

ROBUST MAXWELL SOLVERS FOR LARGE SCALE PARTICLE-IN-CELL SIMULATIONS

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ABSTRACT

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The design of modern devices is impacted heavily by the use and availability of robust, efficient computational tools. This includes modeling devices that use plasma and other space charge like particle accelerators, klystrons, . These devices and phenomena can have fine features and complex geometry. That in turn requires millions and potentially billions of degrees of freedom to properly resolve the physics in the region of interest.

A common computational model to perform this analysis is the particle-in-cell method. It provides a straightforward paradigm to self-consistently solve for the distribution of the plasma as a collection of particles. The prevailing approach to solve for the fields in PIC is the finite difference time domain method, or EM-FDTD PIC. However, in the past decade, considerable effort has been put into defining finite element based PIC schemes, EM-FEMPIC. One major concern of utilizing EM-FEMPIC over EM-FDTD PIC is the computational cost of FEM, which is greater than FDTD, despite the advantages of field and geometry accuracy FEM affords.

This dissertation seeks to advance the state of the art of EM-FEMPIC methods by defining EM-FEMPIC schemes that can accurately solve large-scale problems. First, the requirements of charge conserving EM-PIC schemes are explored for both EM-FDTD PIC and EM-FEMPIC. A clear comparison of methods are made between EM-FDTD PIC and two EM-FEMPIC formulations. Then, a higher order EM-FEMPIC scheme is presented that maintains charge conservation. Finally, two domain decomposition approaches are presented that ameliorate the cost of EM-FEMPIC without compromising the accuracy or physics.

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CHAPTER 1

INTRODUCTION AND BACKGROUND

1.1 Introduction

Plasma is the most abundant state of matter in the universe. It is ionized gas of equal parts positively and negatively charged particles, namely electrons and ions. Plasma is the bulk constituent of stars, solar winds, and natural phenomena such as lightning and the key component in television screens, neon signs, and nuclear fusion. Understanding how plasma interacts with its environments informs the design of novel accelerator technology and beam wave interaction devices. The volume of plasma is approximately charge neutral, though regions may be more positively or negatively charged. This has some interesting repercussions. The charges in plasma can radiate when moving, causing self-interactions in the plasma, as well as be affected by other electromagnetic sources. Plasma generally are good electrical and thermal conductors and even exhibit wave phenomena. The combination of all these features makes plasma very difficult to predict through simple models for the vast number of complicated uses and places it manifests. Thus, computational modeling is often used to study plasma and gain insight into how these behaviors manifest themselves in nature and man-made environments, computational modeling is often used.

Many computational tools have been developed in order to accelerate the design of new devices and better understand nature. This is not to say that modeling plasma is a simple task, even after decades of research and development of these tools. Modeling plasma requires one to solve a multiscale, multiphysics problem to simulate the behavior of many, many particles interacting with themselves and potentially other outside sources. This is an inherently nonlinear problem that has been an open area of research, with many paradigms to solve it. This can be simplified by modeling plasma as the interaction of currents and

the resulting electromagnetic fields. This would require a robust electromagnetic solver at a minimum to model plasma. It would also be wise to consider methods that can leverage high performance computing architecture, considering that modeling electromagnetic devices without sources can require vast amounts of computational resources. In order to accomplish this feat of modeling plasma, it is necessary to improve and create computational tools that specifically accommodate the physics one wishes to model. This work specifically seeks to improve the state of the art for numerically finding dynamic electromagnetic fields with charges.

1.2 Problem Statement

We begin by simplify the physics of the problem by following a kinetic description of the plasma. In this model, the representation of the particles in the system move as result of collisions or electromagnetic forces, which may come from external forces or interactions between particles. Consider a region in space Ω which contains the plasma of interest that is bounded by $\partial\Omega$ with an outward pointing normal vector $\hat{n}$ that points into a vacuum Ω_v . The plasma is represented with particles described with a phase space distribution

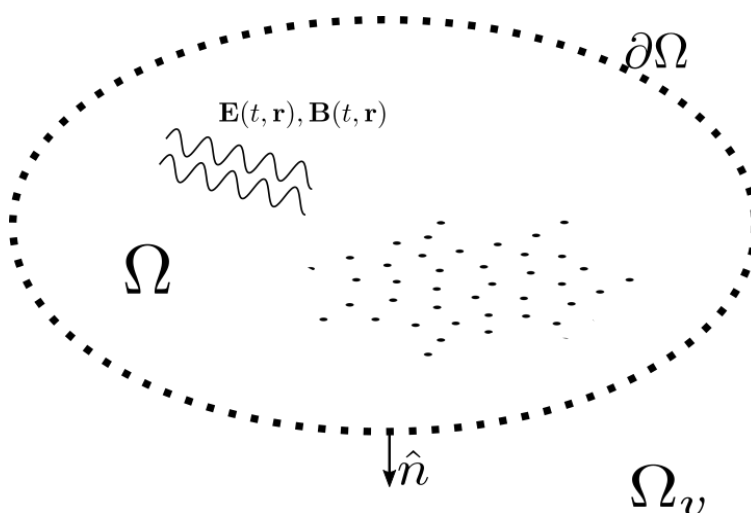


Figure 1.1: Sample Volume Ω with particles

function $f(t, \mathbf{r}, \mathbf{v})$ (PSDF) that satisfies the Vlasov equation

$$\partial_t f(t, \mathbf{r}, \mathbf{v}) + \mathbf{v} \cdot \nabla f(t, \mathbf{r}, \mathbf{v}) + \mathbf{a} \cdot \nabla_v f(t, \mathbf{r}, \mathbf{v}) = 0, \quad (1.1)$$

where $\mathbf{v}$ is the particle velocity and the particle acceleration is defined by the Lorentz force

$$\mathbf{a} = \frac{q}{m} (\mathbf{E}(t, \mathbf{r}) + \mathbf{v} \times \mathbf{B}(t, \mathbf{r})). \quad (1.2)$$

