perfectly electrically conducting (PEC) targets, and another in terms of unknowns defined over a volume, for dielectric targets.

2.2 Scattering from PEC Targets

The surface EFIE is typically used in the analysis of scattering from open PEC surfaces, i.e., metallic screens, plates, etc [75]. This stands in contrast to its counterpart, the Magnetic Field Integral Equation (MFIE), which can only be applied to closed surfaces [76]. When possible, the two are often taken as a linear combination, the Combined Field Integral Equation (CFIE) [77]. As the operators forming the two terms have disjoint null spaces, this formulation avoids becoming ill-conditioned in the vicinity of the null space of either taken in isolation. Still, the form of the EFIE (Fredholm first type) leads to its becoming ill-conditioned at low frequencies - though numerous remedies exist [78, 79, 80] involving
Calderon identities [81]. As the PEC targets of interest for the periodic systems discussed in Chapter 2.4 are primarily FSS, which consist of conducting strips and plates, only the EFIE is explored in what follows. When computational results are presented, it is worth noting that only simple measures (matrix-based preconditioning) have been taken to address problems with conditioning.

2.2.1 Statement of the Problem

Consider a domain, \( \Omega \subset \mathbb{R}^3 \), in which a PEC surface, \( \partial \Omega_C \), equipped with the surface normal vector, \( \hat{n} \), is immersed. The material composition of the background in which \( \partial \Omega_C \) is immersed is homogeneous and linear, and without loss of generality, it is considered to be vacuum characterized by the constitutive parameters \( \varepsilon_0 \) and \( \mu_0 \). Incident on this domain is a plane wave of the form:

\[
\vec{E}_{inc}(\vec{r}) = E_0 e^{-i\vec{\kappa}_0 \cdot \vec{r}}
\]  

(2.17)

Here, \( \vec{\kappa}_0 \) is the associated wavevector with \( \kappa = |\vec{\kappa}_0| \), and \( \vec{E}_0 \in \mathbb{C}^3 \) describes the incident field strength and polarization. The interrogating field gives rise to a scattered field, \( \vec{E}_{scat}(\vec{r}) \), such that the total field can be expressed as a linear superposition, \( \vec{E}(\vec{r}) = \vec{E}_{inc}(\vec{r}) + \vec{E}_{scat}(\vec{r}) \). Using the surface equivalence principle [82, 76], this scattered field can be expressed in terms of a convolution of an equivalent source distribution \( \vec{J}_S(\vec{r}) \) supported by \( \partial \Omega_C \), radiating into an homogeneous domain:

\[
\vec{E}_{scat}(\vec{r}) = -i\kappa \eta \int_{\partial \Omega_C} d^2\vec{r}' \overline{G}(\vec{r}, \vec{r}') \cdot \vec{J}_S(\vec{r}')
\]  

(2.18)
Here, $\eta = \sqrt{\mu_0/\varepsilon_0}$ and $\overline{G}(\vec{r}, \vec{r}')$ is a dyadic Green’s function, defined in terms of the scalar Green’s function $G(\vec{r}, \vec{r}')$ as follows [82]:

$$\overline{G}(\vec{r}, \vec{r}') = \left( I + \frac{\nabla \nabla}{\kappa^2} \right) G(\vec{r}, \vec{r}') \quad (2.19)$$

Here, $I$ is the unit dyad. At this point, it is worth emphasizing that the Green’s function in Equation 2.19 gives the response of the system at $\vec{r}$ due to a point excitation at $\vec{r}'$, in the absence of the PEC surface, $\partial \Omega_C$. The Green’s function is responsible for satisfying the Sommerfeld radiation boundary condition in free space, though often more complicated boundary conditions may be desired. Of particular interest in Chapter 3 will be Green’s functions that generate Bloch-periodic fields over the unit cell boundaries of some array, while also satisfying radiation conditions receding away to infinity [83]. Details of $G(\vec{r}, \vec{r}')$ for such domains are given in Appendix 5.5. What remains of this section will give consideration to the statement of the surface EFIE with an arbitrary $G(\vec{r}, \vec{r}')$.

A Fredholm integral equation of the first type can be posed by enforcing boundary conditions on the tangential electric field over the support of the equivalent currents. This condition can be stated physically as the vanishing of the tangential component of the electric field over $\partial \Omega_C$, or mathematically as:

$$\hat{n} \times \vec{E}_{\text{scat}}(\vec{r}) = -\hat{n} \times \vec{E}_{\text{inc}}(\vec{r}), \quad \forall \vec{r} \in \partial \Omega_C \quad (2.20)$$

$$-i\kappa \hat{n} \times \int_{\partial \Omega_C} d^2\vec{r}' \overline{G}(\vec{r}, \vec{r}') \cdot \vec{J}_S(\vec{r}') = -\hat{n} \times \vec{E}_{\text{inc}}(\vec{r}). \quad \forall \vec{r} \in \partial \Omega_C \quad (2.21)$$

$$\mathcal{T}_S \{ \vec{J}_S \} \left[ \vec{r} \right] = -\hat{n} \times \vec{E}_{\text{inc}}(\vec{r}). \quad \forall \vec{r} \in \partial \Omega_C \quad (2.22)$$
This equality is the surface EFIE. In Section 2.2.2, the details necessary for its discretization are presented, and then later in Section 3.7.1 it will be utilized to study scattering from periodic arrays of PEC structures.

2.2.2 Numerical Details

Having stated the continuous problem, the remaining task is the specification of a set of basis functions for the discrete problem. To this end, an approximate \( \vec{J}_{S,h}(\vec{r}) \) will be defined in terms of functions supported by a simplicial tesselation of \( \partial \Omega_C \), i.e., a triangular mesh of the PEC surface. An exemplary triangular mesh for a periodic scattering problem is illustrated in Figure 2.4.

Linear vector basis functions due to Rao, Wilton, and Glisson [84] (RWG basis functions) will be defined on each interior edge of the mesh. Some of the useful features of these functions are as follows:

- Basis functions are associated with all interior edges of the mesh and compactly supported by the two triangles sharing such an edge.

- Continuity of currents is satisfied across all edges.

- The charge density, i.e., divergence, on the interior of the support is piecewise constant, and globally neutral.

- The charge density is free of line charges on all boundaries of the support.

Per the list of desirable features presented in Section 1.2.2, these functions have the appropriate degree of regularity, are easily integrated/differentiated, and have the added benefit of being physically intuitive. If a more accurate representation of the current is
needed, higher-order vector basis functions [85] may be employed, though they will not be explored in this Dissertation.

Having defined an appropriate basis set, the approximate equivalent surface current is given as:

$$\bar{\mathbf{J}}_S(\mathbf{r}) \approx \bar{\mathbf{J}}_{S,h}(\mathbf{r}) = \sum_{q=1}^{N_q} c_q \mathbf{u}_q(\mathbf{r})$$ (2.23)

Here, the summation is taken over all $N_q$ interior edges of the mesh upon which the $q$th RWG basis function is defined. The discrete form of the EFIE can be posed by i) computing the matrix associated with the Galerkin projection of the integral operator onto the RWG basis and ii) computing the column vector associated with the projection of the right hand side onto the RWG basis. The resultant discrete form is given as:

$$\langle \bar{\mathbf{u}}_r, \mathcal{T}_S\{\bar{\mathbf{J}}_{S,h}\} \rangle_{supp(\bar{\mathbf{u}}_r)} = -\langle \bar{\mathbf{u}}_r, \hat{n} \times \bar{\mathbf{E}}_{inc} \rangle_{supp(\bar{\mathbf{u}}_r)}$$ (2.24)

Here the equation is verified for all $\bar{\mathbf{u}}_r$, and the unknown quantity is the set of $N_q$ complex coefficients $c_q$. The non-local nature of the integral operator makes this a dense system of equations that will, in general, have have $N_q^2$ non-zero entries. Using matrix factorization methods [86], the cost of solution will scale as $O(N_q^3)$, whereas using iterative methods [87] the cost of solution will scale as $O(n_{it}N_q^2)$, where $n_{it}$ is the number of iterations required to achieve a fixed error. The focus of Section 3.7 will be on reducing the cost of iterative solution to $O(n_{it}N_q)$ using the ACE algorithm.
2.3 Scattering from Dielectric Targets

The volumetric formulation of the EFIE is typically applied to scattering from inhomogeneous or thin dielectric structures [88]. Frequently, it is advantageous to instead use the Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) [47] or Müller [48] formulations when studying scattering from dielectrics, as they only require the representation of interfaces between regions in which the medium is piecewise homogeneous. However, they require the doubling of unknowns at these interfaces, as both interior and exterior problems must be posed. Further, as the Müller and PMCHWT formulations require the use of the in-medium wavenumber in the Green’s function, whereas the volumetric EFIE does not, fast methods reliant upon the representation of the Green’s function as some sort of truncated series may require the retention of more terms to achieve the requisite accuracy in lossy or high index media. As ACE is one such method and scattering from such media will be demonstrated in Chapter 2.4, namely noble metals at optical frequencies, the volumetric EFIE will be considered in what follows. Unlike the surface EFIE, this form of the EFIE takes the form of a perturbation on the identity (Fredholm second type), and is typically free of issues with conditioning in practice [89, 90, 91]. However, because it is convenient, matrix-based preconditioning measures will still be applied when generating results.

2.3.1 Statement of the Problem

Consider a domain, \( \Omega \subset \mathbb{R}^3 \), in which a set of dielectric scatterers is embedded, characterized by the spatially varying dielectric function \( \varepsilon(\mathbf{r}, \omega) \). A homogeneous background of vacuum is assumed to exist, such that \( \Omega_D = \text{supp}(\varepsilon(\mathbf{r}, \omega) - \varepsilon_0) \), is compact. The domain
is excited by an incident planewave of the same form as Equation 2.17. The interrogating field gives rise to a scattered field, \( \vec{E}_{\text{scat}}(\vec{r}) \), such that the total field can be expressed as a linear superposition, \( \vec{E}(\vec{r}) = \vec{E}_{\text{inc}}(\vec{r}) + \vec{E}_{\text{scat}}(\vec{r}) \). Using the volumetric equivalence principle [76], this scattered field can be expressed in terms of convolutions with an equivalent source distribution \( \vec{J}_V(\vec{r}) \) supported by \( \Omega_D \), radiating into an homogeneous domain:

\[
\vec{E}_{\text{scat}}(\vec{r}) = -i\kappa \eta \int_{\Omega_D} d^3\vec{r}' \overline{G}(\vec{r}, \vec{r}') \cdot \vec{J}_V(\vec{r}') \tag{2.25}
\]

Here, \( \overline{G}(\vec{r}, \vec{r}') \) is defined in Equation 2.19 and \( \vec{J}_V(\vec{r}) \) is related to the electric displacement, \( \vec{D}(\vec{r}) = \varepsilon(\vec{r}, \omega) \vec{E}(\vec{r}) \), as follows:

\[
\vec{J}_V(\vec{r}) = i\omega C_D(\vec{r}) \vec{D}(\vec{r}), \quad \text{where} \quad C_D(\vec{r}) = \frac{\varepsilon(\vec{r}, \omega) - \varepsilon_0}{\varepsilon(\vec{r}, \omega)} \tag{2.26}
\]

From this substitution, it should be evident that the support of \( J_V(\vec{r}) \) is \( \Omega_D \). Another convenient feature of this substitution is that any discontinuities in the normal component of \( \vec{J}_V(\vec{r}) \) across material interfaces is due to \( C_D(\vec{r}) \) rather than \( \vec{D}(\vec{r}) \), which is normally continuous in the absence of impressed charges.

A Fredholm integral equation of the second type can be posed by enforcing the identity of the total field.

\[
\vec{E}(\vec{r}) - \vec{E}_{\text{scat}}(\vec{r}) = \vec{E}_{\text{inc}}(\vec{r}), \quad \forall \vec{r} \in \Omega_D \tag{2.27}
\]

\[
\vec{D}(\vec{r})/\varepsilon(\vec{r}, \omega) - i\kappa \eta \int_{\Omega_D} d^3\vec{r}' \overline{G}(\vec{r}, \vec{r}') \cdot \left(i\omega C_D(\vec{r}') \vec{D}(\vec{r}')\right) = \vec{E}_{\text{inc}}(\vec{r}), \quad \forall \vec{r} \in \Omega_D \tag{2.28}
\]

\[
\left(\vec{D}(\vec{r})/\varepsilon(\vec{r}, \omega) + \tau_V \{\vec{D}\} [\vec{r}]\right) = \vec{E}_{\text{inc}}(\vec{r}), \quad \forall \vec{r} \in \Omega_D \tag{2.29}
\]
This equality is the volumetric EFIE. In Section 2.3.2, the details necessary for its numerical solution are presented, and then later in Section 3.7.2 it will be utilized to study scattering from periodic arrays of dielectric structures.

2.3.2 Numerical Details

The basis function space that will be utilized for the discrete problem is very similar to the one for the surface EFIE in Section 2.2.2. While the approximate \( \mathbf{D}_h(\mathbf{r}) \) will be defined in terms of functions supported by a simplicial tesselation of \( \Omega_D \), this domain is of a volumetric extent, so the associated simplices are tetrahedra. An exemplary tetrahedral mesh is illustrated in Figure 2.5.

Linear vector basis functions will be used, due to Schaubert, Wilton, and Glisson [88] otherwise known as SWG basis functions. Some of the useful features of these functions are as follows:

- Basis functions are associated with all interior/exterior faces of the mesh and compactly supported by the one or two adjacent tetrahedra.

- Continuity of the electric displacement is satisfied across all faces.

- The charge density, i.e., divergence, on the interior of the support is piecewise constant, and globally neutral.

Similar to RWG basis functions, SWG basis functions have the appropriate regularity, are easy to manipulate, and intuitive. As with the surface EFIE, higher-order vector basis functions [85] are also available, but will not be necessary for the results presented in Chapter 2.4.
Using the SWG basis, the approximate electric displacement is rendered as:

\[ \tilde{D}(\tilde{r}) \approx \tilde{D}_h(\tilde{r}) = \sum_{q=1}^{N_q} c_q \tilde{u}_q(\tilde{r}) \]  

(2.30)

Here the summation is taken over all \( N_q \) faces, both interior and exterior, upon which the \( q \)th SWG basis functions is defined. A discrete form of the volumetric EFIE is derived similar to the discrete form of the surface EFIE, leading to:

\[ \langle \tilde{u}_r, \tilde{D}_h/\varepsilon \rangle_{\text{supp} \tilde{u}_r} + \langle \tilde{u}_r, \mathcal{T}_V \{ \tilde{D}_h \} \rangle_{\text{supp} \tilde{u}_r} = \langle \tilde{u}_r, \tilde{E}_{\text{inc}} \rangle_{\text{supp} \tilde{u}_r} \]  

(2.31)

This equation is verified for all \( \tilde{u}_r \), and the unknown quantities are the \( N_q \) complex coefficients. As with the surface EFIE, this is a dense system of equations that will generally require \( \mathcal{O}(N_q^3) \) operations for a direct solution or \( \mathcal{O}(n_{it}N_q^2) \) for an iterative solution. Section 3.7 will include results that demonstrate the \( \mathcal{O}(n_{it}N_q) \) solution of this form of the EFIE.

2.4 Figures
Figure 2.4: An exemplary triangular mesh used in calculating scattering from a periodic array of PEC split ring resonators.
Figure 2.5: An exemplary tetrahedral mesh used in calculating scattering from a periodic array of dielectric spheres.
Chapter 3: Periodic ACE

3.1 Overview of Periodic ACE

Chapter 2 presented an overview of the IE formulations that will be used to analyzing scattering from periodic structures. The focus of this Chapter will be fast methods for solving them - namely, the ACE algorithm. At first, a generic approach will be taken in which extensions of the ACE algorithm will be presented for a number of long-range interactions in periodic systems - weakly screened Yukawa and low-frequency Helmholtz. The attendant theoretical and implementation-oriented details will be described, including modifications made to the octree structure - a hierarchical decomposition of the domain common to hierarchical fast methods. Results will be presented that validate claims of linear scaling and convergence to arbitrary accuracy. After validating the performance of the kernel evaluation, the ACE algorithm will be applied to the analysis of scattering from PEC and dielectric structures, with details affirming agreement with established codes and measurement, as well as significant acceleration over an unaccelerated reference code.

3.2 Hierarchical Fast Methods

3.2.1 Tree Codes, FMM, and ACE

In Section 1.2.4, the basic philosophy of fast methods for IEs was discussed in terms of reducing the cost of effecting a discrete convolution between a dense $N \times N$ kernel matrix and a vector of length $N$. Classically, the cost of this operation is $O(N^2)$, however, fast methods promise to reduce this cost to $O(N \log^\alpha(N))$ for $\alpha \in (0, 1)$, a geometry-dependent
constant. While this was discussed in the context of the iterative solution of IEs, more generally one might consider the evaluation of the energy of interaction between \( N \) bodies due to a pairwise potential. Here, the unknown to be resolved is simply the convolution itself, rather than its operand. This was in fact the motivation that drove the development of the first tree codes, due to Barnes and Hut [92], and the FMM of Greengard and Rokhlin [93] - the rapid evaluation of the gravitational/Coulombic potential due to a distribution of masses/charges.

In spite of their frequent conflation, tree codes and FMMs represent two distinct approaches to the efficient evaluation of pairwise potentials that are best explained in [94]. The Barnes-Hut tree code [92] was based upon the observation that the gravitational potential at a point due to masses far away can be accurately represented in terms of a truncated multipole expansion of the mass distribution. More generally, in tree codes the interaction between a source-observer pair is computed using one of three options: (i) directly, (ii) at each observation point using the multipole expansion due to a cluster of sources, or (iii) using local expansions at a cluster of observers. FMMs take this set of principles further, introducing aggregation and disaggregation operators, that permit the computation of potentials in an optimal manner [94].

The ACE algorithm is included under the umbrella of FMM-type methods, as it includes both aggregation and disaggregation operators. Classical FMMs rely on constructing a representation of the Green’s function in terms of special functions; for instance, the Coulombic Green’s function is represented in terms of spherical harmonics. The ACE algorithm, on the other hand, is based upon a representation of the Green’s function as a generalized Taylor expansion that is expressed in terms of totally symmetric tensors which reduce the overall
cost relative to other Cartesian methods.

In 2007, ACE was introduced for the evaluation of potentials of the form $r^{-\nu}$ [59]. While it is based on Taylor series expansions, it was shown that it is possible to develop exact aggregation and disaggregation operators. Due to this feature, no further error is introduced in translating the origins of multipole or local expansions, in contrast to FMMs. More interestingly, using the well-known equivalence between traceless Cartesian tensors and Legendre polynomials, it was shown that it is possible to develop relationships, both in terms of cost and operations, between ACE and classical FMM. As ACE is not wedded to addition theorems for special functions, it is possible to apply these to the rapid evaluation of many different potentials. To date, this has also been done for Lienard-Wiechert potentials [95], and diffusion, Klein-Gordon, and lossy wave potentials [96]. Likewise, ACE has also been implemented together with FMM for the wideband analysis of electromagnetic phenomena [97], with analytical error bounds that have been demonstrated via numerical experimentation.

In what follows, the extension of ACE to potentials in periodic systems will be described.

3.2.2 Specialization To Periodic Systems

While FMMs, including ACE, have been studied extensively in the context of non-periodic problems [98, 99, 100], their adaptation to periodic problems is encountered less frequently in the available literature. In particular, virtually all of the previous work on periodic FMMs is for Coulomb systems, with only a few examples of papers on periodic Helmholtz [101, 102] or Yukawa systems [103]. This can be partially attributed to difficulties commonly encountered in periodizing long-range potentials. This can be best seen in terms of the development of periodic Coulomb FMMs. In their seminal paper on the FMM [93],
Greengard and Rokhlin implement periodic boundary conditions, as well as Dirichlet and Neumann, for the two-dimensional Coulomb potential. In this context, the influence of an infinite array of image cells must be computed within some original primitive unit cell. To this end, periodicity is enabled by constructing a multipole expansion for the entire primitive unit cell, acknowledging that each image cell in the periodic lattice will have the same form, and evaluating a lattice sum to construct a periodized local expansion at the original primitive unit cell. For periodic boundary conditions, Schmidt and Lee later extended this approach to three-dimensions incorporating rapidly convergent Ewald summations [104, 105], whereas subsequent work by Berman and Greengard saw the development of a renormalization-based identity for evaluating such summations in two- and three-dimensions [106]. One particularly interesting extension due to Lambert, et al [107] utilizes the hierarchical structure of the FMM to accelerate the aggregation of multipole expansions of periodic image cells recursively, yielding very efficient summations over the periodic lattice. The evaluation of lattice sums becomes more challenging in the case of Yukawa or Helmholtz potentials. In [103], for example, integral representations of the lattice sums are utilized and evaluated by quadrature.

The majority of the previously referenced FMMs incorporate periodic boundary conditions only at the top of the tree, corresponding to a multipole expansion of the entire unit cell. The local expansion due to the influence of the rest of the lattice, excepting the nearfield of the unit cell, is evaluated using lattice sums. At all levels below the top, free space translation operators are used, taking into account not only the effect of boxes lying inside of the unit cell, but nearfield boxes outside of unit cell, as well. In this Dissertation, a slightly different approach is followed, i.e., an addition theorem is developed for the full
periodic Green’s function for multipole-to-local translations. This is very similar in spirit to what has been done using interpolatory methods [108, 109, 110], and in fast time domain methods [111] in electromagnetics. By using a peroidized translation operator, all translations will be restricted to the interior of a single unit cell, reducing the total number of operations required per tree traversal relative to these other methods, at the expense of requiring more complex translation operators and the evaluation of periodic Green’s functions in the nearfield, both of which are relegated to preprocessing. Given differences between test architectures and implementation, it is difficult to draw direct comparisons between timings for our method and others available in the literature. However, extensive results will be provided that demonstrate an exceptional acceleration relative to direct evaluation, and breakeven points that are clearly very competitive with extant methods.

3.3 Statement of the Problem

3.3.1 Continuous Problem

Consider a domain, $\Omega \subset \mathbb{R}^3$, supporting a source distribution, $\rho(\vec{r}) : \Omega \rightarrow \mathbb{R}$, that gives rise to an unknown potential, $\psi(\vec{r})$, governed by the following Helmholtz equation:

$$\left( \nabla^2 + \kappa^2 \right) \psi(\vec{r}) = -\rho(\vec{r}) \quad (3.32)$$

Here, $\kappa \in \mathbb{C}$, such that Equation 3.32 can be continued to a Yukawa problem for purely imaginary $\kappa$, a lossy Helmholtz problem for general complex $\kappa$, or a Coulomb problem for $\kappa = 0$. Assume that $\rho(\vec{r})$ is Bloch-periodic with respect to a $\mu$-dimensional lattice, $\mathcal{L}_\mu$, 

defined as:

\[ \mathcal{L}_\mu := \{ \mathbf{t}(\mathbf{n}_\mu) = \sum_{i=1}^{\mu} n_i \mathbf{a}_i \mid n_i \in \mathbb{Z} \} \]  

(3.33)

Here, \( \mathbf{n}_\mu \) is used as a short-hand notation for the \( \mu \)-tuple \((n_1, \ldots, n_\mu)\), and \( \mathbf{a}_i \) are the primitive vectors associated with some Bravais lattice. One can then define the associated reciprocal lattice, \( \mathcal{L}^*_\mu \):

\[ \mathcal{L}^*_\mu = \{ \mathbf{k}(\mathbf{n}_\mu) = \sum_{i=1}^{\mu} n_i \mathbf{b}_i \mid n_i \in \mathbb{Z} \} \]  

(3.34)

Here, \( \mathbf{b}_i \) are the primitive reciprocal lattice vectors, which together with the primitive lattice vectors satisfy \( \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij} \).

Using these definitions, the Bloch-periodicity of \( \rho(\mathbf{r}) \) can be expressed as follows:

\[ \rho(\mathbf{r} - \mathbf{t}(\mathbf{n}_\mu)) = e^{-i\mathbf{k}_0 \cdot \mathbf{t}(\mathbf{n}_\mu)} \rho(\mathbf{r}) : \mathbf{t}(\mathbf{n}_\mu) \in \mathcal{L}_\mu \]  

(3.35)

Here, \( \mathbf{k}_0 \in \mathbb{R}^\mu \) is the Bloch wavevector describing the phase relationship between values of \( \rho(\mathbf{r}) \) when the argument is translated by a vector in \( \mathcal{L}_\mu \). This condition is derived in Section A.1.1 of the Appendix. It is evident that the specific case of \( \mathbf{k}_0 = 0 \) corresponds to conventional periodicity, wherein \( \rho(\mathbf{r}) \) is left invariant under a translation of the argument by a vector in \( \mathcal{L}_\mu \). Given this constraint on \( \rho(\mathbf{r}) \), it can be characterized over a reduced volume namely the primitive cell, \( \Omega_\mu \subset \Omega \), the minimal set which reflects the translational symmetry of the lattice. One can completely reconstruct \( \Omega \) from a union of primitive cells shifted by all lattice vectors in \( \mathcal{L}_\mu \):

\[ \Omega = \{ \Omega_\mu + \mathbf{t}(\mathbf{n}_\mu) \mid \mathbf{t}(\mathbf{n}_\mu) \in \mathcal{L}_\mu \} \]  

(3.36)
Here, the set \( \Omega_\mu + \mathbf{t}(\mathbf{n}_\mu) = \Omega_{\mathbf{n}_\mu} \) is referred to as the \( \mathbf{n}_\mu \)th image cell, where \( \Omega_{(0,\ldots,0)} = \Omega_\mu \) is the central primitive cell. The measure of space occupied by a single primitive cell in the subspace of the lattice is denoted as \( \mathcal{A}_\mu \) (i.e., \( \mathcal{A}_1 \) = length of the primitive cell, etc.). Figure 3.6 provides a pictorial representation of \( \Omega \) for \( \mu = 2 \).

By the translational invariance of the coefficients in Equation 3.32, that \( \rho(\mathbf{r}) \) is Bloch-periodic is sufficient to guarantee the Bloch-periodicity of \( \psi(\mathbf{r}) \), as well.

\[
\psi(\mathbf{r} - \mathbf{t}(\mathbf{n}_\mu)) = e^{-i\mathbf{k}_0 \cdot \mathbf{t}(\mathbf{n}_\mu)} \psi(\mathbf{r}) : \mathbf{t}(\mathbf{n}_\mu) \in \mathcal{L}_\mu \tag{3.37}
\]

While this will suffice to constrain all boundary conditions for \( \mu = 3 \), for \( \mu = 1 \) and \( \mu = 2 \) there are \( 3 - \mu \) unspecified boundaries. These boundaries are chosen to behave as if unbounded space lies beyond them, as this is frequently the physically relevant choice for numerous applications. More specifically, the situation in which the potential either decays as an observer recedes away from the lattice for complex \( \kappa \), or satisfies a radiation boundary condition for real \( \kappa \) is under consideration.

Having fully specified the problem, i.e., PDE and boundary condition, potential solutions for \( \psi(\mathbf{r}) \) may be constructed.

\[
\psi(\mathbf{r}) = \int_{\Omega_\mu} d\mathbf{r}' G_\mu(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}') \tag{3.38}
\]

Here, \( G_\mu(|\mathbf{r} - \mathbf{r}'|) \) is the appropriate Bloch-periodic Green’s function. Given its rapid and absolute convergence in and away from \( \mathcal{L}_\mu \), the Ewald representation [112] of the Bloch-
The periodic Green's function is utilized.

$$G_\mu(|\vec{r} - \vec{r}'|) = \sum_{\vec{t}(\vec{n}_\mu) \in \mathcal{L}_\mu} e^{-i\vec{\kappa}_0 \cdot \vec{t}(\vec{n}_\mu)} \mathcal{E}_r(|\vec{r} - \vec{r}' - \vec{t}(\vec{n}_\mu)|) + \sum_{\vec{k}(\vec{n}_\mu) \in \mathcal{L}^*_\mu} \mathcal{E}_k(\vec{r} - \vec{r}', \vec{k}(\vec{n}_\mu) + \vec{\kappa}_0)$$

(3.39)

Following the usual convention, the first summation will be referred to as the 'real sum' and the second as the 'reciprocal sum'. The functional form of the terms in the real sum are independent of $\mu$:

$$\mathcal{E}_r(|\vec{r} - \vec{r}' - \vec{t}(\vec{n}_\mu)|) = \sum_{\pm} e^{\pm i\kappa |\vec{r} - \vec{r}' - \vec{t}(\vec{n}_\mu)|} \text{erfc} \left( \eta |\vec{r} - \vec{r}' - \vec{t}(\vec{n}_\mu)| \pm i \frac{\kappa}{2\eta} \right)$$

(3.40)

Here, 'erfc' is the complementary error function, and $\eta \in \mathbb{R}^+$ is referred to as the 'splitting parameter', the value of which controls the relative rate of convergence of the two sums in Equation 3.39. The significance of this parameter is addressed in Section A.1.2 of the Appendix.

The form of the terms in the reciprocal sum depend on the value of $\mu$:

$$\mathcal{E}_k(\vec{r} - \vec{r}', \vec{k}(\vec{n}_\mu) + \vec{\kappa}_0) = \frac{e^{i(\vec{k}(\vec{n}_1) + \vec{\kappa}_0) \cdot \vec{r}_l}}{4\pi A_1} \sum_{\nu=0}^{\infty} \frac{(-1)^\nu}{\nu!} (|\vec{r}_l|\eta)^{2\nu} E_1 + \nu \left( \frac{\alpha^2(\vec{n}_1)}{4\eta^2} \right)$$

(3.41a)

$$= \frac{e^{i(\vec{k}(\vec{n}_2) + \vec{\kappa}_0) \cdot \vec{r}_l}}{4\alpha(\vec{n}_2) A_2} \sum_{\pm} e^{\pm \alpha(\vec{n}_2) |\vec{r}_l|} \text{erfc} \left( \frac{\alpha(\vec{n}_2)/2}{2\eta} \pm \eta |\vec{r}_l| \right)$$

(3.41b)

$$= \frac{e^{i(\vec{k}(\vec{n}_3) + \vec{\kappa}_0) \cdot \vec{r}_l - \alpha^2(\vec{n}_3)/4\eta^2}}{A_3 \alpha^2(\vec{n}_3)}$$

(3.41c)
Here, $E_n$ is the exponential integral of $n$th order, and $\mathbf{r}_l$ and $\mathbf{r}_t$ are projections of $\mathbf{r} - \mathbf{r}'$ parallel and transverse to the span of $\mathcal{L}_\mu$, respectively. The form of $\alpha(\mathbf{n}_\mu)$ is independent of $\mu$:

$$
\alpha(\mathbf{n}_\mu) = \sqrt{|\mathbf{k}(\mathbf{n}_\mu) + \kappa_0|^2 - \kappa^2}
$$

(3.42)

Given the form of $G_\mu(|\mathbf{r} - \mathbf{r}'|)$, and some arbitrary $\rho(\mathbf{r})$ on $\Omega_\mu$, $\psi(\mathbf{r})$ can be evaluated for all $\mathbf{r}$ in $\Omega$. An exemplary discretization of this calculation is considered next, to which the ACE algorithm can be applied to achieve the efficient evaluation of a discrete form of $\psi(\mathbf{r})$.

### 3.3.2 Discrete Problem

Without loss of generality, consider the case where $\rho(\mathbf{r})$ can be expressed in terms of $N$ point sources distributed throughout $\Omega_\mu$:

$$
\rho(\mathbf{r}) = \sum_{s=1}^{N} w_s \delta(\mathbf{r} - \mathbf{r}_s)
$$

(3.43)

Here, $\mathbf{r}_s \in \Omega_\mu$ is the location of the $s$th source, and $w_s$ is its associated weight. Equation 3.38 can be used to write $\psi(\mathbf{r})$ as:

$$
\psi(\mathbf{r}) = \sum_{s=1}^{N} w_s G_\mu(|\mathbf{r} - \mathbf{r}_s|)
$$

(3.44)
The calculation of the mutual interaction between the sources is considered, i.e., Equation 3.38 is evaluated at all source points. This can be recast as a matrix equation as follows:

\[
\psi(\vec{r}_o) = \sum_{s \neq o} G(\|\vec{r}_o - \vec{r}_s\|) \rightarrow \Psi_o = (1 - \delta_{os})G(\|\vec{r}_o - \vec{r}_s\|)Q_s
\]  

(3.45a)

\[
\Psi_o = G_{os}Q_s
\]  

(3.45b)

Here, \(G_{os}\) is an \(N \times N\) matrix in which the self-terms are explicitly excluded and \(Q_s\) and \(\Psi_o\) are \(N \times 1\) column vectors. From this form of the potential, it is evident that the evaluation of \(\Psi_o\) will require \(O(N^2)\) operations and \(O(N^2)\) storage using direct methods. It is the goal of Sections 3.4, 3.5 and 3.6 to demonstrate that the ACE algorithm can be used to reduce the total cost of this computation to \((N)\) in both time and storage. In Section 3.7 it will be demonstrated that this same computational framework can be adapted to the iterative solution of integral equations that arise in electromagnetic scattering problems. It is worth remarking here that the latter Section will be concerned with the resolution of \(Q_s\), given some known \(\Psi_o\).

3.4 Details of the ACE Algorithm

ACE and other FMM-type methods achieve an \(O(N)\) cost in timing and storage by approximating Equation 3.45 as follows:

\[
\Psi_o = G_{os}Q_s \approx G_{os}^{\text{near}}Q_s + \mathcal{T}^{ACE}(Q_s)
\]  

(3.46)
Here, $G_{os}^{near}$ is a sparse matrix, carrying only the entries of $G_{os}$ that arises due to source-observer pairs which are in some metric, ‘near’, and $\tau^{ACE}$ is some composition of operations which approximately effects the remaining ‘far’ source-observer pairs. $\tau^{ACE}$ will be defined explicitly in Section 3.4.4. The ACE algorithm describes the metric that demarcates ‘near’ and ‘far’ interactions based upon a hierarchical decomposition of $\Omega_\mu$, and provides rules for evaluating both terms in Equation 3.46 in a manner requiring $O(N)$ operations and storage.

Such a hierarchical decomposition is achieved by mapping all source and observer points onto a regular octree data structure, henceforth referred to as ‘the tree’. This structure provides a natural metric by which ‘near’ and ‘far’ interactions can be separated, as well as a means by which the application of $\tau^{ACE}$ can be mapped onto the traversal of the tree. With this in mind, the ACE algorithm proceeds along the following steps:

1. Construct the tree based upon discretization of $\rho(\vec{r})$ and $\psi(\vec{r})$ in $\Omega_\mu$.
2. Fill nearfield/farfield interaction lists based upon the structure of the tree.
3. Precompute nearfield matrix elements and ACE translation operators.
4. Compute $\Psi_o$ via sparse nearfield matrix multiplication and tree traversal.

Steps 1-3 constitute pre-processing, which need be performed only once for a fixed source distribution. Step 4 is the only recurring step, required for the repeated evaluation of a potential in which the entries of $Q$ vary, as may be required for the iterative resolution of a linear system of equations. In Sections 3.4.1-3.4.4 each of these steps is described in detail.
3.4.1 Tree Construction

Tree construction is based upon the specification of the desired number of levels, \( N_l \), chosen to optimize the cost and/or error. The primitive cell, \( \Omega_\mu \), is recursively subdivided into boxes of equal volume \( N_l - 1 \) times. A single level of the tree is defined by a set of boxes of equal volume, with 1 being the level with the smallest (‘leaf’) boxes. At a given level, a box subordinate to a larger box at the level above is deemed the child to the larger box, which is deemed its parent. Every box is assigned an address in octal, based upon a canonical octree decomposition, allowing us to readily acquire the ‘genealogy’ of a particular box given its address alone. This method of addressing boxes is called Morton ordering or Z-space filling curves [113]. Each box at the leaf level carries a list of the point sources/observers lying inside its boundaries. Given the hierarchical structure of the tree, it is trivial to determine the point sources/observers subordinate to boxes at lower levels by recursively aggregating children until the leaf level is reached.

As will be explicitly discussed in the next section, the construction of the interaction lists requires the consideration of not just boxes that lie inside of \( \Omega_\mu \), but their nearest images as well. This is done to properly catalog near and far interactions, as is elucidated in the next section. The images of the cell are included by adding two fictitious levels together with the tree hierarchy that represents the nearest images of \( \Omega_\mu \). Figure 3.7 illustrates this modification to the overall structure. Note, these image boxes will not contain any explicit sources or observers, and are not involved in tree traversal. Instead, they only serve as placeholders used in addressing boxes, incurring a negligible computational overhead. Consequently, their contribution to the height of the tree is not considered when it is referenced. As the
addressing scheme of a regular octree follows Morton ordering, boxes inside the primitive cell will fall within a contiguous address space [113]. This provides a simple means by which real boxes can be distinguished from image boxes. As will be discussed in Section 3.4.2, knowledge of the nearest images of the primitive cell are essential in constructing the necessary interaction lists, which this extension of the conventional tree structure provides.

3.4.2 Interaction Lists

Among the most crucial steps in tree-based methods is choosing an appropriate rule for separating ‘near’ and ‘far’ interactions. In non-periodic domains, this demarcation is a relatively straightforward task. Two boxes are considered to be ‘far’ from one another if (i) they are separated by at least one box length and (ii) their parents are not ‘far’ from one another. The first portion of this criterion is naturally tied to the distance between boxes, and ensures that spatial variations in the relative potential of the two domains are limited. The latter portion, on the other hand, ensures that ‘far’ interactions are computed in $\mathcal{O}(N)$ operations.

One of the primary challenges in adapting ACE to periodic domains is constructing a rule that meets both of these needs: minimal spatial variation in the relative potential as well as $\mathcal{O}(N)$ scaling. This is somewhat non-trivial, in that the periodic boundary conditions map the problem onto a domain with a toroidal topology. Consequently, the distance between two boxes is no longer unique, as each box will possess images that effectively contribute to the relative potential through the periodic Green’s function. In determining whether or not
two boxes in the primitive cell are ‘far’ from one another, a rule that gives consideration to all image boxes must be constructed. Such a rule is as follows:

1. The original boxes and all of their images are separated by at least one box length.

2. Among the parents of both the original and image boxes, at least one pair is not ‘far’.

Figure 3.8 illustrates the ‘near’ and ‘far’ boxes for exemplary boxes at different levels of a tree with $N_l \geq 4$. The contents of boxes outlined in blue are stored explicitly in the tree, whereas boxes outlined in red are part of the fictitious extra levels discussed in the previous Section. For both exemplary boxes, it is worth noting the manner in which the nearfield wraps around the unit cell. The source box residing in the upper left corner of the primitive cell will participate in nearfield interactions with observer boxes residing at each of the other 3 corners, in spite of their apparent distance. Poorer error convergence has been observed when using the usual, non-periodic rules for parsing interactions, so this is an important subtlety to keep in mind when adapting extant codes to periodic problems.