In general, the plasma can be composed of many species of particles, but for simplicity, only a single species is considered in this description. The particles are sources, the charge density $\rho(t, \mathbf{r})$ and current density $\mathbf{J}(t, \mathbf{r})$, that are defined in terms of the PSDF as

$$\rho(t, \mathbf{r}) = q \int_{\Omega} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v} \quad (1.3a)$$

$$\mathbf{J}(t, \mathbf{r}) = q \int_{\Omega} \mathbf{v}(t) f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v} \quad (1.3b)$$

and are subject to Newton's equations of motion

$$\mathbf{v}(t) = \partial_t \mathbf{r}(t) \quad (1.4a)$$

$$\mathbf{a}(t) = \partial_t \mathbf{v}(t). \quad (1.4b)$$

The electric field $\mathbf{E}(t, \mathbf{r})$ and magnetic flux density $\mathbf{B}(t, \mathbf{r})$ satisfy Maxwell's equations

$$\partial_t \mathbf{B}(t, \mathbf{r}) = \nabla \times \mathbf{E}(t, \mathbf{r}) \quad (1.5a)$$

$$\partial_t \mathbf{D}(t, \mathbf{r}) = \nabla \times \mathbf{H}(t, \mathbf{r}) - \mathbf{J}(t, \mathbf{r}) \quad (1.5b)$$

$$\nabla \cdot \mathbf{B}(t, \mathbf{r}) = 0 \quad (1.5c)$$

$$\nabla \cdot \mathbf{D}(t, \mathbf{r}) = \rho(t, \mathbf{r}), \quad (1.5d)$$

where the electric flux density $\mathbf{D}(t, \mathbf{r})$ and magnetic field $\mathbf{H}(t, \mathbf{r})$ are related to the electric field and magnetic flux density through the constitutive parameters

$$\mathbf{D}(t, \mathbf{r}) = \varepsilon(t, \mathbf{r}) *_t \mathbf{E}(t, \mathbf{r}) \quad (1.6a)$$

$$\mathbf{B}(t, \mathbf{r}) = \mu(t, \mathbf{r}) *_t \mathbf{H}(t, \mathbf{r}) \quad (1.6b)$$

where $*_t$ is a convolution in time. The permittivity $\varepsilon(t, \mathbf{r}) = \varepsilon_0 \varepsilon_r(t, \mathbf{r})$ and permeability $\mu(t, \mathbf{r}) = \mu_0 \mu_r(t, \mathbf{r})$. This work mostly has Ω composed of free space, implying $\varepsilon_r(t, \mathbf{r}) = \mu_r(t, \mathbf{r}) = 1$, and $1/\sqrt{\mu_0 \varepsilon_0} = c$ where c is the speed of light. The fields also obey the boundary conditions

$$\hat{n} \times (\mathbf{E}_\Omega(t, \mathbf{r}) - \mathbf{E}_{\Omega_V}(t, \mathbf{r})) = 0 \quad (1.7a)$$

$$\hat{n} \times (\mathbf{H}_\Omega(t, \mathbf{r}) - \mathbf{H}_{\Omega_V}(t, \mathbf{r})) = \mathbf{J}_s(t, \mathbf{r}) \quad (1.7b)$$

$$\hat{n} \cdot (\mathbf{D}_\Omega(t, \mathbf{r}) - \mathbf{D}_{\Omega_V}(t, \mathbf{r})) = \rho_s(t, \mathbf{r}) \quad (1.7c)$$

$$\hat{n} \cdot (\mathbf{B}_\Omega(t, \mathbf{r}) - \mathbf{B}_{\Omega_V}(t, \mathbf{r})) = 0 \quad (1.7d)$$

where the subscript denotes whether it is within Ω or in Ω_V . Additionally, it is necessary to also satisfy the continuity equation

$$\partial_t \rho(t, \mathbf{r}) = -\nabla \cdot \mathbf{J}(t, \mathbf{r}) \quad (1.8)$$

which can be derived from (1.5) or from (1.1).

The fields which satisfy (1.5) do not have to be obtained directly from those equations. At times, the wave equation is used instead

$$\nabla \times \mu_r^{-1}(t, \mathbf{r}) *_t \nabla \times \mathbf{E}(t, \mathbf{r}) + c^{-2} \partial_t^2 \varepsilon_r(t, \mathbf{r}) *_t \mathbf{E}(t, \mathbf{r}) = -\partial_t \mathbf{J}(t, \mathbf{r}) \quad (1.9)$$

or

$$\nabla \times \varepsilon_r^{-1}(t, \mathbf{r}) *_t \nabla \times \mathbf{H}(t, \mathbf{r}) + c^{-2} \partial_t^2 \mu_r(t, \mathbf{r}) *_t \mathbf{H}(t, \mathbf{r}) = \nabla \times \varepsilon_r^{-1}(t, \mathbf{r}) *_t \mathbf{J}(t, \mathbf{r}). \quad (1.10)$$

Either both equations can be used to obtain both the electric and magnetic fields, or one can be used and then use one of the curl equations, Faraday's law (1.5a) or Ampere's law (1.5b), to obtain the other field. Regardless of which equation or set of equations are used, the main difficulty remains: to choose a scheme which self-consistently yields the fields and particle positions and velocities that satisfies the Vaslov-Maxwell equation, Newton's equations, Maxwell's equations, and the appropriate boundary conditions.

1.2.1 Preliminaries

The first step in solving the proposed the problem is to discretize problem such that it can be described numerically to be solved on computers. First, divide Ω in to a number of non-overlapping cells, also reffered to as elements. The shape of the cells are typically hexahedra or tetrahedra in three dimensions, or rectangles or triangles in two dimensions. The collection of these cells are called a mesh or grid. In some methods, the hexahedral (rectangular) mesh will be made regular, such that it will be cubic (square), which is called a structured mesh. Otherwise the mesh is called unstructured. The trade-off is that structured grids allow one to take advantage of the orthogonality of the grid, but lose potential accuracy to staircasing errors as Ω is not usually a square or rectangular object. Regardless of the mesh style that is chosen, the mesh will be composed of nodes, edges, faces, and cells. Associated with some feature of the mesh, there is a basis set used to represent or reconstruct some quantity. The discretization of the equations will require approximation of the vector quantities as

$$\mathbf{X}(t, \mathbf{r}) \approx \sum_{i=1}^{N_\gamma} x_i(t) \mathbf{s}_i(\mathbf{r}) \quad (1.11)$$

where N_γ is number of nodes, edges, faces, or cells, and $\mathbf{s}(\mathbf{r})$ is some vector basis set. Similarly, scalar quantities are approximated as

$$Y(t, \mathbf{r}) \approx \sum_{i=1}^{N_\gamma} y_i(t) g_i(\mathbf{r}) \quad (1.12)$$

where $g(\mathbf{r})$ is a scalar basis set. Often, a shorthand will be used to collect the coefficients of the basis sets, or degrees of freedom, into a single vector, e.g. $\mathbf{x} = [x_1(t), x_2(t), \dots, x_{N_\gamma}(t)]$. The choice of the basis sets depends on the quantity being discretized due to conditions on that quantity. For example, a field quantity like the electric field does not require normal continuity across an interface. In fact, in the presence of a surface charge or change in material, the electric field will be normally discontinuous. However, the tangential component of the electric field is always continuous (as we have discounted the possibility

of a fictitious magnetic monopole or current). Furthermore, not every equation defined in the previous section will be turned into an equation that will be solved, yet it still must be satisfied. This will lead to particular choices of basis sets that is explained in detail in Chapter 2.

There are many approaches to to obtain the values of the degrees of freedom that best approximate the quantities of interest. The methods that will be presented later in this chapter and in this work, the finite-difference time domain (FDTD), the finite element method (FEM), and the mixed finite element method (MFEM), are all examples of the method of weighted residuals. Consider a spatial linear operator $\mathcal{L} \circ$ that operates on a function $\mathbf{X}(t, \mathbf{r})$ such that

$$\mathcal{L} \circ \mathbf{X}(t, \mathbf{r}) = \mathbf{U}(t, \mathbf{r}), \quad \forall \mathbf{r} \in \Omega \quad (1.13)$$

subject to boundary condition

$$\mathcal{L}_{\partial\Omega} \circ \mathbf{X}(t, \mathbf{r}) = \mathbf{W}(t, \mathbf{r}), \quad \forall \mathbf{r} \in \partial\Omega \quad (1.14)$$

with boundary operator $\mathcal{L}_{\partial\Omega} \circ$. The method of weighted residuals defines a residual function from (1.13)

$$\mathcal{R}(t, \mathbf{r}) = \mathcal{L} \circ \mathbf{X}(t, \mathbf{r}) - \mathbf{U}(t, \mathbf{r}) \quad (1.15)$$

which is has applied inner product, or tested, with a trial basis set $\tilde{\mathbf{s}}_j(\mathbf{r})$ that has compact support, typically over one cell on the mesh defined in Ω, Ω_c . Ideally, the residual would be equal to zero. However, only an approximation is available through the measurement of residual with a compact support basis set through an inner product that is set to zero

$$\int_{\Omega_c} d\tilde{\mathbf{r}} \tilde{\mathbf{s}}(\tilde{\mathbf{r}}) \cdot \mathcal{R}(t, \tilde{\mathbf{r}}) = 0. \quad (1.16)$$

Provided the residual is defined using (1.11), a system of linear equations can be defined as

$$\sum_{j=1}^{N_\gamma} x_i(t) \langle \tilde{\mathbf{s}}_i(\mathbf{r}), \mathcal{L} \circ \mathbf{s}_j(\mathbf{r}) \rangle = \langle \tilde{\mathbf{s}}_i(\mathbf{r}), \mathbf{U}(t, \mathbf{r}) \rangle \quad (1.17)$$

where $\langle \cdot, \cdot \rangle$ denotes a standard inner product. This can be more simply written as a matrix vector product