Mechanically, the construction of the interaction lists is straightforward. For a given level, the range of addresses which lie inside the primitive cell is known, so an iteration over boxes can be explicitly restricted to only these boxes. This iteration begins at the $(N_l - 1)\text{th}$ level, just below the ‘root’ of the real tree, at which all boxes are ‘near’ each other. At the next level down, the children of these boxes are iterated over, and the ‘near’ versus ‘far’ rule outlined above is applied. As the nearest image boxes are addressed using Morton ordering, both the relative location of an image box given its corresponding real box and its entire ‘genealogy’ can be located. The descent of the tree continues, iterating over only real boxes.
at each level, until all boxes at the leaf level are visited, at which point the interaction lists are complete. These lists are next employed in precomputation, in which they are used to construct a list of the necessary nearfield matrix elements and unique ACE translation operators that need be computed.

3.4.3 Precomputation

Precomputation can be broken into two stages, (i) nearfield matrix elements and (ii) ACE translation operators. In constructing nearfield matrix elements, all unique source-observer pairs are considered, and elements of $G^{\text{near}}$ are computed directly. Precomputation of ACE translation operators is slightly more complex. All farfield interactions are sorted by the distance separating source and observer parent domains in each of the Cartesian coordinates. Given the regularity that our decomposition of the domain imposes (i.e. all boxes at a given level have the same dimensions), and that the ACE translation operators only depend upon the relative separation of two boxes, and not their absolute position, there is significant degeneracy among the ACE translation operators. Consequently, in sorting by domain separation, a subset of unique translation operators can be identified. These can be computed once, stored, and recycled. This is particularly important in periodic ACE, as the calculation of a single unique translation operator will possess $(P + 3)(P + 2)(P + 1)/6$ unique components, each of which is an Ewald-like infinite sum (see Equation 3.51).
3.4.4 Tree Traversal

The evaluation of $T^{ACE}(Q_s)$, in Equation 3.46 proceeds along the five steps presented below. In general, these steps are common to any FMM, though the mathematical details differ from algorithm to algorithm.

1. **Charge-to-Multipole (C2M):** Construct Multipole expansions from point sources in each leaf box.

2. **Multipole-to-Multipole (M2M):** Aggregate Multipole expansions at higher levels of the tree.

3. **Multipole-to-Local (M2L):** Translate Multipole expansions about source domains to Local expansions about observer domains.

4. **Local-to-Local (L2L):** Disaggregate Local expansions at lower levels of the tree.

5. **Local-to-Observer (L2O):** Compute potential at observers from Local expansions in each leaf box.

In what follows, these steps are mathematically codified in terms of Theorems, proofs of which are available in [59]. As these Theorems are reliant upon the language of Cartesian tensors, a brief overview of the necessary notation is provided in exposition.

A Cartesian tensor of rank $n$ is denoted by $A^{(n)}$. In general, such a tensor consists of $3^n$ components from $\mathbb{C}$, indexed by the set $\{\alpha_i \mid i \in \{1, \ldots, n\}, \alpha_i \in \{1, 2, 3\}\}$, where an individual component is given as $A^{(n)}_{\alpha_1 \ldots \alpha_n}$. A totally symmetric tensor is one in which $A^{(n)}_{\alpha_1 \ldots \alpha_n}$ is independent of any permutation on the indices, and can be represented by $(n+1)(n+2)/2$
independent components. Consequently, one can index components of the totally symmetric
tensor, $A^{(n)}$, as $A[n_1, n_2, n_3]$, where $n_i$ is the number of times that index $i$ occurs and
$n_1 + n_2 + n_3 = n$. An $n$-fold contraction between two tensors is denoted by $\cdot n \cdot$, such that
$C^{(m-n)} = A^{(m)} \cdot n \cdot B^{(n)}$. Finally, an $n$-fold product of a rank 1 tensor, $\mathbf{r}$, with itself is
denoted by $\mathbf{r}^{(n)}$. More details concerning Cartesian tensors and notation can be found in
References [59] and [114].

To provide context for the ACE Theorems, an exemplary scenario is constructed in which
consideration is given to the computation of potentials observed in a domain $\Omega_{obs} \subset \Omega_\mu$, due to sources in a domain $\Omega_{src} \subset \Omega_\mu$. The two domains are well-separated in the sense
that they are in each others’ farfield. The linearity of the ACE framework implies that
potentials in $\Omega_{obs}$ due to other farfield source clusters can be found using the same procedure.
Superordinate to the two domains of interest are their respective parent domains, $\Omega_{src} \subset
\Omega_{src}^p$ and $\Omega_{obs} \subset \Omega_{obs}^p$. The centroids of these domains are located at $\mathbf{r}_{src}$, $\mathbf{r}_{src}^p$, $\mathbf{r}_{obs}$, and
$\mathbf{r}_{obs}^p$. This scenario is illustrated in Figure 3.9.

Using these notations the steps of the tree traversal process, as outlined in the beginning
of this Section, are effected using the following five Theorems.

**Theorem 3.4.1 (Charge-to-Multipole Expansion (C2M)).** The potential, $\psi(\mathbf{r}_o)$, at
any point $\mathbf{r}_o \in \Omega_{obs}$, due to $S$ sources at points $\mathbf{r}_s' \in \Omega_{src}$ with strength $q_s$ ($s \in \{1,2,\ldots,S\}$)
can be expressed in terms of a Cartesian multipole expansion.

\[ \psi(\mathbf{r}_o) = \sum_{s=1}^{S} w_s G_\mu(|\mathbf{r}_o - \mathbf{r}'_s|) = \sum_{n=0}^{\infty} M^{(n)} \cdot n \cdot \nabla^{(n)} G_\mu(\mathbf{r}_o - \mathbf{r}_{src}), \quad (3.47a) \]

\[ M^{(n)} = \sum_{s=1}^{S} (-1)^n q_s \frac{n!}{n!} (\mathbf{r}'_s - \mathbf{r}_{src})_n \quad (3.47b) \]

**Theorem 3.4.2 (Multipole-to-Multipole Expansion (M2M)).** A multipole expansion of \( S \) sources about \( \mathbf{r}_{src} \), \( O^{(n)} \), can be expressed in terms of a multipole expansion about the point \( \mathbf{r}_{psrc}^{p} \).

\[ M^{(n)} = \sum_{s=1}^{S} (-1)^n q_s \frac{n!}{n!} (\mathbf{r}'_s - \mathbf{r}_{src}^{p})_n = \sum_{m=0}^{n} \sum_{P(m,n)} \frac{m!}{n!} (\mathbf{r}_{src}^{p} - \mathbf{r}_{src})^{(n-m)} O^{(m)} \quad (3.48a) \]

\[ O^{(n)} = \sum_{s=1}^{S} (-1)^n q_s \frac{n!}{n!} (\mathbf{r}'_s - \mathbf{r}_{src})_n \quad (3.48b) \]

Here, it is important to note that Equation 3.48a is mathematically equivalent to Equation 3.47b. In other words, no additional error is incurred in shifting the origin of a multipole expansion, using Equation 3.48a instead of Equation 3.47b. It is this detail of the ACE algorithm which leads to an error which is completely independent of the height of the tree, a feature which is demonstrated to machine precision in [59, 97, 96].

**Theorem 3.4.3 (Multipole-to-Local Translation (M2L)).** For a multipole expansion about \( \mathbf{r}_{src}^{p} \), \( M^{(n)} \), a local expansion \( L^{(n)} \) that produces the same potential in \( \Omega_{obs}^{p} \) is given
\[ \psi(\mathbf{r}_o) = \sum_{n=0}^{\infty} (\mathbf{r}_o - \mathbf{r}_p^o)^{(n)} \cdot n \cdot \mathbf{L}^{(n)} \]  
(3.49a)

\[ \mathbf{L}^{(n)} = \sum_{m=n}^{\infty} \frac{1}{n!} \mathbf{M}^{(m-n)} \cdot (m-n) \cdot \nabla^{(m)} \mathbf{G}_\mu(|\mathbf{r}_o^p - \mathbf{r}_{src}^p|) \]  
(3.49b)

Here, the set of tensors, \( \nabla^{(m)} \mathbf{G}_\mu(|\mathbf{r}_o^p - \mathbf{r}_{src}^p|) \), where \( m \in \mathbb{N} \), is required. This set is otherwise known as the translation operator. The elements of these tensors correspond to coefficients of a Taylor series expansion of the Green’s function about \(|\mathbf{R}| = |\mathbf{r}_o^p - \mathbf{r}_{src}^p|\).

For a rank \( p \) tensor component of the translation operator, its individual components are written as:

\[ \nabla^{(p)} \mathbf{G}_\mu(|\mathbf{R}|) \left[ px, py, pz \right] = \partial_{px} \partial_{py} \partial_{pz} \mathbf{G}_\mu(|\mathbf{R}|) : px + py + pz = p \]  
(3.50)

As the Ewald representation is utilized for \( \mathbf{G}_\mu(|\mathbf{R}|) \), the necessary partial derivatives are applied to each term of Equation 3.39, yielding:

\[ \nabla^{(p)} \mathbf{G}_\mu(|\mathbf{R}|) \left[ px, py, pz \right] = \sum_{\mathbf{t}^{(p)}} e^{i\mathbf{k}_0 \cdot \mathbf{t}^{(p)}} \partial_{px} \partial_{py} \partial_{pz} \mathbf{\epsilon}_r(|\mathbf{R} + \mathbf{t}^{(p)}|) \ldots \]

\[ + \sum_{\mathbf{k}^{(p)}} \partial_{\mathbf{k}_x} \partial_{\mathbf{k}_y} \partial_{\mathbf{k}_z} \mathbf{\epsilon}_k(|\mathbf{R} + \mathbf{k}^{(p)}| + \mathbf{k}_0) \]  
(3.51)

Relatively convenient closed-form expressions for each term of these summations are provided in Section A.2 of the Appendix to facilitate implementation.

**Theorem 3.4.4 (Local-to-Local Expansion (L2L)).** A local expansion \( \mathbf{O}^{(n)} \) centered
about $\mathbf{r}_{\text{obs}}^p$ can be expressed in terms of a local expansion about the point $\mathbf{r}_{\text{obs}}$, using:

$$L^{(n)} = \sum_{m=n}^{\infty} \binom{m}{m-n} O^{(m)} \cdot (m-n) \cdot (\mathbf{r}_{\text{obs}} - \mathbf{r}_{\text{obs}}^p)^{(m-n)}$$  \hspace{1cm} (3.52)

Finally, the potential at a point $\mathbf{r}_\alpha$ in $\Omega_\alpha$ can be computed from the local expansion centered about $\mathbf{r}_\alpha$.

**Theorem 3.4.5 (Local-to-Observer (L2O)).** The potential, $\psi(\mathbf{r}_\alpha)$ can be expressed in terms of $L^{(n)}$, a local expansion centered about $\mathbf{r}_{\text{obs}}$, using:

$$\psi(\mathbf{r}_\alpha) = \sum_{n=0}^{\infty} L^{(n)} \cdot n \cdot (\mathbf{r}_\alpha - \mathbf{r}_{\text{obs}})^{(n)}$$  \hspace{1cm} (3.53)

### 3.5 Cost Analysis

The computational cost of the ACE algorithm has been previously analyzed in detail for non-periodic problems [59]. It is worth noting that this analysis is predicated upon the consideration of a randomly uniform distribution, and deviations from non-ideal scaling, i.e., $O(N \log(N))$, will be evident for highly skewed distributions. In what follows, a brief review of the dominant costs is provided and minor differences which arise in adapting ACE to periodic systems are highlighted.

Consider a primitive cell in which $N$ co-located source/observer points are randomly distributed. These points are mapped onto an $N_l$ level tree, where the number of boxes at level $l$ is $B_l$ and $B_{l-1} = 8B_l$. The average number of unknowns per leaf box is denoted $s$, i.e. $N/s = B_1$, and the total number of boxes at all levels $\sum_{l=1}^{N_l} B_l \sim \frac{N}{s} \sim B_1$. The total cost
of evaluating Equation 3.46, truncating all expansions at \( P \)th order, can be broken down into nearfield (NF), C2M, M2M, M2L, L2L, and L2O costs, each of which is summarized below:

1. **NF:** \( s^2 \) operations per ‘nearfield’ neighbor \( \times 27 \) ‘nearfield’ neighbors per leaf box \( \times B_1 \) leaf boxes: \( C_{NF} = 27Ns \)

2. **C2M:** \( s \) operations per component \( \times \sim \frac{P^3}{6} \) unique multipole components \( \times B_1 \) leaf boxes: \( C_{C2M} = \frac{N}{6}P^3 \)

3. **M2M:** \( \sim \frac{P^6}{720} \) operations per M2M translation \( \times \sim B_1 \) M2M translations: \( C_{M2M} = \frac{N}{s}P^6 \)

4. **M2L:** \( \sim \frac{P^6}{720} \) operations per ‘farfield’ neighbor \( \times \sim 56 \) ‘farfield’ neighbors per box \( \times \sim B_1 \) boxes: \( C_{M2L} = 56\frac{N}{s}P^6 \)

5. **L2L:** Same as M2M: \( C_{L2L} = \frac{N}{s}P^6 \)

6. **L2O:** Same as C2M: \( C_{L2O} = \frac{N}{6}P^3 \)

This leaves us with the total cost:

\[
C_{tot} = N \left( 27s + \frac{P^3}{3} + 58\frac{P^6}{720s} \right) \sim \mathcal{O}(N) \quad (3.54)
\]

The multiplicative factor behind \( N \) is minimized by a density of \( s \approx \frac{P^3}{18} \). As discussed in Section 3.4.1, rather than specifying a minimum box size to achieve this ideal density of unknowns prior to constructing the tree, the number of levels, \( N_l \), is specified. Knowing
that $B_1 = 8^{N_l-1}$, this ideal density of unknowns is then realized for $N_l = \left\lfloor 1 + \log_8\left(\frac{18N}{P^3}\right) \right\rfloor$.

Excepting an improvement made since the publication of [59], this is essentially the same cost structure. In the original publication, the number of ‘farfield’ neighbors per box is given as 189, here it has been reduced to 56. This is achieved by taking advantage of the exact up/down tree traversal operations in ACE. In situations in which a box is in the ‘farfield’ of all of the children of a given parent, the M2L translation will occur at the level of the parent. For a given box, there will be $27 - 8 = 19$ such parent level interactions, and $64 - 27 = 37$ child level interactions, leading to 56 such interactions in aggregate. This change in the way ‘farfield’ interactions are treated is independent of whether ACE is being used for periodic or non-periodic problems.

The only significant difference in cost between periodic and non-periodic ACE is in the prefactors in the C2M and M2L costs. The 27 ‘nearfield’ neighbors per leaf box and 56 ‘farfield’ neighbors per box are upper bounds, and in the case of non-periodic ACE, only realized for boxes that have no faces touching the boundary of the computational domain. For boxes on the boundary, however, both the number of near and far interactions will be reduced, the net effect of which is a practically negligible change in the optimal value for $s$ and the overall prefactor. In periodic ACE, however, boundary boxes essentially participate in near and far interactions as if they were on the interior of the computational domain, given our revised rule for filling interaction lists. In this sense, periodic ACE is actually closer to the idealized cost given above.
3.6 Kernel Results

In Section 3.6.1 and 3.5 results are presented validating the accuracy and linear scaling of the ACE algorithm. In both Sections results were obtained using a kernel version of the code that only evaluates Equation 3.46.

3.6.1 Error Convergence

In demonstrating error convergence, only the contributions to the total potential arising due to farfield interactions are considered. \( \Psi^\text{ACE}_o = \mathcal{T}^\text{ACE}(Q_s) \) is computed using the ACE algorithm whereas \( \Psi^\text{direct}_o = G_{os}Q_s - G_{os}^{\text{near}}Q_s \) is computed directly. This difference is not explicitly computed, rather nearfield pairs are simply ignored in evaluating the potential. This is done to allay any concerns about numerical cancellation in the reference data. The relative error in the \( L_2 \)-norm is reported in all numerical experiments:

\[
\varepsilon_{\text{far}} = \sqrt{\sum_{o=1}^{N} \frac{|\Psi^\text{ACE}_o - \Psi^\text{direct}_o|^2}{|\Psi^\text{direct}_o|^2}} \quad (3.55)
\]

As farfield contributions will tend to be slightly smaller than those due to nearfield interactions, this is in some sense a ‘worst-case’ metric for error, and one can typically expect an order of magnitude improvement in the error for the entire potential.

In Figure 3.10, convergence in the number of ACE harmonics is illustrated for \( \mu = 1, \mu = 2, \) and \( \mu = 3 \). This result was achieved using a numerical experiment with the following conditions: 8192 point sources were distributed randomly over the unit cube, which also
served as the primitive unit cell, and the farfield contribution to the total potential arising due to their mutual interaction is computed both with ACE and without ACE. The order at which the ACE expansions were truncated was varied from $P = 1$ to $P = 10$ and the relative error in only the farfield contribution to the potential was recorded.

The convergence is monotonic in $P$, and achieves an acceptable level of accuracy even for small values of $P$, e.g., the error is $< 1\%$ for $P \geq 3$. For $P \geq 6$, the rate of convergence decreases. This can be attributed to error in reconstructing higher order terms in the Ewald sum. As $|\tilde{t}(\mathbf{n}_\mu)|$ and $|\tilde{k}(\mathbf{n}_\mu)|$ increase in the real and reciprocal sums, the individual terms will exhibit a slower convergence in $P$. This is most intuitively accessible in terms of the reciprocal sum, in the individual terms become increasingly oscillatory as $|\tilde{k}(\mathbf{n}_\mu)|$ increases. However, as these terms will make an increasingly smaller contribution to the overall summation, the rate of convergence of the sum in aggregate will be dominated by terms with small $|\tilde{t}(\mathbf{n}_\mu)|$ and $|\tilde{k}(\mathbf{n}_\mu)|$. However, as the reconstruction error approaches the level at which these contributions enter the total sum, their poorer convergence will give rise to the observed non-uniformity in $P$-convergence. Otherwise, the rate of convergence is essentially independent of the type (Helmholtz or Yukawa) as well as $\mu$, and further results will be restricted to $\mu = 2$ for clarity of presentation.

In demonstrating the accuracy and applicability of ACE to a wide range of practical problems, it is interesting to analyze convergence at a fixed value of $P$ as $\kappa$ varies. Recall that $\kappa$ is inversely proportional to the screening length for the Yukawa potential, and the wavelength for the Helmholtz potential, motivating the introduction of a unitless length scale, $\lambda = 2\pi/(\kappa(A_\mu)^{1/\mu})$. This scale roughly defines how rapidly the potential will vary over a unit cell, i.e., the number of wavelengths in a unit cell for the Helmholtz potential.
That the ACE algorithm maintains a high degree of accuracy at a fixed value of $P$ for a broad range of relevant $\lambda$ values for both Helmholtz and Yukawa potentials is made evident in Figure 3.11. Here 1000 unknowns are distributed over a cube of unit volume and the farfield error is evaluated at a fixed value of $P = 6$, for both the Helmholtz and Yukawa potentials with $\mu = 2$ and $\lambda$ ranging from 0.5 to 1024. The error decreases uniformly for $\lambda > 0.5$ from $\sim 10^{-1} - 10^{-2}$ at $\lambda = 0.5$ to $\sim 10^{-7}$ at $\lambda = 1024$. This is essentially due to the fact that as $\lambda$ increases, slowly varying terms become increasingly dominant in the Green’s function. To examine the degradation in error as $\lambda$ decreases, it is useful to consider previous results and analysis for the non-periodic Helmholtz kernel, as presented in [97]. Here, the authors allude to a decrease in the efficiency of the ACE algorithm at a fixed accuracy, i.e. as $\lambda$ becomes small relative to a box length, $P$ must be increased to achieve the same relative error. This type of behavior is similarly evident in the periodic Helmholtz and Yukawa potentials. Numerical experimentation indicates that the periodic and non-periodic ACE expansions degrade at approximately the same rate as wavelength is decreased at fixed $P$. While increasing $P$ somewhat alleviates this, as $\lambda$ decreases, $P$ will become prohibitively large at some point in maintaining a desired level of accuracy, limiting the viability of ACE.

To this end, it is worthwhile to examine this apparent limitation in the context of the physical relevance of small values of $\lambda$. Consider $\lambda = 0.5$ ($\kappa = 4\pi$), the value for which error is highest in Figure 3.11. For the Yukawa potential, $\lambda = 0.5$ corresponds to a strongly screened system, in as far as second nearest neighbor cells will introduce a correction to the potential less than 0.001% of the correction due to the nearest neighbor cells. In such a strongly screened system, the interactions are better handled by short-range acceleration,
that may be as simple as maintaining interaction lists for a truncated potential. Physically relevant values of \( \lambda \) will instead be on the order of or greater than a primitive cell length \( (A_1^{1/\mu}) \), i.e. a weakly screened system for which the ACE algorithm is demonstrably accurate. For the Helmholtz potential, rather than strong screening, small values of \( \lambda \) correspond to increasingly oscillatory behavior. Fortunately, most physically relevant conditions for the periodic Helmholtz potential involve values of \( \lambda \) which correspond to systems in which the period of oscillation is on the order of, or greater than a primitive cell length. Typically frequency selective structures, metamaterials, and photonic crystals, to name but a few applications, consist of subwavelength unit cells (i.e. \( \lambda \geq 1 \) on our scale), to which the ACE algorithm is also very well-suited.

3.6.2 Computational Cost

In Figures 3.12 and 3.13 scaling of the precomputation and tree traversal times with the number of point sources, \( N \), are presented. Timings are presented for 5 different values of \( P \) to demonstrate that linear scaling can be achieved at arbitrary precision. In generating these results, \( N \) sources were distributed randomly over a unit cube on a \( \mu = 2 \) lattice with \( |\vec{a}_1| = |\vec{a}_2| = 1 \) and \( \kappa = 2\pi \). As the cost has a very weak \( \mu \) dependence, only \( \mu = 2 \) is presented as it will be of interest for applications, and the scaling is essentially the same for \( \mu = 1 \) and \( \mu = 3 \). The number of levels at each value of \( N \) is increased, from 3 to 6, maintaining an average density of unknowns per leaf box of 80. The precomputation times in Figure 3.12 include the time required for tree construction as well as the calculation of all unique translation operators that will be later applied during tree traversal. This is a one time cost that is presented to demonstrate two things: i.) precomputation scales weakly
with the number of source/number of levels and ii.) the scaling is independent of $P$.

The tree traversal timings in Figure 3.13 include the time required for all 5 steps of the tree traversal process. These results are intended to demonstrate that linear scaling is achieved independent of $P$. A linear regression indicates an $N^{1.01}$ scaling for all values of $P$, except for $P = 1$, in which the scaling is $N^{1.09}$.

3.7 ACE for Scattering from Periodic PEC and Dielectric Targets

Throughout the remainder of this Chapter, the integration of the periodized ACE algorithm into both surface and volumetric EFIE solvers will be presented. Up until now, all of the results presented are for simple kernel tests in which scalar convolutions of the form given in Equation 3.38 are accelerated. Two fundamental concerns must be addressed in adapting what has been presented up to this point to the EFIE:

- The potential integrals in the EFIE are vector quantities.

- In Equation 3.38, the unknown quantity is the result of the convolution. In an integral equation, the unknown quantity is the operand upon which the convolution is acting.

Each of these concerns will be addressed in sequence.

In the context of an EFIE solver, the role of the potential is played by a vector quantity, namely:

$$
\vec{E}_{\text{scat}}(\vec{r}) = -i\kappa\eta \int d\vec{r}' \vec{G}(\vec{r}, \vec{r}') \cdot \vec{J}(\vec{r}')
$$

(3.56)

As is evident in Equations 2.22 and 2.29, the Galerkin projection of convolutions of this form are essential components of both EFIEs. As the source ($\vec{J}$) and observed ($\vec{E}_{\text{scat}}$) fields are vector quantities, three separate trees are necessary, to accommodate each of the vector
components. Otherwise, as the Green’s function is a dyadic quantity, one might think a ‘dyadic M2L translation operator’ necessary. In practice, however, this is dealt with in one of two ways. As the component of $\overline{G}$ coefficient to $I$ is diagonal, it can be disregarded as being potentially problematic. The only modification that is necessary is due to the term that is coefficient to $\nabla \nabla$, i.e., the off-diagonal contribution. To effect this portion of the Green’s function, either the derivative terms can be transferred to the source and testing basis functions, yielding a four tree scheme, or the derivatives can be applied to the Local Expansion polynomials. The former will be more computationally intensive, whereas the latter will reduce the accuracy of the ACE expansion, by effectively removing two polynomial orders from the Local expansion.

Turning to the issue of the unknown quantity being the operand of the convolution, rather than the result, it suffices to again consider the scalar convolution in Equation 3.45. Iterative solvers based upon Krylov subspace methods [87] can be used to solve for $Q$. Such a solver generates a minimal sequence of vectors, \( \{Q^i|i \in 1, \ldots, n_{it}\} \), in the range of $G$ from which an approximate solution to Equation 3.45 can be constructed, such that $|G_{os} Q^n_{nit} - \Psi_o| \leq \varepsilon$, where $\varepsilon$ is some designated tolerance for error. The most costly part of the iterative solution process is the matrix-vector product, through which test solutions are generated and tested, leading to an $O(n_{it} N^2)$ cost. To this end, the ACE algorithm is used to accelerate the necessary $O(N^2)$ matrix-vector products to $O(N)$, yielding an $O(n_{it} N)$ overall cost.

In the following two subsections, results for an ACE accelerated EFIE solver are presented. In so far as the problem statements given in Sections 2.2.1 and 2.3.1 were agnostic to the choice of Green’s function, it is important to note that all of the results are presented for Bloch-periodic Helmholtz problems on a square lattice with $\mu = 2$. Section 2.2 uses a
surface formulation of the EFIE for the resolution of scattering from PEC targets, as stated in 2.2. Section 2.3 uses a volumetric formulation for the resolution of scattering dielectric targets, as stated in 2.3. In both Sections, the focus is on first demonstrating accuracy in reproducing either data from the literature or a reference code, and then on demonstrating that a considerable speedup is achieved using the ACE algorithm.

### 3.7.1 PEC Targets

As validation of the ACE accelerated surface EFIE code for PEC targets, power transmission spectra of a number of interesting structures are presented. In all cases, the transmission coefficient is given for the (0,0) Floquet mode on a dB scale. When making comparisons between the unaccelerated reference code and the ACE accelerated code, the same iterative methods, preconditioners, and convergence criteria are utilized and all infinite sums are evaluated to a residual relative error \( \leq 0.1\% \). With the exception of the Minkowski fractal, which is compared to a structure with dimensions found in [111], all geometries are specified in normalized units, wherein each cell is taken to be a square of area unity, and all frequencies are scaled such that the unit frequency corresponds to unity wavelength.

In Figure 3.14, the accuracy of the ACE accelerated solver is established by comparing it to an unaccelerated reference code converged to a low residual error (\( \leq 0.001\% \)). The geometry under consideration is a Jerusalem cross with \( N = 85 \) unknowns, which fits inside of a \( 0.87 \times 0.87 \) square in our normalized units. Across all frequencies, the ACE accelerated code and the reference code are in excellent agreement, and the absolute error in the transmission coefficient is strictly less than 1% (typically \( < 0.1\% \)). In general, even for such a low residual, the ACE algorithm and the unaccelerated reference code require the same number of TFQMR
Next, a result is provided that gives an indication of low breakeven point that can be achieved with an efficient implementation. In Figure 3.15, the ACE code is compared to the unaccelerated code for an Omega split ring structure with \( N = 356 \) unknowns. This structure fits inside of a \( 0.95 \times 0.8 \) rectangle, with the longer dimension parallel to the split, and a gap of 0.11 units between layers. In this test, a slightly more permissive residual is achieved (\( \leq 0.01\% \)), and the observables remain in good agreement. This particular geometry was chosen to show the conditions under which the total time to solution for both the ACE and unaccelerated codes are commensurate, in this case an average of 30 seconds per solution.

The next example (Figure 3.16) demonstrates a considerable acceleration in the time to solution for a larger problem - a Minkowski fractal FSS with dimensions taken from [111] with \( N = 2,148 \) unknowns. Here, GMRES is used with a residual error \( \leq 1\% \). For frequencies above 1 GHz, a diagonal preconditioner is utilized, whereas an ILU preconditioner is utilized below. Using an unaccelerated reference code, the average time to solution is 4,440 seconds (74 minutes) per frequency. For the ACE accelerated code, the average time to solution is 108 seconds (1.8 minutes) per frequency. From this results, it is evident that a speedup of 40x can be achieved for a structure that is relatively small by the standards of free space fast methods, while retaining accuracy.

In Figure 3.17, accuracy is validated for a layered structure with \( N = 3,206 \) unknowns. This geometry is inspired by a Minkowski fractal structure, and consists of 2 pairs of complementary patterns, the largest of which is bounded by a square of dimension \( 0.95 \times 0.95 \), for a total of 4 layers separated by 0.24 units in the \( \hat{z} \) direction. Here, TFQMR with an ILU preconditioner is utilized to achieve a residual \( \leq 0.1\% \). The average time to solution for the
ACE code is 314 seconds per frequency (\(\sim 5.2\) minutes), relative to 6,530 seconds (\(\sim 109\) minutes) per frequency for the unaccelerated code.

In Figure 3.18, surface currents for a number of structures with exceptionally high electrical densities (N=7,552 and N=20,992) are shown. Both structures have transverse dimensions that fit inside of a square of dimension 0.95 \(\times\) 0.95 and were generated via fractalization of a simple primitive structure. The first structure is based upon a triply iterated cross aperture, whereas the second structure is based upon a triply iterated Sierpinski carpet. While the first structure consists of a single layer, the second consists of 2 complementary pairs for a total of 4 layers separated by 0.16 units in the \(\hat{z}\) direction. For the first structure, the average time to solution is 1,220 seconds (\(\sim 20\) minutes) using ILU preconditioned TFQMR with a tolerance \(\leq 0.1\%\) for \(P = 7\) harmonics and \(N_l = 5\) levels. For the second structure, it is 11,200 seconds (\(\sim 3.1\) hours) using diagonal preconditioned GMRES with a tolerance \(\leq 1\%\) for \(P = 7\) harmonics and \(N_l = 6\) levels. Extrapolation based upon the unaccelerated code yields average solution times of \(\sim 11.8\) and \(\sim 91.3\) hours, respectively, without ACE.

3.7.2 Dielectric Targets

As with the surface EFIE solver in the previous section, validation is based upon the reproduction of power transmission/reflection spectra for the volumetric EFIE solver for dielectric targets. All results in this section were generated by a diagonal-preconditioned TFQMR solver with a tolerance of \(\leq 0.1\%\). All periodic Green’s function evaluations, in both the Ewald and Floquet representations, are converged to an accuracy of \(\leq 0.001\%\). All ACE translation operators were evaluated to a similar accuracy. Unless otherwise indicated, a tree with \(N_l = 5\) and \(P = 7\) ACE harmonics are utilized, to guarantee an error of \(\sim 0.01\%\)
in reconstructing potentials.

The first result is given in Figure 3.19. In it, the accuracy of the ACE accelerated code is established in reproducing power transmission through an infinite dielectric slab of width 20 nm as the angle of incidence and polarization is varied at a fixed wavelength, \( \lambda = 400 \) nm. A similar result is presented in [115], wherein a layered-medium formulation is compared against an analytic calculation. Here, a periodic volumetric formulation is utilized, wherein the unit cell has an edge length of 80 nm. As is evident, our ACE accelerated code reliably reproduces the analytic solution at both TE and TM polarization, at arbitrarily shallow incidence, for both positive and negative relative permittivities.

The results in Figure 3.20 and Figure 3.21 are intended to illustrate i) agreement of the ACE accelerated VIE code with established results from the literature and ii) acceleration relative to an unaccelerated reference code. The structure in Figure 3.20 is an electromagnetic bandgap structure with applications in microwave engineering. The reference data is taken from [116], wherein a hybrid finite element-boundary integral formulation is utilized. The ACE accelerated code is in good agreement with the established result, and a 37\( \times \) speedup relative to the unaccelerated code is achieved. The result in Figure 3.21 is taken from [117] wherein an analytic calculation is performed using Mie theory. Good agreement is again found between ACE and the established result and a 46\( \times \) speedup relative to our reference code is achieved. This structure has been used elsewhere in the literature as validation of a periodic FMM code, wherein the authors report 4–18 minutes per solution on an 8 processor platform [118]. As a surface integral equation formulation is utilized, as well as parallelism, it is difficult to draw a direct comparison between our results. Taking these differences into consideration, it is safe to at least claim that the ACE accelerated code is competitive with
the state of the art.

The next result is intended to demonstrate the utility of the ACE algorithm in studying models for novel experimental applications. It has been understood for many years that a number of the optical effects common in the wings of butterflies, such as their deep coloring or iridescence, arise due to periodic nanostructures that occur naturally in the scales covering these wings, on top of any chemical coloring (i.e. pigment) that may exist [17, 119, 120]. The blue coloring of the *Morpho* butterfly is partially due to a photonic bandgap (PBG) in the blue portion of the visible spectrum. This PBG is supported by a periodic ribbing in the material covering the butterfly’s wings on the scale of visible wavelengths [17]. Previously, Huang, et al.[18] have performed an extensive analysis of the optical properties of not just naturally occurring wings, but coated and synthetic wings made from Al$_2$O$_3$. A simple model that replicates the blue structural coloring of these types of structures has been constructed, albeit one that is both thinner and oriented differently than the one in [18]. The reflectance of this structure are given in Figure 3.22. Here, a single unit cell with $|\vec{a}_1| = |\vec{a}_2| = 320$ nm is outlined in red. The height of the structure out of plane is 280 nm and the diameter of the larger cylinders is 130 nm, with a center-center spacing of 160 nm between nearest neighbors. The smallest cylinders of diameter 20 nm with axes in the plane of periodicity are oriented along the polarization vector of the incident field, with a center-center spacing of 70 nm out of the plane of periodicity. Dielectric constants for Al$_2$O$_3$ were interpolated from [121] and the resultant mesh has $N = 10,782$ unknowns. It is worth noting that the unit cell is artificially enlarged to ensure that it is cubic. This both simplifies tree construction and increases the number of degrees of freedom for demonstrative purpose, and is not, in principal, necessary. In this result, the unaccelerated time to solution was extrapolated based
upon the nearfield matrix fill time for ACE alone, neglecting the time for iterative solution, so the speedup factor of $46 \times$ is actually representative of a lower bound on the acceleration.

The final result, in Figure 3.23, is a demonstration of capability in solving a very densely discretized structure with a highly dispersive dielectric response. This structure is inspired by [122], wherein a yellow-light fishnet metamaterial made of layered Al$_2$O$_3$ and silver on an ITO substrate is simulated and fabricated. Here, a structure with the same periodicity and nanostrip widths but without tapering and an unmodified dielectric function for Ag is modeled. The well-established Johnson and Christy permittivity for Ag [123] is utilized here, while the authors of [122] have phenomenologically increased the collision rate to account for surface roughness, grain boundaries, and size effects. Thusly, a direct comparison of results is not possible. The resultant mesh has $N = 147,374$ unknowns, and was solved using ACE with 6 levels and $P = 5$. TFQMR was applied with diagonal preconditioning to arrive at an error of $< 3\%$ with an average of 188 iterations per frequency at 20 frequencies. The average time per iteration was 3.18 minutes, and the average total time to solution was 896 minutes. Extrapolating the nearfield matrix fill time indicates that the matrix fill process alone would require 256,500 minutes using the unaccelerated reference code with the same parameters, yielding a lower bound on the speedup of $\sim 286 \times$.

3.8 Figures
Figure 3.6: An exemplary periodic domain for $\mu = 2$. The central primitive cell, as well as its 8 closest image cells are illustrated. The support of some arbitrary $\rho(\vec{r})$ is represented by the blue shaded areas.
Figure 3.7: The primitive unit cell (blue) and the 15 implicit image cells (red) involved in the enlarged tree. The original tree has $N_I = 2$, whereas the enlarged tree has $N_I = 4$. Rather than octal addresses, decimal addresses are given to provide a simpler view of the ordering.
Figure 3.8: ‘Near’ (blue) and ‘far’ (light blue) interactions for source boxes (dark blue) at different levels of the tree. The contents of the red image cells are not actually stored, but need to be considered in constructing interaction lists.
Figure 3.9: Illustration of the exemplary scenario described above. Only the primitive cell is represented. The leaf level domains are highlighted in dark blue, whereas the parent domains are highlighted in lighter blue.
Figure 3.10: Convergence of the relative error in reconstructing the farfield contribution to the potential for both Helmholtz and Yukawa systems with $\mu = 1$, $\mu = 2$, and $\mu = 3$, with $\kappa = \pi$. 8192 sources are distributed over the unit cube, which is also the primitive cell for all tests.
Figure 3.11: Farfield error as a function of $\lambda = 2\pi/\kappa$ for 1000 points randomly distributed over the unit cube at a fixed ACE order, $P = 6$, and $\mu = 2$. 
Figure 3.12: Demonstration of sublinear scaling of the precomputation time for ACE expansions of different orders. These results are generated for a Helmholtz problem with $\mu = 2$. 
Figure 3.13: Demonstration of linear scaling of the tree traversal timing for ACE expansions of different orders. These results are generated for a Helmholtz problem with $\mu = 2$. 
Figure 3.14: (Top) Plot of surface currents on Jerusalem cross. (Bottom) Power transmission spectrum at oblique incidence ($\theta = 45^\circ$, $\phi = 0^\circ$) with $\vec{E}_0 = \sqrt{2}/2 (\hat{x} - \hat{z})$. TFQMR with a diagonal preconditioner was utilized to achieve a residual $\leq 0.001\%$. $P = 7$ harmonics and $N_l = 3$ levels were used in the ACE algorithm.
Figure 3.15: (Top) Plot of surface currents on an Omega split ring structure. (Bottom) Power transmission spectrum for an Omega SRR at normal incidence ($\theta = 0^\circ, \phi = 0^\circ$) for $\vec{E}_0 = \hat{x}$. GMRES with a diagonal preconditioner was utilized to achieve a residual $\leq 0.01\%$. $P = 7$ harmonics and 3 levels were used in the ACE algorithm.
Figure 3.16: (Top) Surface currents on the Minkowski fractal FSS. (Bottom) Power transmission spectrum for a Minkowski fractal FSS.
Figure 3.17: (Left) Power transmission spectrum for a 4 layer structure at normal incidence with $\vec{E}_0 = \hat{x}$ using $N_l = 4$ and $P = 7$. (Right) plot of surface currents as viewed from the side of a single unit cell.
Figure 3.18: (Top) N=7,552 unknown structure excited at normal incidence with $\vec{E}_0 = \hat{x}$. (Bottom) N=20,992 unknown structure excited at normal incidence with $\vec{E}_0 = \hat{x}$. 
Figure 3.19: Validation of the ACE accelerated code against an analytic solution for scattering from a homogeneous dielectric slab of width 20 nm with $\epsilon = \pm 4$. 
Figure 3.20: Validation against scattering from an electromagnetic bandgap structure solved using FE-BI in [116]. The discretization has $N = 6,030$ unknowns. Average time to solution (without acceleration): $\sim 813$ minutes. Average time to solution (ACE acceleration): $\sim 23$ minutes. Total speedup: $\sim 37 \times$. 
Figure 3.21: Validation against scattering from an array of polystyrene spheres ($\epsilon_r = 2.56$) solved analytically in [117]. The discretization has $N = 7,328$ unknowns. Average time to solution (without acceleration): $\sim 2006$ minutes. Average time solution (with acceleration): $\sim 43$ minutes. Total speedup: $\sim 46 \times$. 
Figure 3.22: (Top) Scale geometry with $N = 10,782$ unknowns. (Bottom) Calculated reflectivity of a single model butterfly scale. Average time to solution (without acceleration): $\sim 1430$ minutes. Average time to solution (ACE acceleration): $\sim 31$ minutes. Total speedup: $\sim 46 \times$. 