$$\underline{\mathbf{A}}\mathbf{x} = \mathbf{u} \quad (1.18)$$

where $\underline{\mathbf{A}} \in \mathbb{R}^{N_\gamma \times N_\gamma}$ with elements $\underline{\mathbf{A}}_{ij} = \langle \tilde{\mathbf{s}}_i(\mathbf{r}), \mathcal{L} \circ \mathbf{s}_j(\mathbf{r}) \rangle$ and $\mathbf{u} \in \mathbb{R}^{N_\gamma}$ with elements $\mathbf{u}_j = \langle \tilde{\mathbf{s}}_j(\mathbf{r}), \mathbf{U}(t, \mathbf{r}) \rangle$. Often, the choice of $\tilde{\mathbf{s}}(\mathbf{r})$ is made to be the same as $\mathbf{s}(\mathbf{r})$, which would result in a Galerkin method. It is stressed again that $\mathbf{s}(\mathbf{r})$ itself should satisfy the differential equations and boundary conditions [53]. It is also noted that (1.18) could have been derived through other approaches, such as Rayleigh-Ritz method [6] or through the use of calculus of variations [58]. In later sections and chapters, (1.5) and (1.7) will be used in place of (1.13) and (1.14) to derive FDTD, FEM, and MFEM. Section 2 in particular demonstrates how FDTD, FEM, and MFEM are all related through this framework.

1.3 Particle-in-Cell

One of the most used methods to model plasma is particle-in-cell (PIC). It follows the kinetic approach to modeling plasma by tracking the motion of particles, as each particle has a position and velocity with which it is associated. Often, the particles are representative of groups of particles called macroparticles. Because the interest is most often in the bulk behaviour of the particles, reducing the number of particles modeled this way reduces computational burden without greatly changing the overall behaviour of the plasma. This representation of the plasma then needs to be incorporated with the discretization of the electromagnetic system, a process called mapping the plasma to the mesh. Again, a plasma is a collection of charged particles, and is interpreted as charge and current that is being included in the electromagnetic system. This provides a complete description of the discretized electromagnetic system that can be solved for the fields, which are self-consistent and can be used to accelerate the particles.

The PIC method is a cycle that repeats this process of mapping the position and velocity of particles under the influence of the fields found through some field solver. The basic

steps of the PIC method are as follows

1. Map charge and current to the mesh
2. Solve for the fields including the macroparticles
3. Interpolate the fields at the macroparticle positions
4. Push the macroparticles to new positions.

The motion of the macroparticles is determined by (1.4), typically discretized by staggered finite differences in time such that

$$\mathbf{v}^{n+\frac{1}{2}} = \mathbf{v}^{n-\frac{1}{2}} + \frac{q}{m} (\mathbf{E}^n + \mathbf{v}^n \times \mathbf{B}^n) \quad (1.19a)$$

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \Delta_t \mathbf{v}^{n+\frac{1}{2}}. \quad (1.19b)$$

The preceding equation is typically evolved using what is called the Boris push [18], which preserves the phase of the system while being an explicit method. Other explicit formulations tend to have errors in phase space and implicit methods are typically deemed too expensive to calculate given the number of particles that are in the system at any given time. Additionally, modifications have been made to the Boris push to be valid in the relativistic range, where particles move close to the speed of light [166]. The fields are obtained by any number of methods, depending on the relative physics. When the particles are traveling much slower than the wave speed, one can solve Poisson's equation to yield an electrostatic PIC (ES-PIC) method [135, 163, 162, 64]. However, we focus on the more general case of electromagnetic PIC (EM-PIC) formulations, where the magnetic field (or flux) can be significant. Most commonly, FDTD is used as the field solver, a FDTD-PIC formulation [169]. This formulation not only has been used to codify EM-PIC by the likes of Birdsall, Langdon, Eastwood, and others [16, 77], but has continued to see extensive use [179, 72, 151, 101, 1]. This is due to some of the benefits of FDTD which are highlighted in the next section. However, there has been significant development of FEM-PIC which uses FEM as the field solver in EM-PIC.

1.4 Finite-Difference Time-Domain

The earliest approach of FDM was the finite-difference time-domain (FDTD) or Yee-method, developed by Yee in 1966 [189]. In this method, finite differences are used to approximate the time derivatives and curl operators of (1.5a) and (1.5b). The degrees of freedom are the electric field and magnetic field defined on the edges of staggered cubical or rectangular mesh, often called a structured grid. The two equations are also staggered in time to make an explicit Leapfrog time marching scheme. The time step size is limited by a Courant–Friedrichs–Lewy condition determined by the size of the mesh cells. Unconditionally stable time marching schemes have been developed for FDTD, but most commonly focus on the Leapfrog method. The simplicity of FDTD makes it a powerful tool for analysis, implemented very simply with the recurrence formulations that define the method using a simple stencil. Its popularity over the decades has created a wealth of implementations, including on high performance architectures. It has been used to analyze and model many problems including electromagnetic scattering, antennas, photonics, and [159, 102, 134, 82]. It has also been used extensively to model kinetic plasmas, which will be discussed at length in Section 2.

However, FDTD is not without its limitations. The structured grids used results in geometric errors in representing more complex geometry. This can be remedied somewhat by sub-cell and sub-grid formulations which increase the resolution of regions of the mesh, sacrificing stability and control of the accuracy [57]. Higher order spatial representations are typically limited to expanding the stencil and are not as accessible as other methods. Therefore, often the solution is to increase the resolution of the mesh by creating more cells. Furthermore, these approaches to improve geometric and field accuracy can exacerbate another limitation: the time step size. As stated, the time step size is limited by the smallest features in the mesh, making analyzing certain systems very time consuming from the sheer number of time steps needed to observe the desired phenomena. Some of these problems were remedied by the adaption of FEM for electromagnetics.