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Figure 3.23: Demonstration of capability in solving a large scattering problem ($N = 147,374$) inspired by a metamaterial design presented in [122]. An average of 188 iterations per frequency was required, with an average time per iteration of 3.18 minutes, and an average total solution time of 896 minutes.
Chapter 4: DG for the Transient Maxwell Problem

4.1 Overview of Time Domain DG

The primary focus of this Chapter is the solution of the time domain Maxwell Equations. This is in contrast to the previous Chapters on IEs in a number of ways. Whereas the unknowns of interest were previously equivalent currents that give rise to fields that satisfy the Maxwell Equations, here the unknowns of interest are the fields themselves. Further, while time harmonic excitations were previously considered, now transient excitations are considered that permit the extraction of observables over a band of frequencies from a single simulation.

4.2 Time Domain Maxwell Equations

4.2.1 Statement of the Problem

Consider a domain, $\Omega \subset \mathbb{R}^3$, in which some distribution of non-dispersive matter characterized by isotropic constitutive parameters $\varepsilon(\mathbf{r})$ and $\mu(\mathbf{r})$ is immersed. The EM fields will
satisfy the Maxwell Equations:

\[ \varepsilon(\vec{r}) \frac{\partial \vec{E}(\vec{r}, t)}{\partial t} = \nabla \times \vec{H}(\vec{r}, t) + \vec{J}(\vec{r}, t) \] (4.57a)

\[ \mu(\vec{r}) \frac{\partial \vec{H}(\vec{r}, t)}{\partial t} = -\nabla \times \vec{E}(\vec{r}, t) \] (4.57b)

\[ \nabla \cdot \vec{D}(\vec{r}, t) = \rho(\vec{r}, t) \] (4.57c)

\[ \nabla \cdot \vec{B}(\vec{r}, t) = 0 \] (4.57d)

Additionally, the source charge and current satisfy the continuity equation:

\[ \frac{\partial \rho(\vec{r}, t)}{\partial t} + \nabla \cdot \vec{J}(\vec{r}, t) = 0 \] (4.58)

It is assumed that the sources are quiescent and autonomous, as their time evolution does not need to be solved for, but is instead impressed at \( t = 0 \). Of primary concern will be the resolution of \( \vec{E}(\vec{r}, t) \) and \( \vec{H}(\vec{r}, t) \) from Equations 4.57b and 4.57a, assuming that the initial conditions, \( \vec{E}(\vec{r}, 0) \) and \( \vec{H}(\vec{r}, 0) \) are given and satisfy Equations 4.57d and 4.57c.

Considerable economy can be realized by introducing the conservation form of Equations 4.57b and 4.57a. To this end, \( \vec{E}(\vec{r}, t) \) and \( \vec{H}(\vec{r}, t) \) can be united into a 6-vector \( \vec{q}(\vec{r}, t) \) that obeys the following:

\[ Q(\vec{r}) \frac{\partial \vec{q}(\vec{r}, t)}{\partial t} = -\nabla \cdot \vec{F}(\vec{q}(\vec{r}, t)) + \vec{S}(\vec{r}, t) \] (4.59)

The constitutive parameters are contained in the \( 6 \times 6 \) diagonal matrix, \( Q(\vec{r}) \):

\[ Q(\vec{r}) = \begin{pmatrix} \varepsilon(\vec{r}) & 0 \\ 0 & \mu(\vec{r}) \end{pmatrix} \] (4.60)
The conserved quantities (i.e., the fields) form a 6-vector, $\mathbf{q}(\mathbf{r}, t)$:

$$
\mathbf{q}(\mathbf{r}, t) = \begin{pmatrix}
\mathbf{E}(\mathbf{r}, t) \\
\mathbf{H}(\mathbf{r}, t)
\end{pmatrix}
$$

(4.61)

These conserved quantities are tied to a tensor current:

$$
\mathbf{F}(\mathbf{q}(\mathbf{r}, t)) = \begin{pmatrix}
-\hat{u}_i \times \mathbf{H}(\mathbf{r}, t) \\
\hat{u}_i \times \mathbf{E}(\mathbf{r}, t)
\end{pmatrix}
$$

(4.62)

where $\hat{u}_i$ is the $i$th Cartesian unit vector, as well as a 6-vector source term:

$$
\mathbf{S}(\mathbf{r}, t) = \begin{pmatrix}
0 \\
\mathbf{J}(\mathbf{r}, t)
\end{pmatrix}
$$

(4.63)

The remainder of this Chapter will focus on the discretization of this form of the Maxwell Equations within the DG framework (Section 4.2.2) and results that validate its proper implementation (Section 4.2.3) germane to the applications being explored in Chapter 5.

4.2.2 Numerical Details

4.2.2.1 Modal and Nodal DG Basis Functions

The basis functions utilized in discretizing Equation 4.59 are a set of globally discontinuous higher-order polynomials. To this end, both $\mathbf{E}_h(\mathbf{r}, t)$ and $\mathbf{H}_h(\mathbf{r}, t)$ are defined in terms of a collection of local expansions restricted to each element of a simplicial tessellation of $\Omega \approx \Omega_h = \bigcup_{e=1}^{N_e} T_e$. These expansions may be of either a ‘nodal’ or ‘modal’ character. While
these expansions are equivalent by construction, each will have attendant advantages that will be utilized in the discretization process.

The nodal expansion is of the form:

$$\begin{align*}
\vec{E}(\vec{r}, t) &\approx \vec{E}_h(\vec{r}, t) = \sum_{e=1}^{N_e} \sum_{p=1}^{N_p(e)} \vec{E}_h(\vec{r}_{ep}^e, t) l_p^e(\vec{r}) \\
\vec{H}(\vec{r}, t) &\approx \vec{H}_h(\vec{r}, t) = \sum_{e=1}^{N_e} \sum_{p=1}^{N_p(e)} \vec{H}_h(\vec{r}_{ep}^e, t) l_p^e(\vec{r})
\end{align*}$$

(4.64)

(4.65)

Here, the sum on $e$ is taken over each of the $N_e$ tetrahedra, upon which a set of $N_p(e)$ interpolatory polynomials, $l_p^e(\vec{r})$, are defined. These polynomials interpolate on a set of $N_p(e)$ points defined by the global coordinates $\vec{r}_{ep}^e \subset T_e$. Each of the $N_e$ local expansions is complete to polynomial order $\Pi(e)$, with the following relationship between order and cardinality:

$$N_p(e) = \frac{(\Pi(e) + 1)(\Pi(e) + 2)(\Pi(e) + 3)}{6}$$

(4.66)

In the nodal framework, the unknown will be the 3-vector-valued functions of time $\vec{E}_h(\vec{r}_{ep}^e, t)$ and $\vec{H}_h(\vec{r}_{ep}^e, t)$, i.e., the solution fields evaluated at the interpolation nodes. The specific interpolating nodes that will be used in practice minimize the Lebesgue constant associated with the interpolation, and are derived in [36] - the Lebesgue constant being a prefactor that describes the distance a given interpolant is from the best possible polynomial approximation.
The modal expansion is of the form:

\[
\mathbf{E}_h(\mathbf{r}, t) = \sum_{e=1}^{N_e} \sum_{p=1}^{N_p(e)} \mathbf{c}_{E,p}^e(t) \psi_p^e(\mathbf{r}) \quad (4.67)
\]

\[
\mathbf{H}_h(\mathbf{r}, t) = \sum_{e=1}^{N_e} \sum_{p=1}^{N_p(e)} \mathbf{c}_{H,p}^e(t) \psi_p^e(\mathbf{r}) \quad (4.68)
\]

Again, the sum on \(e\) is taken over all tetrahedra, upon which a set of \(N_p(e)\) modal polynomials, \(\psi_p^e(\mathbf{r})\), are defined. These polynomials are element-wise orthogonal, such that:

\[
\langle \psi_p^e, \psi_q^e \rangle_T^e \sim \delta_{p,q} \quad (4.69)
\]

Each of the local expansions is complete to polynomial order \(\Pi(e)\) and obeys the order-cardinality relationship in Equation 4.66. The unknowns, \(\mathbf{c}_{E,p}^e(t)\) and \(\mathbf{c}_{H,p}^e(t)\) are 3-vector-valued functions of time that are the local expansion coefficients for \(\mathbf{E}_h(\mathbf{r}, t)\) and \(\mathbf{H}_h(\mathbf{r}, t)\) restricted to tetrahedron \(e\). The specific modal polynomials that are utilized are a minimal set of products of Jacobi polynomials derived in [36].

It is useful to consider why these two equivalent expansions are necessary. In what follows, the modal basis will be used whenever elementary calculus is required, e.g., integration or differentiation. It is possible to perform these operations on the modal polynomials as they have a simple closed form. For simplicial elements, there is in fact no closed form expression for the nodal interpolating polynomials, so these operations cannot be applied directly. However, as will be discussed in Section 4.2.2.2, the off-diagonal matrix elements will consist of surface integrals over the faces of the \(N_e\) tetrahedra. In the modal basis, these integrals will generally give rise to dense off-diagonal blocks. The nodal polynomials,
however, have the nice property that these blocks will be sparse due to the fact that interpolating polynomials associated with nodes that do not lie on a given face, are identically zero on that face. To this end, the general philosophy will be to compute the unknowns in the nodal basis, but to evaluate matrix elements in the modal basis and then transform them into the nodal basis. The form of the requisite elements will be given below in Section 4.2.2.2, whereas explicit details concerning their evaluation are contained in [36].

4.2.2.2 DG Discretization

The discretization process in DG is somewhat more involved than it was with the IEs of Chapter 2. As before, however, it begins with the projection of Equation 4.59 onto an arbitrary nodal testing function, $l_p^e(\vec{r})$:

$$\langle l_p^e, Q \frac{\partial \vec{q}_h}{\partial t} \rangle_{Te} = -\langle l_p^e, \nabla \cdot \vec{F}(\vec{q}_h) \rangle_{Te} + \langle l_p^e, \vec{S} \rangle_{Te}$$ (4.70)

The key ‘trick’ in the DG discretization scheme is to apply integration by parts to the divergence term twice. The first integration by parts yields:

$$\langle l_p^e, Q \frac{\partial \vec{q}_h}{\partial t} \rangle_{Te} = -\langle l_p^e, \vec{n} \cdot \vec{F}^*(\vec{q}_h) \rangle_{F_e} + \langle \nabla l_p^e, \vec{F}(\vec{q}_h) \rangle_{Te} + \langle l_p^e, \vec{S} \rangle_{Te}$$ (4.71)

Here, $\vec{F}^*(\vec{q}_h)$ is called the ‘numerical flux’. It takes the place of the usual boundary term arising from integration by parts, which is ill-defined, given the element-wise definition of basis functions. In other words, because the basis functions do not explicitly constrain continuity across faces, the fields at the boundary are inherently multi-valued, making the definition of a boundary term in the integration by parts ambiguous. A second integration
by parts yields the following:

\[
\langle l^e_p, Q \frac{\partial \vec{q}_h}{\partial t} \rangle_{T_e} = -\langle l^e_p, \nabla \cdot \vec{F}(\vec{q}_h) \rangle_{T_e} + \langle l^e_p, \vec{n} \cdot \left( \vec{F}(\vec{q}_h) - \vec{F}^*(\vec{q}_h) \right) \rangle_{F_e} + \langle l^e_p, \vec{S} \rangle_{T_e} \tag{4.72}
\]

This returns the problem to a strong form, and provides insight into how \( \vec{F}^*(\vec{q}_h) \) should be defined. As the boundary term in Equation 4.72 should vanish for solutions to the Maxwell equations, the numerical flux should be designed in such a way as to numerically enforce inter-element boundary conditions, as they are not explicitly built into the function space. To this end it is useful for \( \vec{F}^*(\vec{q}_h) \) to take the form of an upwind flux, first derived for Finite Volume Methods [124, 67]:

\[
\vec{n} \cdot \left( \vec{F}(\vec{q}_h) - \vec{F}^*(\vec{q}_h) \right) = \left( \begin{array}{c}
-\vec{n} \times \left( Z^+ \left[ [\vec{H}_h] \right] - \vec{n} \times \left[ [\vec{E}_h] \right] \right) \\
\frac{2}{2\left\{ \{ Z \} \right\}} \vec{n} \times \left( Y^+ \left[ [\vec{E}_h] \right] + \vec{n} \times \left[ [\vec{H}_h] \right] \right)
\end{array} \right) \tag{4.73}
\]

It is important to note that this choice of the flux is not unique. In fact, in so far as this flux introduces a term proportional to \( \vec{E}_h \) in Ampere’s law, and \( \vec{H}_h \) in Faraday’s law, this particular form will render the final discrete system dissipative. Consequently, one might consider removing these terms to yield what is known as a ‘central flux’. While this flux can be used with symplectic integrators to guarantee discrete energy conservation [125], it does not damp spurious modes that arise in a nodal DG framework [126].

If Equation 4.72 is made to hold for all \( l^e_p \), it describes a system of \( 6N \) ODEs in \( 6N \) unknowns, where \( N = \sum_{i=1}^{N_e} N_p(e) \). Here, the unknowns are \( \vec{E}_h(\vec{r}_p, t) \) and \( \vec{H}_h(\vec{r}_p, t) \), the field values at all interpolation nodes as a function of time. To this end, Equation 4.72 is called the ‘semi-discrete form’ of the problem, in so far as it remains un-discretized in time. For
convenience, it is re-written in terms of the field components $\vec{E}_h$ and $\vec{H}_h$:

$$
\langle l_p^e, \varepsilon \frac{\partial \vec{E}_h}{\partial t} \rangle_{Te} = -\langle l_p^e, \nabla \times \vec{H}_h \rangle_{Te} + \langle l_p^e, \vec{F}_E\{\vec{E}_h, \vec{H}_h\} \rangle_{Fe} \tag{4.74a}
$$

$$
\langle l_p^e, \mu \frac{\partial \vec{H}_h}{\partial t} \rangle_{Te} = \langle l_p^e, \nabla \times \vec{E}_h \rangle_{Te} + \langle l_p^e, \vec{F}_H\{\vec{E}_h, \vec{H}_h\} \rangle_{Fe} + \langle l_p^e, \vec{J} \rangle_{Te} \tag{4.74b}
$$

Here $\vec{F}_E$ and $\vec{F}_H$ are the relevant components of the upwind flux in Equation 4.73. The features of the matrices that this form generates are as follows:

1. The matrix elements associated with the elemental inner products taken alone form a block-diagonal matrix. Each element generates an $N_p(e) \times N_p(e)$ block.

2. The matrix elements associated with the trace inner products taken alone contribute to both diagonal and off-diagonal blocks. Each interior face produces gives diagonal and off-diagonal contributions, exterior faces produce only diagonal contributions. Boundary conditions are enforced through these terms, details of which are given in Section 4.2.2.3.

Specific details of the matrix elements themselves can be found in [36].

The final step is the time discretization of Equation 4.74. As both matrices on the LHS are block-diagonal, it is convenient to integrate this system of ODEs using an explicit method. In particular, a low-storage fourth order Runge-Kutta [127] is applied. Attendant to this choice is the limitation that the time step used in this integration, $\Delta t$, is limited by a CFL-like condition [67] that gives the maximum stable time step. In practice, the time step is chosen as:

$$
\Delta t = C \frac{h}{c \max(N_p(e)^2)} \tag{4.75}
$$
Here, \( C \leq 1 \) is a scale factor that can be used to decrease the time step beyond the minimum required for stability, \( c \) is the speed of light in the units of the problem, the factor of \( N_p(e)^2 \) accounts for the reduction in the distance between interpolation nodes at higher order, and \( h \) is a mesh-dependent quantity given as:

\[
h = \min_{\Omega_h} \frac{2}{3} \left( \frac{\text{Volume of } T_e}{\min_{F_e} \text{(Area of face)}} \right)
\]  

(4.76)

This will hold for straight-edged tetrahedra, for which the factor of \( 2/3 \) comes from the volumetric and surface Jacobians associated with transforming onto reference elements. For all results, \( C = 1 \) to achieve the largest stable time step.

### 4.2.2.3 Boundary Conditions

The final piece of the DG framework worth remarking on is the enforcement of boundary conditions. Simply put, these are imposed by restricting the form of \( [\vec{E}_h] \) and \( [\vec{H}_h] \) at interior or exterior boundaries. In particular, in so far as \( \vec{E}_h^- \) and \( \vec{H}_h^- \) are set by the problem solution, \( \vec{E}_h^+ \) and \( \vec{H}_h^+ \) must be specified. For PEC boundaries, these are given as:

\[
\vec{E}_h^+ = -\vec{E}_h^-
\]  

(4.77a)

\[
\vec{H}_h^+ = \vec{H}_h^-
\]  

(4.77b)

Heuristically, one might view this as enforcing the vanishing of the tangential \( \vec{E}_h \) field by constraining the field on the positive trace as to cancel it. Similarly, for PMC boundaries
these are given as:

\[ \vec{E}^+_h = \vec{E}^-_h \]  
\[ \vec{H}^+_h = -\vec{H}^-_h \]  

(4.78a)

(4.78b)

This can be heuristically justified in an analogous way. To realize a simple Silver-Müller boundary condition, the following conditions are enforced [128, 129]:

\[ \vec{E}^+_h = -\vec{E}^-_h \]  
\[ \vec{H}^+_h = -\vec{H}^-_h \]  

(4.79a)

(4.79b)

This form is perhaps not as physically transparent as the PEC and PMC boundary conditions. However, one can see that the upwind flux in Equation 4.73 vanishes when the usual Silver-Müller relationship between tangential \( \vec{E}_h \) and \( \vec{H}_h \) is satisfied. It is also frequently useful to enforce a Dirichlet boundary condition when the fields at a boundary are known analytically. In this case, the positive traces are given as:

\[ \vec{E}^+_h = -\vec{E}^-_h + 2\vec{E}_{enf} \]  
\[ \vec{H}^+_h = -\vec{H}^-_h + 2\vec{H}_{enf} \]  

(4.80)

(4.81)

Here, \( \vec{E}_{enf} \) and \( \vec{H}_{enf} \) are the enforced fields, and this condition can be physically reconciled as forcing the positive traces of both fields to cancel the negative trace, and adding in the imposed fields.

The final type of boundary condition to be discussed arises in the total field/scattered
field formalism [49]. This formalism is typically applied in the context of imposing the incident field in scattering problems. Here, it will be useful in representing the fields due to a point-dipole excitation, \( \vec{J}(\vec{r}, t) \), of the form:

\[
\vec{J}(\vec{r}, t) = \vec{d}_s j_s(t) \delta(\vec{r} - \vec{r}_s)
\]  

(4.82)

Here, \( \vec{d}_s \) is the orientation of the dipole, \( \vec{r}_s \) is its location, and \( j_s(t) \) is the temporal signature of the current driving it. The nearer one gets to the point excitation, the more poorly approximated the fields will be due to the smooth polynomial basis functions being employed. The total field/scattered field formalism can be used to remove the singular portion of the field from numerical consideration, and has been applied to this end for the treatment of line sources in DG [128]. To achieve this, the fields are decomposed into incident and scattered components:

\[
\vec{E}_h = \vec{E}_{h,\text{inc}} + \vec{E}_{h,\text{scat}}
\]  

(4.83a)

\[
\vec{H}_h = \vec{H}_{h,\text{inc}} + \vec{H}_{h,\text{scat}}
\]  

(4.83b)

A boundary is demarcated around the point source, outside of which the total fields \( \vec{E}_h \) and \( \vec{H}_h \) are solved, and inside which only the scattered components \( \vec{E}_{\text{scat}} \) and \( \vec{H}_{\text{scat}} \) are solved. This scenario is illustrated in Figure 4.24. \( \vec{E}_{h,\text{inc}} \) and \( \vec{H}_{h,\text{inc}} \) are the fields generated by the source satisfying the Maxwell Equations in free space. Explicit expressions for these fields are given in Section A.3 of the Appendix. At the boundary between the the total and scattered field regions, a boundary condition must be imposed that ensures that the two regions remain consistent. Rather than restricting the form of \( \begin{bmatrix} \vec{E}_h \end{bmatrix} \) and \( \begin{bmatrix} \vec{H}_h \end{bmatrix} \) through
the positive traces, however, this boundary condition is enforced by augmenting the existing value by the incident field at the boundary. In other words, the jumps are instead given as:

\[
\begin{align*}
\left[ \vec{E}_h \right] &= \vec{E}^+_h - \vec{E}^-_h \pm \vec{E}_{h,inc} \\
\left[ \vec{H}_h \right] &= \vec{H}^+_h - \vec{H}^-_h \pm \vec{H}_{h,inc}
\end{align*}
\] (4.84a)

Here, the + sign is utilized when the positive trace is within the scattered field region, and the − sign is utilized when the positive trace is in the total field region.

4.2.2.4 Non-Conformal Discretizations

In Section 1.2.5, the ability of the DG framework to accommodate non-conformal meshes was briefly discussed. To this end, when working with such meshes there are no changes to the discretization, and Equation 4.74 continues to yield the appropriate matrix elements. However, the evaluation of the matrix elements arising due to the trace terms will change, and requires non-trivial modifications as far as implementation is concerned. To see this, one might consider the many ways in which two meshes might meet at a non-conformal interface. Rather than being aligned, as would be the case in a conformal mesh, the triangular faces at the non-conformal boundary can overlap in four different ways, illustrated in Figure 4.25.

To this end, new data structures must be introduced to deal with a number of assumptions that can no longer be made:

1. An element may now have arbitrarily many neighbors, rather than one per face (i.e., a maximum of four). Similarly, each face is no longer associated with at most two abutting tetrahedra.
2. The interpolation nodes on two overlapping faces will no longer be exactly degenerate. This degeneracy is used to simplify the evaluation of matrix elements a great deal in conformal meshes, as they can be computed on a reference element, stored, and scaled when they are applied in the Runge-Kutta integration.

In modifying an existing DG implementation to support these assumptions, this new data type will consist of a list of the separate polygonal fragments that tessellate the non-conformal interface, each node of which includes the following information:

- Indices of the faces and elements that comprise the fragment.
- Area of the fragment.
- Interpolation operators that map from the associated DG basis nodes on both traces onto a set of degenerate quadrature nodes, derived from [130].
- Matrix elements associated with the overlap of basis functions on the fragment.

First, however, one must generate a description of the fragments themselves. This is most easily accomplished using polygon clipping algorithms [131]. Such an algorithm has been implemented, and an exemplary non-conformal interface processed by it is illustrated in Figure 4.26.

4.2.3 Validation

In this Section, results validating a Fortran implementation of the scheme discussed above are presented. These results are intended to demonstrate the correctness of the code for later use. In sequence, results will be demonstrated that illustrate the following:
• Higher order accuracy of the DG method in terms of convergence of analytically known cavity fields in the $L^\infty$ norm.

• Solution of an inhomogeneous Maxwell Equation in which a point dipole excites a PEC cavity, yielding its spectrum of modes.

• Implementation of piecewise homogeneous materials, as indicated by the modal spectrum of a partially filled cavity.

• Convergent representation of the fields due to a dipole in free space using Dirichlet, total field/scattered field, and absorbing boundary conditions.

The first result validates the proper higher order convergence of the DG implementation, and is inspired by an example in [36]. Here initial conditions for a TM$_{1,1}$ cavity mode are imposed as the boundary data on a PEC cavity, and the resultant $\vec{E}(\vec{r},t)$ and $\vec{H}(\vec{r},t)$ are integrated out for many cycles. Results are presented in Figure 4.27 that demonstrate convergence in both polynomial order and the edge length, $h$. The error in the $L^\infty$ norm is estimated from a sampling of the field at 10,000 randomly chosen points on the interior of the cavity at the peak of the fifth cycle of the cavity mode. It is evident that the error can be reduced by either increasing the polynomial order, $N_p$, or decreasing $h$.

The next sequence of results is the reconstruction of a set of cavity modes from the fields generated by a dipolar current source excited by a broadband pulse, inspired by results in [132]. A cubic 1 m PEC cavity is meshed, and 5 dipolar current sources are distributed throughout, with random positions and orientations. Each source is excited by the derivative of a Gaussian-modulated pulse with center frequency 540 MHz and an effective bandwidth of 660 MHz. The fields are evolved for 1000 ns, and recorded at 20 random positions throughout
the cavity. The discrete Fourier spectrum is computed for each electric field component at each position. The resultant cavity modes are identified by an averaging of the spectra over all observers and electric field components, and the results are illustrated in Figure 4.28. It is evident that the location of the first 21 modes are in good agreement with analytic results. This validates the ability of this implementation to reproduce the spectral response of a PEC structure.

The next result in this sequence validates the implementation of piecewise homogeneous dielectric materials. The eigenmodes of a cubic 1m cavity filled partially (40%) with a material for which \( \varepsilon_r = 2 \) were computed analytically and numerically. Results are illustrated in Figure 4.29. Again, the cavity is excited by 5 dipole point excitations, with randomly chosen positions and orientations, each driven by the derivative of a Gaussian-modulated pulse with center frequency 270 MHz and an effective bandwidth 400 MHz. The fields are evolved for 800 ns, and the discrete Fourier spectrum is computed from 20 samples at random positions throughout the cavity. As before, the resultant cavity modes are identified by an averaging of the spectra over all observers and electric field components. The location of the first 20 modes are in good agreement with analytic results. In the case of nearly degenerate modes, the numerically computed peaks are not always split. To see this splitting, a longer simulation could be run to achieve a better spectral resolution.

Next, a result is presented illustrating the correct implementation of Dirichlet, total field/scattered field, and Silver-Müller boundary conditions. A sphere of radius 1m is meshed with a desired edge length of \( \lambda/5 \) and three separate tests are run. In the first, a 0.5m sphere is removed from the center of the domain, and Dirichlet boundary conditions are applied on both the interior and exterior faces. Electric and magnetic fields due to a dipole source at
the center of the sphere are imposed on both surfaces, for a current with the time signature of a Gaussian pulse with center frequency 300 MHz and bandwidth 300 MHz. The pulse is allowed to propagate through the computational domain, and the relative $L^2$ error is computed after it has passed for polynomial orders 1 through 5. In the next test, the same source is utilized, but the Dirichlet boundary condition is only applied at the exterior face, where it should exactly capture the outgoing character of the fields propagating into an unbounded medium. At the interior face, the total field/scattered field boundary condition is applied, and the 0.5m sphere that was removed is again inserted. This region is treated as a scattered field region, and the exterior spherical shell is treated as a total field region. $L^2$ error is computed in both regions under the same conditions. The final test uses the same geometry, but rather than applying a Dirichlet boundary condition at the exterior face, a Silver-Müller boundary condition is imposed. Again, the $L^2$ error is computed throughout the domain. The results of this sequence of tests are given in Figure 4.30

Here, there are two points worth noticing. First, the rate of convergence for the total field/scattered field plus Dirichlet test is greater than that of the pure Dirichlet test. This is due to the fact that the computational domains are different. In the pure Dirichlet test, there is no interior to the spherical shell, for which the scattered field region is defined in the other test. Second, the convergence for the total field/scattered field plus absorbing boundary condition saturates, whereas neither of the other tests do. This is due to the presence of spurious scattering from the boundary of the computational domain. More can be learned about the nature of this error by considering the time signature of the absolute error integrated over only the spatial extent of the domain. This is illustrated in Figure 4.31.
While the total field/scattered field plus absorbing boundary condition error converges uniformly in polynomial order up until $t \approx 10$ ns, beyond this time, all orders have the same time signature. This error is not due to a deficiency in the choice of representation, as it eventually overtakes the error in the 1st order total field/scattered field plus Dirichlet data, but is instead due to spurious reflections at the approximate absorbing boundary condition. Normalizing the error in terms of the amplitude of the exciting field indicates that slightly less than 1% of the power incident on this boundary is spuriously reflected, which is consistent with the level at which the relative error was found to saturate in Figure 4.30. This is a well-known issue associated with utilizing a Silver-Müller condition of this order. To reduce the size of these reflections, the termination of the domain could be placed further from the source, or an alternative transparent boundary condition could be applied, such as a perfectly matched layer, or a pole condition-based truncation. The implementation and exploration of these types of boundary conditions are left to future work, and the level of reflection associated with this simple boundary condition must simply be left as a caveat to the user.

Having established the validity of numerous components of the DG implementation, all of the necessary components of the code are suitably vetted for the application to be presented in Chapter 5.

4.3 Figures
Figure 4.24: Total field/scattered field separation for imposing fields due to a dipole source. The location of the source is indicated by the arrow, the red annulus is the total field region and the blue circle is the scattered field region. At the boundary between the two regions, the condition in Equation 4.84 is enforced.

Figure 4.25: Four distinct types of fragments that can occur in a tetrahedral non-conformal mesh.
Figure 4.26: Quadrature at a non-conformal interface. Triangles on one side of the interface are outlined in black, triangles on the other are outlined in red. Blue points indicate the vertices of fragments, and green points indicate the quadrature points used for integration. Fragments have been further decomposed into triangles upon which a symmetric higher order quadrature is defined [130]. Some pathologies are also illustrated, as a result of finite precision arithmetic.
Figure 4.27: Error in $\bar{E}(\vec{r}, t)$ of a TM$_{1,1}$ cavity mode in the $L^\infty$ norm after 5 cycles. Convergence is demonstrated with respect to edge length and polynomial order.
Figure 4.28: Eigenmodes of an empty 1m cubic cavity.
Figure 4.29: Eigenmodes of a 1m cubic cavity for which the bottom 40% is filled with a material with $\varepsilon_r = 2$, with free space elsewhere.
Figure 4.30: Convergence of the relative $L^2$ error of the fields due to a point dipole excited by a Gaussian modulated pulse with center frequency 300 MHz and bandwidth 300 MHz at the center of a 1m spherical domain. Boundary conditions are imposed using pure Dirichlet, Dirichlet plus total field/scattered field, and absorbing plus total field/scattered field boundary conditions.
Figure 4.31: Absolute $L^2$ error of the fields due to a point dipole excited in the same manner as in Figure 4.30.
Chapter 5: DG-QED for Cavity Mediated Energy Transfer

5.1 Overview of Energy Transfer

In this Chapter, the time domain Maxwell solver discussed in Chapter 4 is applied to the analysis of systems in which a number of quantum mechanical subsystems interact through their mutual coupling to the EM field. This type of modeling can be applied to the spectrum of applications identified in Section 1.1.2, including energy transfer and quantum information. Here, results will be limited to proofs of concept. In Section 5.2, details of the modeling formalism will be identified. The quantum mechanical subsystems will be described in terms of a set of two-level quantum systems (2LSs) that are coupled to the EM field through a multipolar Hamiltonian truncated at the dipole level. The quantum master equation that describes the evolution of the reduced density matrix associated with only the 2LSs will be given, and coefficients will be identified in terms of quantities that can be computed using a classical Maxwell solver. In Section 5.2, an algorithm for extracting the relevant model parameters from a sequence of classical time domain Maxwell solutions is presented. Section 5.3 will include results that illustrate two proofs of concept, namely spontaneous emission in the vicinity of a PEC plane, and the coupling of two quantum dots in a semiconductor microcavity. Finally, Section 5.4 will outline future work.
5.2 Cavity QED Formalism

5.2.1 Model Hamiltonian and Master Equation

Consider an open domain, \( \Omega \subset \mathbb{R}^3 \), with boundary \( \partial \Omega \), some subset of which may be PEC, \( \partial \Omega_C \), and a distribution of classical dielectric matter characterized by the dielectric function
\[
\varepsilon(\mathbf{r}, \omega) = \varepsilon_0 \left( \varepsilon'(\mathbf{r}, \omega) + i \varepsilon''(\mathbf{r}, \omega) \right)
\]
with analytic properties consistent with the Kramers-Kronig relations [133]. For simplicity, it is assumed that the matter is non-magnetic and characterized by permeability \( \mu_0 \), noting that the extension to magnetic media will require nothing that is not analogously encountered in accommodating a dispersive dielectric. Some distribution of \( N_d \) two-level systems (2LSs) is contained within \( \Omega \), such that the \( m \)th 2LS is characterized by the position of its centroid, \( \mathbf{r}_m \), transition frequency \( \omega_m \), and dipole transition moment \( \mathbf{d}_m \). The Hilbert space of each 2LS consists of the usual complex 2-vectors of unit norm, which are operated upon by the usual local SU(2) basis, i.e., the Pauli matrices plus the identity \( \{ \hat{I}_m, \hat{\sigma}_m^x, \hat{\sigma}_m^y, \hat{\sigma}_m^z \} \). Raising/lowering operators are built from these matrices, \( \hat{\sigma}_m^{\pm} = \frac{1}{2}(\hat{\sigma}_m^x \pm i \hat{\sigma}_m^y) \), and used to define dipole transition operators
\[
\hat{\mathbf{d}}_m = \mathbf{d}_m \hat{\sigma}_m^{-} + \mathbf{d}_m^* \hat{\sigma}_m^{+}.
\]
The 2LSs will be coupled to the electromagnetic field within a multipolar formalism, truncated at the electric dipole level [19, 134].

\[
\hat{H} = \int d\mathbf{r} \int_0^{\infty} d\omega \omega \hat{\mathbf{f}}^\dagger(\mathbf{r}, \omega) \hat{\mathbf{f}}(\mathbf{r}, \omega) + \sum_{m=1}^{N_d} \hbar \omega_m \hat{\sigma}_m^{+} \hat{\sigma}_m^{-} - \sum_{m=1}^{N_d} \int d\omega \left[ \hat{\mathbf{d}}_m \cdot \hat{\mathbf{E}}(\mathbf{r}_m, \omega) + h.c. \right]
\]

Here, \( \hat{\mathbf{f}}(\mathbf{r}, \omega) \) and its adjoint are bosonic fields that obey the usual equal-frequency, equal-space commutation relations that generate the EM field, with the quantum fields, \( \hat{\mathbf{E}}(\mathbf{r}_m, \omega) \)
and \( \hat{B}(\vec{r}_m, \omega) \), obeying:

\[
\hat{E}(\vec{r}_m, \omega) = i \sqrt{\frac{\hbar}{\pi}} \frac{\omega^2}{c^2} \int_{\Omega} d\vec{r}' \sqrt{\tilde{\varepsilon}'(\vec{r}', \omega)} \overline{G}(\vec{r}_m, \vec{r}', \omega) \cdot \hat{f}(\vec{r}', \omega) \tag{5.86}
\]

\[
\hat{B}(\vec{r}_m, \omega) = i \omega \nabla \times \hat{E}(\vec{r}_m, \omega) \tag{5.87}
\]

Here, \( \overline{G}(\vec{r}, \vec{r}', \omega) \) is the classical dyadic Green’s function for the electric field that satisfies the following inhomogeneous vector Helmholtz equation:

\[
\nabla \times \nabla \times \overline{G}(\vec{r}, \vec{r}', \omega) - \frac{\omega^2}{c^2} (\tilde{\varepsilon}'(\vec{r}, \omega) + i \tilde{\varepsilon}''(\vec{r}, \omega)) \overline{G}(\vec{r}, \vec{r}', \omega) = \delta(\vec{r} - \vec{r}') \tag{5.88}
\]

subject to the constraint that the generated fields obey classical boundary conditions on \( \partial \Omega \), and throughout materials described by \( \tilde{\varepsilon}(\vec{r}, \omega) \).

Using this Hamiltonian, the Heisenberg equations of motion can be derived in the usual way for some operator, \( \hat{O} \):

\[
\frac{d\hat{O}}{dt} = \frac{i}{\hbar} \left[ \hat{H}, \hat{O} \right] \tag{5.89}
\]

Here, \( \hat{O} \) may be any of the relevant dynamical variables, e.g., \( \hat{\sigma}_m^- \), \( \hat{\sigma}_m^+ \), and \( \hat{f}(\vec{r}, \omega) \). As there is a continuum of EM field variables, it is favorable to integrate them out, and to instead study the reduced density matrix, \( \hat{\rho}_s(t) = \text{Tr}(\hat{\rho})_{EM} \). The subscript indicates that the trace is evaluated over the EM field variables, and that only the 2LS sector of the Hilbert space remains in the reduced density matrix. A master equation that governs the evolution of this quantity has been derived in the limit that the relative detuning between 2LSs is small over...
the scale of frequency variations in the system Green’s function [134]. It is given as:

\[
\frac{\partial \hat{\rho}_s}{\partial t} = -i \sum_{m=1}^{N_d} \tilde{\omega}_m \left[ \hat{\sigma}_m \cdot \hat{\rho}_s \right] + i \sum_{m \neq n} g_{m,n} \left[ \hat{\sigma}_m \hat{\sigma}_n \cdot \hat{\rho}_s \right] - \ldots
\]

\[
\ldots \frac{1}{2} \sum_{m,n} \Gamma_{m,n} \left( \hat{\sigma}_m \hat{\sigma}_n \cdot \hat{\rho}_s - 2 \hat{\sigma}_n \hat{\rho}_s \hat{\sigma}_m + \hat{\rho}_s \hat{\sigma}_m \hat{\sigma}_n \right)
\]

(5.90)

Here, \(\tilde{\omega}_m = \omega_m - g_{m,m}\) is the Lamb-shifted transition frequency, and the quantities \(g_{m,n}\) and \(\Gamma_{m,n}\) can be derived from the classical dyadic Green’s function governed by Equation 5.88:

\[
g_{m,n} = \frac{\tilde{\omega}_n^2}{\hbar \varepsilon_0 c^2} \vec{d}_m \cdot \Re \{ \overline{\mathbf{G}}(\vec{r}_m, \vec{r}_n, \tilde{\omega}_n) \} \cdot \vec{d}_n
\]

(5.91)

\[
\Gamma_{m,n} = \frac{2 \tilde{\omega}_n^2}{\hbar \varepsilon_0 c^2} \vec{d}_m \cdot \Im \{ \overline{\mathbf{G}}(\vec{r}_m, \vec{r}_n, \tilde{\omega}_n) \} \cdot \vec{d}_n
\]

(5.92)

For canonical systems in which \(\overline{\mathbf{G}}(\vec{r}, \vec{r}', \omega)\) has a closed-form expression, these parameters can be computed, and the master equation can be integrated numerically using something simple, such as Runge-Kutta. In general \(\overline{\mathbf{G}}(\vec{r}, \vec{r}', \omega)\) has no closed-form expression, and it is necessary to consider methods for numerically generating relevant samples of \(\overline{\mathbf{G}}(\vec{r}, \vec{r}', \omega)\). In what follows, the manner in which the time domain Maxwell solver from Chapter 4 can be used to this end will be discussed.