1.5 Finite Element Method

The earliest works in FEM were outside of the electrical engineering discipline. It is credited to the appendix of a paper by Courant [40] in 1943, but it would not be until the late 1960s when Arlett, Bahrani, and Zienkiewicz [7] and Silvester [150] would apply the method to electromagnetics examining waveguides and cavities. Despite studying the time harmonic Helmholtz equation, the process for formulating the FEM system remains much the same. Here, Ω can be subdivided with triangles or tetrahedra in addition to rectangles/rectangular prisms where degrees of freedom and associated basis functions are defined. This generates a sparse, but typically not diagonal, system of equations that can be solved. Importantly, in the earliest works, scalar basis functions associated with the nodes of the mesh were used. However, when extended to the vector wave equation, spurious modes were found which were caused by not properly satisfying Gauss' law and the associated boundary conditions [80]. In order to overcome this problem, many approaches were developed [73, 184, 137], but the most popular method is using vector basis functions [123, 29]. Importantly, these basis sets, first proposed by [180], only have tangential continuity at the element boundaries, which correctly satisfies the boundary condition for fields (1.7a) without violating the boundary condition for fluxes (1.7d). With this development, accurate results could be reported for not only the wave equation, but Maxwell equations as well.

The introduction of vector basis functions for FEM allowed for the exploration of more problems in EM. FEM for the wave equation has been used to model many electromagnetic problems such as circuits, antennas, scattering, and other plasma-related phenomena [175, 99, 81, 186, 93]. In order to do large scale analysis, different approaches have been developed to avoid having to solve all the equations simultaneously. Some approaches like discontinuous Galerkin [79, 36, 67, 25] or element level dual field [100] approaches use flux or field continuity conditions to enable solving (1.9) on an element level. Other domain decomposition methods (DDM) [173, 55] are designed to solve the problem in

larger groupings of elements, and using various boundary conditions to ensure satisfaction of boundary conditions. One drawback of solving (1.9) and (1.10) specifically is that it does not implicitly constrain Gauss' law. Therefore, some began solving (1.5a) and (1.5b), by introducing another basis function with normal continuity across cell faces, to create a mixed finite element method (MFEM) [20, 24, 76, 140]. This method is the primary focus of this thesis.

1.6 Open Problems

The creation of more powerful EM-PIC methods requires advancing the underlying field solver technology. EM-PIC is by no means new and has been thoroughly explored using FDTD, as well as implementations in FEM [109], as well as MFEM [130, 115, 88]. However, examining each case reveals deficiencies. The shortcomings of FDTD, namely greater accuracy without greatly increasing spatial discretization, has driven the push toward using FEM and MFEM. At the time of writing, FEM-PIC approaches cannot use exact current mapping, instead relying on pseudocurrents to enforce the continuity equation [106]. MFEM implementations have not utilized unconditionally stable time marching, nor taken advantage of higher order spatial basis sets. Attempts to perform large scale analysis have been restricted to FDTD-PIC and discontinuous Galerkin FEM-PIC methods which still require divergence cleaning to maintain charge conservation. The approach for large scale analysis using MFEM (and by extension, MFEM-PIC) relies on performing a sparse approximate inverse. However, as will be explored in Chapter 2, there are connections between FDTD, FEM, and MFEM that can be explored to make more robust field solvers, and by extension, better EM-PIC methods. This work uses improvements to MFEM as a means to define and formalize the guiding principles to define robust EM-PIC methods. Furthermore, the improvements and ideas presented here can be extended to modeling other sources beyond kinetic plasmas.

1.7 Goals and Outline

In this dissertation, I present methods to reduce the cost of MFEM-based EM-PIC. The principle contributions of this work are as follows:

1. Apply various advances in FEM to MFEM, namely
 - unconditionally stable time marching,
 - higher order spatial basis sets,
 - domain decomposition, and
2. Apply these advances to modeling plasmas and space charge with charge conserving PIC schemes
3. Explore the uses and benefits of an underutilized variant of MFEM, DH-MFEM, particularly with respect to DH-MFEM-PIC.

The outline of the dissertation is as follows.

Chapter 2 is prescribed to develop charge conserving current mapping schemes in FEM. It examines what properties are necessary to create a charge-conserving current mapping scheme for EM-PIC. Comparisons are made between FDTD and two formulations of MFEM. Chapter 3 presents a EM-MFEMPIC scheme using higher order spatial basis functions. The use of higher order basis functions allows for a reduction of degrees of freedom for a desired level of accuracy compared to previous lowest order descriptions. It also presents a scheme to satisfy Gauss' magnetic law that is valid for higher order schemes. Chapter 4 presents two domain decomposition schemes for MFEM and applies them to EM-FEMPIC. The cost of solving large problems is reduced by solving a dual problem on fictitious, non-overlapping boundaries. This allows for a speed up in computational time while maintaining the required charge conservation properties.

CHAPTER 2

RUBRICS FOR CHARGE CONSERVING CURRENT MAPPING IN FINITE ELEMENT PARTICLE IN CELL METHODS

2.1 Introduction

Modeling plasmas and other charged media as sources is a needed capability to better understand and design many real-world devices. Of the many techniques to model this phenomena, the particle-in-cell (PIC) method has been a popular approach. A wide variety of fields depend on PIC as a computational method, ranging from fundamental science of space weather, nuclear fusion, atomic processes on one hand, to high technology applications like particle accelerators, coherent electromagnetic radiation sources, and plasma processing devices on the other. PIC, at a glance works as follows; charged media, represented as a collection of particles, move in a domain under the influence of fields that are due to motion of these particles. This calls for self consistent solution of Maxwell's equations in conjunction with equation of motion. Given application drivers stated earlier, there has been extensive development of EM-PIC methods [45, 98, 63, 38]. Several of these have been used extensively in the design of devices [104, 30, 60]. While traditional application were electrically large *albeit* geometrically simple, there is burgeoning interest in devices with significantly geometric complexity but smaller footprint. As a result, there is need for EM-PIC methods with greater capabilities [109].

But before we delve extensively into nuances and needs of modern EM-PIC codes, it helps to understand a bit of history of challenges that have been overcome in developing EM-PIC methods. The principal challenge in EM-PIC modeling is self-consistency of solving Maxwell's equation together with equations of motion so as to actually capture dynamics of the distribution function. Challenges lies in incorporation of sources (and their variation over time) consistently into Maxwell's equation. As a result, there has been

extensive work in understanding how one may develop methods that conserve charge [33, 32, 153]. Early development of EM-PIC methods largely relied on finite difference time domain (FDTD-PIC), as did addressing many of the aforementioned challenges [171, 91]. More recent PIC development has seen extensive development mixed finite element methods (MFEM-PIC) and discontinuous-Galerkin (DG-PIC) as the EM field solver [88, 120, 78].

These developments are specially pertinent as EM-PIC models that can more accurately capture geometry and physics with greater computational efficiency would soon be necessary to modeling physics ranging from novel accelerators to high frequency semiconductor devices. As the complexity of system to be modeled increases one needs EM-PIC suites that leverage advances in both finite element and particle methods. But as is to be expected, integrating the two calls for ensuring that self-consistency is preserved. This implies that discrete solutions of Maxwell's equations together with Newton's laws satisfy *all* of Maxwell's equations together with the equation of continuity at every time step. This is easier said than done. Errors can manifest themselves as spurious charges and currents. To overcome these, it is possible to use procedures such as divergence cleaning to correct the erroneous fields that arise. Approaches to correct the fields include using Lagrange multipliers [106], solving Poisson's equation at multiple time steps [18, 91], or changing the field solver [148]. However, there can be a significant computational cost to using these methods. Of course, a more desirable alternative is to prescribe a rubric in which charge is conserved as well as there is no space charge/current.

Developing computational methods that are inherently charge conserving has been a topic of interest as long ago as there have been EM-PIC codes [26, 44]. The benefits of having a charge conserving scheme are apparent; they avoid additional work necessary to effect divergence cleaning. Unfortunately, their development has always been closely tied to a particular EM-solution technique, be in FDTD-PIC [171, 51] or MFEM-PIC [130, 115]. The latter is novel in that it develops a method that relies on *de-Rham* maps to define the

proper basis sets for representing the electric field and magnetic flux density. In effect, the primal quantities are defined based on Faraday’s laws. The current mapping schemes demonstrate how they recover the results found in the early literature [171, 51]. As methods developed have been solver specific, significant attention has not been paid to examining the underlying mathematical structure and why that is necessary for charge conservation. In this work, we seek to do just that.

While unusual, we start our analysis at the particle approximation of the distribution function and develop a simple *albeit* rigorous approach to demonstrate charge continuity relationships between charge density and currents. The exposition in this paper straightforward and uses the sifting property of the delta function. This is unlike that in presented in [51] that relies on an discrete approximation. As an added benefit, this approach lays the groundwork for developing conditions for mapping particles and fields on any discrete grid, and consistently evolving their position and strength. In effect, we create a uniform framework and criterion that is necessary to solve all of Maxwell’s equation consistently, thereby satisfying charge conservation as well. The rubrics prescribed are in agnostic to the method used to solve Maxwell’s equations. Indeed, we demonstrate how these are applicable to FDTD and (M)FEM. We also use a these rubrics to develop a novel MFEM-PIC scheme that uses electric flux density and the magnetic field (DH-MFEM-PIC) and validate its properties including charge conservation, satisfaction of Gauss’ law as well as comparison against quasi-analytic data.

The rest of the paper is organized as follows: After defining the EM-PIC problem in Section 2.2 and its discretization using particle approaches, we define the three rules in Section 2.3 in the context of preserving the spatial and temporal connections between Gauss’ law and Ampere’s law. In Section 2.4, we provide examples on how FDTD and two formulations of a variant of FEM, the mixed finite element method (MFEM), satisfy the three conditions. One of these is novel in that it relies on the electric flux density and the magnetic field (DH-MFEM). Next, in Section 2.5, we provide results that show

what happens when the conditions are violated as well as affirm the correct behavior of MFEM when the conditions are met. In addition, several results are provided for the DH-MFEM-PIC that demonstrate necessary features for a number of examples (charge conservation, satisfaction of Gauss' laws, correctness against quasi-analytical data). In an Appendix, we present details of the MFEM discretizations and other proofs.