5.2.2 Extraction of Model Parameters

In general, a complete description of \(\overline{\mathbf{G}}(\vec{r}, \vec{r}', \omega)\) would require the solution of Equation 5.88 for all source-observer pairs in \(\Omega\), at all frequencies. Fortunately, Equation 5.90 only requires samples for a finite number of source-observer pairs, namely \(N_d^2\), at frequencies in
the set of 2LS transition frequencies, \( \{ \omega_m | m \in 1 \ldots N_d \} \). These samples can be extracted from field data generated from \( N_d \) separate solutions of the classical time domain Maxwell Equations. The \( m \)th simulation will consist of the following:

1. A point dipole excitation at \( \vec{r}_m \), oriented along the direction defined by \( \vec{d}_m \) is excited by the derivative of a Gaussian modulated pulse. To this end, the source term is rendered:

\[
\vec{J}_m(\vec{r}, t) = \vec{d}_m \frac{d}{dt} \left( \sin(\omega_c(t - t_d)) e^{-\frac{(t-t_d)^2}{2\sigma^2}} \right) \delta(\vec{r} - \vec{r}_m) \tag{5.93}
\]

\[
\vec{J}_m(\vec{r}, t) = \vec{d}_m \tilde{j}(t) \tag{5.94}
\]

Here, \( t_d \) is some shift in time chosen to ensure that the system is approximately quiescent at \( t = 0 \), and \( \omega_c \) and \( \sigma \) define the center frequency and bandwidth of the frequency interval over which \( \overline{G}(\vec{r}, \vec{r}', \omega) \) is desired.

2. The total classical electric field will be recorded at each of the remaining \( N_d - 1 \) 2LSs, and the scattered electric field will be recorded at the \( m \)th 2LS. These data will be Fourier transformed to yield \( \vec{E}(\vec{r}_n, \omega) \) and \( \vec{E}_{scat}(\vec{r}_m, \omega) \).

3. Entries of the dyadic Green’s function can then be extracted from:

\[
\vec{E}(\vec{r}_n, \omega) = -i\omega \mu_0 \overline{G}(\vec{r}_n, \vec{r}_m, \omega) \cdot \vec{J}_m(\vec{r}_m, \omega) \tag{5.95}
\]

\[
\vec{E}_{scat}(\vec{r}_m, \omega) = -i\omega \mu_0 \overline{G}_{scat}(\vec{r}_m, \vec{r}_m, \omega) \cdot \vec{J}_m(\vec{r}_m, \omega) \tag{5.96}
\]
Here the scattered field dyadic Green’s function, $\mathbf{G}_{scat}(\vec{r}, \vec{r}', \omega)$ is defined as:

$$\mathbf{G}(\vec{r}, \vec{r}', \omega) = \mathbf{G}_0(\vec{r}, \vec{r}', \omega) + \mathbf{G}_{scat}(\vec{r}, \vec{r}', \omega)$$ (5.97)

Where $\mathbf{G}_0(\vec{r}, \vec{r}', \omega)$ is the free space dyadic Green’s function. This quantity is so-defined as to regularize the singular behavior of $\mathbf{G}(\vec{r}, \vec{r}', \omega)$ as $\vec{r} \to \vec{r}'$.

4. From these samples, $g_{n,m}$ and $\Gamma_{n,m}$ can be computed. The self-terms, $g_{m,m}$ and $\Gamma_{m,m}$, must be augmented by the free space contribution due to $\mathbf{G}_0(\vec{r}, \vec{r}', \omega)$ in Equation 5.97. These contributions are simply the Lamb shift and emission rate of an isolated emitter in free space.

5.3 DG-QED Results

5.3.1 Spontaneous Emission Above a PEC Half-Space

Analytical results due to Wylie and Sipe [135, 136] for a single quantum emitter above a PEC half-space are used to validate the presented method of calculation. Here, Equation 5.90 reduces to a single parameter, $\Gamma$, where the subscript has been removed. $\Gamma$ sets the rate of spontaneous emission, which will changing depending upon whether or not the emitter’s dipole moment is parallel or perpendicular to the plane of the half-space. The respective rates, $\Gamma_\parallel$ and $\Gamma_\perp$, are most easily expressed normalized against the free space spontaneous
emission rate, $\Gamma_0 = \frac{\omega^3 |\mathbf{d}|^2}{3\hbar \varepsilon_0 c^3}$:

$$\Gamma_\parallel/\Gamma_0 = 1 - \frac{3}{2} \left[ \frac{\cos(\eta)}{\eta^2} + \left( \frac{1}{\eta} - \frac{1}{\eta^3} \right) \sin(\eta) \right]$$

$$\Gamma_\perp/\Gamma_0 = 1 + 3 \left[ \frac{\sin(\eta)}{\eta^3} - \frac{\cos(\eta)}{\eta^2} \right]$$

(5.98) (5.99)

Here, $\eta = 2\omega z/c$ is a unitless parameter describing the distance of the emitter from its own image in the half-space, rationalized by the emission wavelength.

The equivalent image problem is simulated, using the DG solver from Chapter 4. Here, a dipolar current source is placed at the center of a spherical domain and excited with the derivative of a Gaussian pulse. Free space termination is simulated using an absorbing boundary condition, and a 2nd order complete basis is utilized. The original problem and its equivalent image problem are illustrated in Figure 5.32. The Green’s function is extracted using the procedure outlined in Section 5.2.2, from which the normalized emission rates are computed. The numerical results are compared against the analytic results in Equation 5.98 in Figure 5.33. The agreement between the computed rate and the analytic rate is as expected. The $L^2$ error in the fields is on the order of 1% throughout the simulation domain. Slightly larger deviations exist in the computed rates, and are most evident in the tail of the parallel-oriented decay rate. This is attributed to additional error incurred in interpolating the discrete Fourier spectrum.

The calculation was attempted for $\eta < 1$, corresponding to the emitter being less than 0.08\(\lambda\) from the PEC surface. While this type of nearfield calculation is possible, it becomes very difficult to resolve the imaginary part of the Green’s function. This can be rationalized in terms of the singular behavior of the half-space dyadic Green’s function. The real part
diverges as $\sim (z/\lambda)^{-1}$, whereas the imaginary part goes to a constant. Consequently, while the fields may be resolved well in the $L^2$ norm, this may be dominated by the representation of the large real part, rather than the small imaginary part, requiring a significant increase in the order of the DG basis. As this will also require a decrease in the element size to represent the scattered field region, the CFL-like condition will become even more restrictive, and the accurate calculation of the extreme nearfield of the emitter rapidly becomes a computationally expensive endeavor.

5.3.2 Energy Transfer in a Semiconductor Nanocavity

In the next result, the coupling parameters associated with two quantum dots inside of a semiconductor nanocavity are analyzed. To this end, each quantum dot is modelled as a 2LS with a simple excitonic transition yielding the gap between the ground and excited states. Here, a cavity is formed from by a 260 nm thick layer of GaAs ($n = 3.5$) sandwiched between two AlAs/GaAs Distributed Bragg Reflectors (DBR) ($n = 3.0, n = 3.5$), each consisting of 6 alternating quarter-wave slabs. Previously, others have analytically characterized long-range energy transfer processes between quantum dots in free space [137, 138], as well as in such a cavity with more DBR layers [139], and at shorter ranges in a planar PEC microcavity [140]. A mesh of the computational domain, with dimensions, is illustrated in Figure 5.34.

The procedure for extracting inter-2LS couplings as outlined in Section 5.2.2 is implemented to study the coupling of a quantum dot at the center of this structure, with another placed a distance $d$ away from it along the axis of the cavity. The moments of both dots are aligned, and oriented such that they point along the short edge of the computational domain, and negligible fields are radiated in this direction. The coupling parameters are
investigated over a spectrum of energies centered at 1.36 eV, the cutoff of a guided mode of the system, with a FWHM of 0.68 eV. Fields are evolved for a period of time sufficient for the entire pulse to pass through the domain, and for the cavity fields to return to a quiescent state. Snapshots of the electric field intensity are illustrated in Figure 5.35.

In this image, the first snapshot is taken as the current source amplitude is peaked. The second and third are taken after the source has died down to a negligible level and give some indication of the guided mode structure being excited. By the end of the simulation, the fields have died down to the extent that they are unobservable on the scale of the visualization, i.e., they are at least 3 orders of magnitude below the peak.

The electric field component parallel to the exciting dipole is sampled along the central axis of the GaAs nanocavity, and Fourier transformed to give an indication as to how the cavity dresses propagation. The interval over which the field is sampled is indicated in the top part of Figure 5.35. Figure 5.37 illustrates the Fourier transformed field component over the spectral range for which the energy of the exciting current is above 10% of its peak, from a distance of 40 nm from the exciting source, to the edge of the computational domain 1040 nm away. For reference, Figure 5.36 illustrates the same quantity over the same scale, but in free space.

The Gaussian nature of the excitation is evident in the free space data in Figure 5.36. That the cavity strongly modifies this field distribution is then evident in Figure 5.37. While it is still evident that the fields are generated by a source with a Gaussian spectrum, it is clear that the cavity dramatically modifies this even at short range. One of the more relevant features is that the spectral content at and below 1.36 eV appears to be reduced relative to the content above this energy. This is a cutoff effect, in so far as 1.36 eV corresponds to an
in-GaAs wavelength of 260 nm, the height of the cavity, for which TE and TM guided modes exist [139]. Spectral content above this energy/below this wavelength will be able to match the dispersion relation of these modes and propagate, while content below this energy/above this wavelength will evanesce. In so far as this mode has a finite Q, this cutoff is not strict, and energy is coupled into leaky modes rather than evanescing as they would in a lossless cavity. These leaky modes exist independent of wavelength over the interval of interest. As the DBRs being modeled only consist of 3 layers above and below the cavity, the Q is not as high as is often experimentally realized, and some fields are still evident below the guided mode cutoff. Even so, the strong field between 1.36 and 1.9 eV from 250 nm to 540 nm can still be attributed to the dipole coupling to some low- to moderate-Q TE guided mode.

Next, the inter-2LS light-matter couplings are extracted using the procedure outlined in Section 5.2.2. In Figures 5.39 and 5.38, the modulus of the inter-2LS Green’s functions are illustrated for the DBR cavity and in free space for reference. In free space, a strong short-range interaction is evident, corresponding to the tail of the usual Förster energy transfer, scaling as $d^{-3}$. Further away, this scaling transitions to a slower $d^{-1}$, as the radiated fields begin to dominate. The situation is very much different in the DBR cavity. Here, a cutoff effect is evident in the short-range portion of the interaction, in which the strength of the inter-2LS coupling is diminished over a band of energies near the cavity cutoff. Further away, the interaction is enhanced by at least an order of magnitude relative to free space, both above and below cutoff. Below cutoff, the interaction strength decays more slowly than in free space. Above cutoff, the interaction is oscillatory, with a sharp suppression of the interaction corresponding to nodes of the cavity field evident in Figure 5.37, on top of a weak decay. For a higher Q structure, it is expected that the relative enhancement/suppression of
the interaction above cutoff would be more significant, with a maximum on resonance with
the guided mode, and the coupling to the leaky modes below cutoff would yield a slowly
decaying but weaker interaction. In particular, the results in [139] indicate that in a higher
Q DBR system with the system dipoles aligned in the same way, the resonant interaction is
mediated by a TE mode that gives rise to a characteristic $d^{-1/2}$ decay in the interaction
strength. A similar long-range interaction is evident in the results of the calculation in this
Section - while the relative size of the enhancement/suppression above and below cutoff is
different, the distance-dependence of the cavity-mediated interaction scales similarly.

To consider the interaction in more detail, the real and imaginary parts of the Green’s
function are plotted for 2LSs with transitions in three regimes - below cutoff, at cutoff, and
above cutoff in Figures 5.40, 5.41, and 5.42. Again, it is evident that the oscillations in the
net interaction strength become stronger at or above cutoff, corresponding to suppression at
the nodes of the guided mode observed in Figure 5.37. By resolving the real and imaginary
parts of the Green’s function individually, the relative strength of the coherent and incoherent
terms in Equation 5.90 interactions can be determined. This type of knowledge is especially
useful for quantum information applications in which the preservation of coherence is vital.

5.4 Future Work

Ultimately, the analysis of higher Q structures is desirable, both to see more dramatic
effects in terms cavity-mediated interactions, and to explore systems of relevance to quantum
information applications. To increase the Q of the structure studied in Section 5.3.2, a
number of steps might be taken. The simplest would be to add more layers to the DBRs
forming the cavity. This would increase the computational effort required for the solution of
the problem, but is otherwise tractable given enough CPU hours. Another, would be to use a higher contrast in index between DBR layers. The GaAs/AlAs example presented has a relatively low dielectric contrast simply because it is experimentally possible to realize this type of structure. While computational methods have no such restrictions, this does raise questions of relevance. However, even with these strategies, some other issues arise in the accurate analysis of high Q systems using time domain methods. One is evident in Figure 4.28. Here, the modal structure of a PEC cavity was resolved using a technique similar to the one employed in this Chapter. Theoretically, the modes being interrogated have an infinite Q, in so far as there are no losses in the system being modeled. Instead, a spurious numerical linewidth is evident, that makes it appear as if these modes have a finite lifetime due to the finite duration of the time signature from which they are extracted. Further, the dissipative nature of the upwind flux introduces numerical losses that contribute to this broadening, especially as longer simulations are required to resolve higher Q resonances. Ultimately, this is not a significant deficiency for energy transfer applications, and further explorations of systems similar to the one in Section 5.3.2 will be carried out. So long as the light-matter coupling is weak to moderate, this approach is eminently practical. However, as the transition into strongly coupled CQED is approached, as would be the case with quantum information applications, the high fidelity representation of cavity Q will become increasingly important.

To this end, a reasonable solution is to model the Q factor directly, by solving a Maxwell eigenproblem on an open domain. The discretization of the Maxwell eigenproblem is possible within the DG framework, so the underlying basis functions and code base can be reused. Immediately, one may be concerned that the eigenanalysis may be polluted by spurious
modes \(^1\), as is the case in nodal CG frameworks [141], however, the use of interior penalty (IP) factors [142] has been shown to alleviate this in DG. To this end, Buffa and Perugia [143] have outlined a set of conditions necessary for declaring that a DG discretization is free of spurious modes, and have subsequently shown that numerous IP and local DG schemes meet these criteria. Even in the case of non-conformal meshing, spurious solutions have been empirically demonstrated to be of little concern [65].

Even so, this analysis has been carried out for problems on closed domains. A structure with a finite Q is necessarily defined on an open domain. While the Silver-Müller boundary condition used earlier in this Dissertation can be used to effect this, it has some disadvantages as it must be placed sufficiently far from a given structure that the fields incident on it must be transverse, lest spurious reflections arise. A PML [40] can be used to bring the effective boundary closer, and will generally result in smaller spurious reflections. However, i.) PML optimization will become an issue, ii.) the PML may itself give rise to spurious modes, and iii.) error may be less controllable than would be desired for high Q systems. Even with a PML, if the open domain has some structure, as was the case with the DBR result presented in Section 5.3.2, it is lost in the finite truncation of the computational domain, i.e., the PML does not preserve layering of media, and neither does the Silver-Müller boundary condition. In practice, this can be mitigated by constructing a mesh that is sufficiently large that the absence of infinite stratification is not noticeable for a point source excitation at its center, and this is exactly what was done in Section 5.3.2. Ideally, however, a method that can achieve the same result with a smaller mesh while preserving this structure is desirable.

To this end, future work will see the development of an IPDG framework for a pole

\(^1\)Fundamentally, this would also be an issue for the transient analysis, as was explored in the last section of [126].
condition-based transparent boundary conditions that requires a simpler optimization, has been shown to produce nice error bounds for CG methods, and accommodates unbounded inhomogeneities. The crux of this method is the identification of the Sommerfeld radiation condition with conditions on the holomorphic extension of the Laplace transform of the asymptotic field [44, 45]. Considerable work has been done in realizing a numerically tractable means of generating solutions that satisfy these conditions. Perhaps the most successful approach to date is based upon the Möbius transform of the Laplace transform of the asymptotic field [46]. Further, these methods involve the use of infinite elements, which can be constructed in such a way as to allow for the explicit modeling of infinite stratification for structures like a DBR, and have already been applied to this end for planar waveguiding structures for scalar wave problems [144]. These methods can also be applied in the time domain, and implementing them provides a logical first step towards achieving a more accurate analysis of lossy cavities within the time domain framework already developed in this Chapter, prior to shifting the theoretical focus to one based upon eigenanalysis.

In switching over to an eigenanalysis-based approach, a question naturally arises germane to the underlying quantum mechanical model - how can the master equation coefficients be extracted from the Green’s function if the method outlined in Section 5.2.2 determines them from time domain data? The Green’s function can instead be constructed using a resolvent formalism, i.e., an expansion in eigenfunctions/eigenvalues of the field. While this will suffice for extracting parameters for the model identified in Section 5.2, alternative models may also prove promising in eliciting more detailed physics. In particular, a modified Maxwell eigenproblem was recently proposed in [27], in which the full light-matter eigenstates for a system with multiple quantum subsystems can be resolved directly. This formalism also
includes the proper treatment of the non-local susceptibility associated with coupling to an exciton, as would be relevant to a more first principles treatment of field-mediated coupling between quantum dots.

This raises one final issue to be confronted in future work. In the theory in Section 5.2, the light-matter coupling is still fundamentally phenomenological, in so far as the dipole moments have not been related to any higher theory that derives the 2LS parameters from something like an electronic structure model. To this end, closing the loop and performing ab initio electronic structure calculations to inform the QED model would provide a level of detail that has not yet been realized. Actual computation of excitonic wavefunctions may require the retention of terms beyond the dipolar truncation of the multipolar Hamiltonian given in Equation 5.85. Recent experiments have shown that in plasmonic systems with strong field gradients, the light-matter coupling can become sensitive to corrections that arise beyond the dipole approximation, justifying the application of this level of modeling [145].