2.2 Problem Statement and Formulation

Consider a domain Ω whose boundaries are denoted by $\partial\Omega$. It is assumed that domain comprises of charged species that exist in a background medium defined by ε_0 and μ_0 , the permittivity and permeability of free space; for simplicity of the exposition, we consider only one species. It is also assumed that there exists an electromagnetic field, both impressed and arising from motion of the charged species. Both the fields and the charged species evolve in time. The evolution of the charged species is modeled via a fluid approximation and those of fields using Maxwell's equations. To this end, we assume that the particle distribution function (PDF) $f(t, \mathbf{r}, \mathbf{v})$ must satisfy the Vlasov-Maxwell equation

$$\partial_t f(t, \mathbf{r}, \mathbf{v}) + \mathbf{v} \cdot \nabla f(t, \mathbf{r}, \mathbf{v}) + \frac{q}{m} [\mathbf{E} + \mathbf{v} \times \mathbf{B}] \cdot \nabla_v f(t, \mathbf{r}, \mathbf{v}) = 0. \quad (2.1)$$

The electric field $\mathbf{E}(t, \mathbf{r})$ and magnetic flux density $\mathbf{B}(t, \mathbf{r})$ satisfy Maxwell's equations

$$-\partial_t \mathbf{B}(t, \mathbf{r}) = \nabla \times \mathbf{E}(t, \mathbf{r}) \quad (2.2a)$$

$$\partial_t \mathbf{D}(t, \mathbf{r}) = \nabla \times \mathbf{H}(t, \mathbf{r}) - \mathbf{J}(t, \mathbf{r}) \quad (2.2b)$$

$$\nabla \cdot \mathbf{B}(t, \mathbf{r}) = 0 \quad (2.2c)$$

$$\nabla \cdot \mathbf{D}(t, \mathbf{r}) = \rho(t, \mathbf{r}), \quad (2.2d)$$

where fields and fluxes are related through constitutive parameters

$$\mathbf{B}(t, \mathbf{r}) = \mu_0 \mathbf{H}(t, \mathbf{r}) \quad (2.3a)$$

$$\mathbf{D}(t, \mathbf{r}) = \varepsilon_0 \mathbf{E}(t, \mathbf{r}). \quad (2.3b)$$

The moments of the particle distribution function yield the the charge density $\rho(t, \mathbf{r})$ and current density $\mathbf{J}(t, \mathbf{r})$, defined as

$$\rho(t, \mathbf{r}) = q \int_{\Omega} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v} \quad (2.4a)$$

$$\mathbf{J}(t, \mathbf{r}) = q \int_{\Omega} \mathbf{v}(t) f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}. \quad (2.4b)$$

It follows from the above equations that charge and current densities are related via the equation of continuity

$$-\partial_t \rho(t, \mathbf{r}) = \nabla \cdot \mathbf{J}(t, \mathbf{r}). \quad (2.5)$$

Further, assume that these equations satisfy the initial conditions arising from

$$\nabla \cdot \mathbf{D}(0, \mathbf{r}) = \rho(0, \mathbf{r}) \quad (2.6a)$$

and

$$\nabla \cdot \mathbf{B}(0, \mathbf{r}) = 0 \quad (2.6b)$$

To complete the description of the problem, we will assume that the boundary of the domain $\partial\Omega$ may be partitioned into several subdomains, Γ_i , such that $\Gamma := \cup_i \Gamma_i$. Each Γ_i has a boundary condition, either Dirichlet (Γ_D), Neumann (Γ_N), or impedance (Γ_I). The boundary conditions are defined as

$$\hat{n} \times \mathbf{E}(t, \mathbf{r}) = \Psi_D(t, \mathbf{r}) \text{ on } \Gamma_D \quad (2.7a)$$

$$\hat{n} \times \frac{\mathbf{B}(t, \mathbf{r})}{\mu_0} = \Psi_N(t, \mathbf{r}) \text{ on } \Gamma_N \quad (2.7b)$$

$$\hat{n} \times \frac{\mathbf{B}(t, \mathbf{r})}{\mu_0} - \gamma \hat{n} \times \hat{n} \times \mathbf{E}(t, \mathbf{r}) = \Psi_I(t, \mathbf{r}) \text{ on } \Gamma_I \quad (2.7c)$$

where $\hat{n}$ the vector normal to the surface $\partial\Omega$, γ is the surface admittance defined as $\sqrt{\epsilon_0/\mu_0}$, and $\Psi_D(\mathbf{r}, t)$, $\Psi_N(\mathbf{r}, t)$, and $\Psi_I(\mathbf{r}, t)$ represent some function. These equations describe a self consistent set that must be solved numerically. In what follows, we describe the numerics necessary to do so.

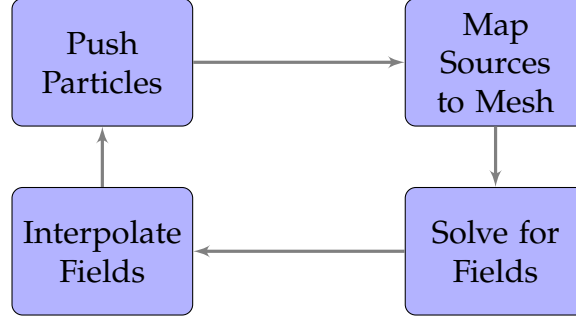


Figure 2.1: Flow of typical EM-PIC simulation.

2.3 Self consistent modeling framework

While we do not solve the Vlasov system directly, we follow the usual practice of representing the particle distribution function using a collection of basis sets and then evolving the trajectory of these in using Newton’s law in concert with Maxwell equations. The basis sets are defined on a cell or simplicial complex which discretizes a volume Ω bounded by $\partial\Omega$. The mesh consists of N_g nodes, N_e edges, N_f faces, and N_v volumes (in three dimensions).