5.5 Figures
Figure 5.32: (Left) A single quantum emitter above a PEC half-space. (Right) Its equivalent image problem. Arrows indicate the direction of the associated dipole moments.
Figure 5.33: Analytical and numerical spontaneous emission rate of a two-level system above a PEC half-space with its dipole moment parallel and perpendicular to the interface.
Figure 5.34: Mesh of the GaAs nanocavity in which energy transfer between two 2LSs is analyzed. All exterior boundaries are terminated with a Silver-Müller boundary condition.
Figure 5.35: Images of the electric field magnitude at three points in time. All images are taken from a plane cut halfway through the short axis of the mesh in Figure 5.34. (Top) At the peak of the exciting current. The black line indicates the path along which the fields are sampled to generate the Green’s function. (Middle) Half way through the simulation, the exciting current pulse is 4 orders weaker than at peak. (Bottom) Three quarters of the way through the simulation, the exciting current pulse is 20 orders weaker than at peak.
Figure 5.36: Distance dependence of the Fourier spectrum of the electric field component parallel to an exciting dipole in free space.
Figure 5.37: Distance dependence of the Fourier spectrum of the electric field component parallel to an exciting dipole in the center of the DBR cavity.
Figure 5.38: $\log_{10}$ of the modulus of the inter-2LS Green’s function in free space.
Figure 5.39: $\log_{10}$ of the modulus of the inter-2LS Green’s function in the cavity.
Figure 5.40: The inter-2LS Green’s function in the cavity for two systems with a transition below cutoff.
Figure 5.41: The inter-2LS Green’s function in the cavity for two systems with a transition resonant with the cutoff.
Figure 5.42: The inter-2LS Green’s function in the cavity for two systems with a transition above the cutoff.
APPENDICES
A.1 Bloch-Periodic Green’s Functions

The intent of Sections A.1.1 and A.1.2 is the clarification of details concerning the Bloch-periodic Green’s function used in Chapters 1.4 and 2.4. Derivations of the Bloch-periodicity condition and the Ewald representation of the Green’s functions are included.

A.1.1 Bloch-Periodicity Condition

The Bloch-periodic Green’s function for the Helmholtz equation is the solution to the following inhomogeneous PDE:

\[
\left( \nabla^2 + \kappa^2 \right) G_\mu(\mathbf{r},\mathbf{r}') = \sum_{\mathbf{t}(\mathbf{n}_\mu) \in \mathcal{L}_\mu} e^{i\vec{\kappa}_0 \cdot \mathbf{t}(\mathbf{n}_\mu)} \delta(\mathbf{r} - \mathbf{r}' - \mathbf{t}(\mathbf{n}_\mu))
\] (100)

Physically, \(G_\mu(\mathbf{r},\mathbf{r}')\) describes the scattering of a planewave excitation of unit intensity and wavevector \(\vec{\kappa}_0 \in \mathbb{R}^3\) on linear \(\delta\)-localized obstructions at the points of \(\mathcal{L}_\mu\). One is typically concerned with elastic scattering, i.e., \(\kappa = |\vec{\kappa}_0|\), though much of the subsequent derivation will remain agnostic to this.

Before deriving \(G_\mu(\mathbf{r},\mathbf{r}')\), it is useful to apply symmetry principles to derive the Bloch-periodicity condition cited in Equation 3.37. Consider a linear operator, \(\hat{T}_{\mathbf{t}(\mathbf{m}_\mu)}\) that translates the relative coordinates \(\mathbf{r} - \mathbf{r}'\) by \(\mathbf{t}(\mathbf{m}_\mu) \in \mathcal{L}_\mu\). Applying this operator both sides of Equation 100 yields:

\[
\hat{T}_{\mathbf{t}(\mathbf{m}_\mu)} \left( \nabla^2 + \kappa^2 \right) G_\mu(\mathbf{r},\mathbf{r}') = \sum_{\mathbf{t}(\mathbf{n}_\mu) \in \mathcal{L}_\mu} e^{i\vec{\kappa}_0 \cdot \mathbf{t}(\mathbf{n}_\mu)} \delta(\mathbf{r} - \mathbf{r}' - \mathbf{t}(\mathbf{n}_\mu) - \mathbf{t}(\mathbf{m}_\mu))
\] (101)
Substituting \( \vec{t}(\vec{l}_\mu) = \vec{t}(\vec{m}_\mu) + \vec{t}(\vec{n}_\mu) \), noting that the sum of \( \vec{t}(\vec{n}_\mu) \) over \( \mathcal{L}_\mu \) is equivalent to summing \( \vec{t}(\vec{l}_\mu) \), and restoring the dummy index \( l \) to \( n \) yields:

\[
\hat{T}_{\vec{t}(\vec{m}_\mu)} \left( \nabla^2 + \kappa^2 \right) G_{\mu}(\vec{r}, \vec{r}') = e^{-i\vec{\kappa}_0 \cdot \vec{t}(\vec{m}_\mu)} \sum_{\vec{t}(\vec{n}_\mu) \in \mathcal{L}_\mu} e^{i\vec{\kappa}_0 \cdot \vec{t}(\vec{n}_\mu)} \delta(\vec{r} - \vec{r}' - \vec{t}(\vec{n}_\mu)) \tag{102}
\]

As \( \hat{T}_{\vec{t}(\vec{m}_\mu)} \) commutes with the Helmholtz operator, it can be determined that \( G_{\mu}(\vec{r}, \vec{r}') \) obeys:

\[
\hat{T}_{\vec{t}(\vec{m}_\mu)} G_{\mu}(\vec{r}, \vec{r}') = G_{\mu}(\vec{r} - \vec{r}' - \vec{t}(\vec{m}_\mu)) = e^{-i\vec{\kappa}_0 \cdot \vec{t}(\vec{m}_\mu)} G_{\mu}(\vec{r} - \vec{r}') \tag{103}
\]

Which is the defining characteristic of a Bloch-periodic function.

A.1.2 Ewald Representation

For brevity of the resultant expressions, assume that \( \vec{\kappa}_0 = 0 \), noting that it is trivial to restore in the resultant expressions given the relation in Equation 103. The simplest representation of \( G_{\mu}(|\vec{r} - \vec{r}'|) \) is the direct one, in which it is furnished in terms of a summation of the associated free space Green’s functions translated over \( \mathcal{L}_\mu \).

\[
G_{\mu}(|\vec{r} - \vec{r}'|) = \sum_{\vec{t}(\vec{n}_\mu)} G(|\vec{r} - \vec{r}' - \vec{t}(\vec{n}_\mu)|) \tag{104}
\]

Here, the relevant free space Green’s function is given as:

\[
G(|\vec{r} - \vec{r}'|) = \frac{e^{-i\kappa|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|} \tag{105}
\]
It is evident that for real $\kappa$, Equation 104 will yield a conditionally convergent sum. Consequently, an alternative representation of the Green’s function is essential for computational purposes. The Ewald representation [112] is one such representation that converges spectrally both in and away from the $\mu$-lattice. The starting point for this representation is the following integral representation of the Green’s function in Equation 105:

$$
G(|\vec{r} - \vec{r}'|) = \frac{e^{-i\kappa|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|} = \frac{1}{2\pi^{3/2}} \int_{0}^{\infty} d\sigma e^{-\sigma^2|\vec{r} - \vec{r}'|^2 + \frac{\kappa^2}{4\sigma^2}}
$$

(106)

A derivation of this identity via a simple substitution is given in [146]. In so far as Equation 106 has a real-valued integrand along the real line, yet the result is ostensibly complex-valued, this is a particularly interesting identity. To this end, in order for the integral to be well-defined, the path of integration must be carefully deformed to avoid non-analyticity as $\sigma \to 0$ on the real line. The contour appropriate for this, can be traced back to Ewald [147], and is discussed in a bit more detail in [83].

The next step of the derivation is the splitting of the integration in Equation 106 over $[0, \infty)$ into separate integrals on $[0, \eta]$ and $[\eta, \infty)$, where $\eta \in \mathbb{R}^+$. The periodic Green’s function can then be represented as:

$$
G_{\mu}(|\vec{r} - \vec{r}'|) = \sum_{\vec{t}(\vec{n}_\mu) \in \mathcal{L}_\mu} \int_{0}^{\eta} d\sigma \ \mathcal{G}(\sigma, |\vec{r} - \vec{r}' + \vec{t}(\vec{n}_\mu)|) + \sum_{\vec{t}(\vec{n}_\mu) \in \mathcal{L}_\mu} \int_{\eta}^{\infty} d\sigma \ \mathcal{G}(\sigma, |\vec{r} - \vec{r}' + \vec{t}(\vec{n}_\mu)|)
$$

(107)

Here, the form of $\mathcal{G}(\sigma, |\vec{r} - \vec{r}' + \vec{t}(\vec{n}_\mu)|)$ is evident from Equation 106. In the first term, summation and integration are exchanged, and then the Poisson summation identity is applied
In this form, the integrals in both the real and reciprocal sums can be evaluated [149], leading to the Ewald representation of the periodic Green’s function in Equation 3.39.

A.2 Periodic Translation Operator Components

In this Section, expressions are provided for the terms in the summation in Equation 3.51. For brevity of the resultant expressions, it is assumed that $\kappa_0 = 0$, noting that it is trivial to restore in the resultant expressions. First, the terms in the real sum are considered. The integral representation of the real sum terms given in Equation 107 can be used to arrive at an expression that avoids the differentiation of complementary error functions. To this end, the derivatives are pulled inside of the integral and applied to the integrand prior to integration:

$$\nabla^{(p)} \mathcal{E}_T(\vec{R}) [p_x, p_y, p_z] =$$

$$= \frac{1}{2\pi^{3/2}} \int_{\eta}^{\infty} d\sigma \left( -\sigma^2 |\vec{R}|^2 + \frac{\kappa^2}{4\sigma^2} \right)$$

$$= \frac{1}{2\pi^{3/2}} \int_{\eta}^{\infty} d\sigma (-\sigma)^p H_{p_x}(\sigma R_x) H_{p_y}(\sigma R_y) H_{p_z}(\sigma R_z) e^{-\sigma^2 |\vec{R}|^2 + \frac{\kappa^2}{4\sigma^2}}$$

$$= (-1)^p \frac{1}{2\pi^{3/2}} \int_{\eta}^{\infty} d\sigma \sum_{m=0}^{p} C_m^{p_x, p_y, p_z} e^{-\sigma^2 |\vec{R}|^2 + \frac{\kappa^2}{4\sigma^2}}$$
Here, $C_{m}^{p_{x}p_{y}p_{z}}$ is the coefficient of the term which is $m$th order in $\sigma$ in the product of Hermite polynomials in Equation 109b. To evaluate this integral in closed form, expand the $\exp(\kappa^2/4\sigma^2)$ term in a Laurent series in $\sigma$.

\[
\nabla(p)\mathcal{E}_{r}(|\vec{R}|) [p_{x}, p_{y}, p_{z}] =
\]

\[
= \frac{(-1)^{p}}{2\pi^{3/2}} \int_{\eta}^{\infty} d\sigma \sum_{m=0}^{p} C_{m}^{p_{x}p_{y}p_{z}} \sum_{\nu=0}^{\infty} \frac{(\kappa/2\sigma)^{2\nu}}{\nu!} \sigma^{p+m} e^{-\sigma^2|\vec{R}|^2}
\]

\[
= \frac{(-1)^{p}}{2\pi^{3/2}} \sum_{m=0}^{p} \sum_{\nu=0}^{\infty} C_{m}^{p_{x}p_{y}p_{z}} \int_{\eta}^{\infty} d\sigma \frac{(\kappa/2\sigma)^{2\nu}}{\nu!} \sigma^{p+m} e^{-\sigma^2|\vec{R}|^2}
\]

\[
= \frac{(-1)^{p}}{4\pi^{3/2}|\vec{R}|} \sum_{m=0}^{p} \sum_{\nu=0}^{\infty} C_{m}^{p_{x}p_{y}p_{z}} \frac{(\kappa^2|\vec{R}|^2/4)^{\nu}}{\nu!} \Gamma \left( \frac{p+m+1}{2} - \nu, \eta^2|\vec{R}|^2 \right)
\]

Here, $\Gamma(n, x)$ is the incomplete Gamma function of $n$th order. It is worth noting that all sums over incomplete Gamma functions are rapidly convergent for physically relevant values of the arguments, and recurrence relations are utilized to rapidly compute each term.

The derivation of the translation operator components corresponding to terms in the reciprocal sum is much simpler, and only the final expressions are presented:

\[
\nabla(p)\mathcal{E}_{k}(\vec{R}, \vec{k}(\vec{n}_{\mu})) [p_{x}, p_{y}, p_{z}] =
\]

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\[ \begin{align*}
= (i k_x p_x e^{i \vec{k} \cdot \vec{R}_l / 4 \pi A_1} \sum_{\nu=0}^{\infty} \frac{(-\eta^2)^\nu}{\nu!} E_{1+\nu} \left( \frac{\alpha^2(n_1)}{4 \eta^2} \right) \times \ldots \\
& \quad \sum_{m=0}^{\nu} \frac{\nu}{m} \frac{(2\nu-2m)!}{(2\nu-2m-p_y)!} \frac{(2m)!}{(2\nu-2m-p_y)!} R_y^{2\nu-2m-p_y} R_z^{2m-p_z} \\
& \quad (\mu = 1) \\
& \quad (111a) \\
= (i k_x p_x e^{i \vec{k} \cdot \vec{R}_l / 4 \pi A_2 \alpha(n_2)} \sum_{\pm}^{\nu} (\pm 1)p_z \times \ldots \\
& \quad \sum_{m=1}^{p_z} \frac{\nu}{m} \frac{(-\eta)^m}{(\alpha(n_2))^{m-p_z}} \frac{2}{\sqrt{\pi}} H_{m-1} \left( \frac{\alpha(n_2)}{2 \eta} \pm \eta R_z \right) e^{-\frac{\alpha(n_2)^2}{4 \eta^2} - \eta^2 R_z^2} \ldots \\
& \quad \ldots (\alpha(n_2))^p_z e^{\pm \alpha(n_2) R_z \text{erfc} \left( \frac{\alpha(n_2)}{2 \eta} \pm \eta R_z \right)} \ldots (\mu = 2) \\
& \quad (111b) \\
= (i k_x p_x e^{i \vec{k} \cdot \vec{R}_l / 4 \pi A_3 \alpha(n_3) / 4 \eta^2} \sum_{\pm}^{\nu} (\pm 1)p_z \times \ldots \\
& \quad \sum_{m=1}^{p_z} \frac{\nu}{m} \frac{(-\eta)^m}{(\alpha(n_3))^{m-p_z}} \frac{2}{\sqrt{\pi}} H_{m-1} \left( \frac{\alpha(n_3)}{2 \eta} \pm \eta R_z \right) e^{-\frac{\alpha(n_3)^2}{4 \eta^2} - \eta^2 R_z^2} \ldots \\
& \quad (\mu = 3) \\
& \quad (111c)
\end{align*} \]

Here, \( R_i \) is the projection of \( \vec{R} \) along the \( i \)-axis, \( E_n(x) \) is the \( n \)th exponential integral and \( H_n(x) \) is the \( n \)th Hermite polynomial. For \( \mu = 1 \), it is assumed that the lattice lies along the x-axis, and for \( \mu = 2 \), it is assumed that the lattice lies in xy-plane.

A.3 Time-Domain Field of a Dipole

For convenience, the time-domain electric and magnetic fields emitted by a classical dipole are presented. To this end, a nice reference is a 2004 paper by Nevels and Jeong [150], in which authors provide a detailed derivation of the time-domain dyadic Green’s function for electric and magnetic currents and fields using the propagator formalism. As only electric
dipole currents are germane to this dissertation, the relevant results are the following two $3 \times 3$ blocks of the full $6 \times 6$ dyad:

$$
\overline{G}_{e,e}(|\vec{r} - \vec{r}'|, t - t') = \overline{G}_{e,e}(|\vec{R}|, \tau) = -\frac{\delta'(ct - |\vec{R}|)}{4\pi|\vec{R}|} \mathcal{I} - \nabla \nabla \frac{U(ct - |\vec{R}|) - U(-|\vec{R}|)}{4\pi|\vec{R}|}
$$

(112)

$$
\overline{G}_{h,e}(|\vec{r} - \vec{r}'|, t - t') = \overline{G}_{h,e}(|\vec{R}|, \tau) = \eta \nabla \times \frac{\delta(ct - |\vec{R}|)}{4\pi|\vec{R}|} \mathcal{I}
$$

(113)

Here, the second subscript indicates the type of current generating the field, and the first subscript indicates the type of field being generated, i.e., it is of interest to consider electric currents generating electric and magnetic fields. Using this form of the dyadic Green’s function, the free space electric and magnetic fields generated by a current of the form given in Equation 4.82 can be rendered as:

$$
\vec{E}(\vec{r}, t) = \int_{-t}^{0} d\tau \ \overline{G}_{e,e}(|\vec{R}_s|, \tau) \cdot \vec{d}_s j_s(t - \tau)
$$

(114)

$$
\vec{H}(\vec{r}, t) = \int_{-t}^{0} d\tau \ \overline{G}_{h,e}(|\vec{R}_s|, \tau) \cdot \vec{d}_s j_s(t - \tau)
$$

(115)

Here, $\vec{R}_s = \vec{r} - \vec{r}_s$ and it has been assumed that $j_s(t)$ was off prior to $t = 0$.

Evaluating the integral in Equation 114, it is clear that $\vec{E}(\vec{r}, t)$ can be separated into farfield and nearfield components, i.e, fields that decays as $|\vec{R}_s|^{-1}$, and those that decay more rapidly:

$$
\vec{E}(\vec{r}, t) = \vec{E}_{ff}(\vec{r}, t) + \vec{E}_{nf}(\vec{r}, t)
$$

(116)

The farfield contributions come from the term proportional to $\mathcal{I}$ in $\overline{G}_{e,e}$, as well as the
portion of the $\nabla^2$ term that differentiates the Heaviside functions twice:

$$\tilde{E}_{ff}(\vec{r}, t) = [\mathbf{R}_S(\tilde{d}_S \cdot \mathbf{R}_S) - \tilde{d}_S] \frac{j_s'(t - |\mathbf{R}_S|/c)}{4\pi|\mathbf{R}_S|}$$  \hfill (117)

The nearfield contribution arises due to the remaining portion of the $\nabla^2$ term:

$$\tilde{E}_{nf}(\vec{r}, t) = [\tilde{d}_S - 3\mathbf{R}_S(\tilde{d}_S \cdot \mathbf{R}_S)] \left( \frac{j_s(t - |\mathbf{R}_S|/c)}{4\pi|\mathbf{R}_S|^2} + \frac{q(t - |\mathbf{R}_S|/c)}{4\pi|\mathbf{R}_S|^3} \right)$$  \hfill (118)

Here, $q(t)$ is the amount of charge deposited on the dipole at time $t$, $q(t) = \int_{0}^{t} dt j_s(t)$. Evaluating the integral in Equation 115, the expression for $\tilde{H}(\vec{r}, t)$ is as follows:

$$\tilde{H}(\vec{r}, t) = \eta \tilde{d}_S \times \mathbf{R} \left( \frac{j_s(t - |\mathbf{R}_S|/c)}{4\pi|\mathbf{R}_S|^2} + \frac{j_s'(t - |\mathbf{R}_S|/c)}{4\pi|\mathbf{R}_S|} \right)$$  \hfill (119)

Here, the nearfield/farfield separation is obvious.
BIBLIOGRAPHY