This process of modeling the charged media can be described as the EM-PIC cycle as seen Fig. 2.1. It begins with mapping the charged particles on the grid, forming a discretized representation of $\rho(t, \mathbf{r})$ and $\mathbf{J}(t, \mathbf{r})$. These discretized currents and charges act as sources in discretized Maxwell solvers, and are used to evolve the fields for one time step. The “new” fields and flux densities are then used update the locations of the charges and thereby obtain currents (and charges). The cycle then repeats. What is apparent from the the above are the the nuances of what ensures self consistent modeling of Maxwell and Vlasov systems discrete grids; this is the focus of this Section.

2.3.1 Sampling the distribution function, and equation of continuity

To begin, we start with representing the particle distribution function using

$$f(t, \mathbf{r}, \mathbf{v}) = \sum_{p=1}^{N_p} S(\mathbf{r} - \mathbf{r}_p(t)) \delta(\mathbf{v} - \mathbf{v}_p(t)) \quad (2.8)$$

where shape functions, $S(\mathbf{r})$, represent the spatial support of particles. It follows from the definitions in (2.4) that $\rho(t, \mathbf{r})$ and $\mathbf{J}(t, \mathbf{r})$ can be represented as

$$\rho(t, \mathbf{r}) = q \sum_{p=1}^{N_p} S(\mathbf{r} - \mathbf{r}_p(t)) \quad (2.9a)$$

$$\mathbf{J}(t, \mathbf{r}) = q \sum_{p=1}^{N_p} \mathbf{v}_p(t) S(\mathbf{r} - \mathbf{r}_p(t)). \quad (2.9b)$$

Given the discrete representation of the distribution function, it can be shown that the equation of continuity is still holds in this discrete/particle setting. While this has been proven by Eastwood [51], the approach we take is straightforward, and exploits the sifting property of the delta function. Specifically, we use the definition $\mathbf{r}_p(t) = \mathbf{r}_{0p}(t) + \int_0^t d\tau \mathbf{v}_p(\tau)$ and the identity

$$\delta(\mathbf{r} - \mathbf{r}_p(t)) = \delta(\mathbf{r} - \mathbf{r}_{0p}(t)) \star_s \left(\mathbf{r} - \int_0^t d\tau \mathbf{v}_p(\tau) \right) \quad (2.10)$$

Using this identity, it can be shown that (see Appendix)

$$\partial_t \delta(\mathbf{r} - \mathbf{r}_p(t)) = -\nabla \cdot [\mathbf{v}_p(t) \delta(\mathbf{r} - \mathbf{r}_p(t))] \quad (2.11)$$

The equation of continuity follows via

$$\begin{aligned} -\partial_t \rho(t, \mathbf{r}) &= -q \sum_{p=1}^{N_p} \partial_t S(\mathbf{r} - \mathbf{r}_p(t)) = -q \sum_{p=1}^{N_p} S(\mathbf{r}) \star \partial_t \delta(\mathbf{r} - \mathbf{r}_p(t)) \\ &= \nabla \cdot \left[q \sum_{p=1}^{N_p} \mathbf{v}_p(t) S(\mathbf{r} - \mathbf{r}_p(t)) \right] = \nabla \cdot \mathbf{J}(t, \mathbf{r}). \end{aligned} \quad (2.12)$$

Of course, this is not the only identity that can be derived. As shown in the Appendix, another relationship pertinent to this paper that follows from the spectral representation of (2.10) is

$$\rho(t, \mathbf{r}) = \rho(0, \mathbf{r}) - q \nabla \cdot \sum_{p=1}^{N_p} \int_{\mathbf{r}_p(0)}^{\mathbf{r}_p(t)} d\tilde{\mathbf{r}} S(\mathbf{r} - \tilde{\mathbf{r}}(t)) \quad (2.13)$$

As shown in the Appendix, this can be transformed into a line integral along the path taken by each particle. Our analysis, thus far, has dwelt on the representation of the distribution

function and its moments, viz., the charge and current. As is evident from (2.12) that the equation of continuity is satisfied when the distribution function is represented by arbitrarily shaped particles. Next, we address mapping/measuring these charges and currents on grid (and how they interact with Maxwell's equations).

2.3.2 Self-consistent solution of Maxwell's Equations with active sources

For self consistency, one needs to solve Maxwell's equations with sources defined by (2.9). In this pursuit, we discretize Maxwell's equations in space with a collection of cells on which we define basis functions to represent fields and sources. Additionally, a temporal discretization is chosen such that a consistent solution for Newton's laws is obtained to update the position *and* trajectory of the particle. It is well known that *de-Rham* diagrams [160, 47] provide appropriate map between fields, fluxes and sources in Maxwell's equations. In addition, one needs additional framework to ensure that charges and currents are correctly measured and integrated in time. In what follows, we discuss each in turn.

2.3.2.1 *de-Rham* complex

To begin, *de-Rham* diagrams establish relations between field, fluxes and sources. These diagrams replicate Maxwell's equations in the discrete world; there exists extensive literature on their use in developing finite elements [46, 8]. In a nutshell, these permit the definition of Whitney spaces that can be used to represent primary quantities (ϕ , $\mathbf{E}$, $\mathbf{B}$) or their duals (ρ , $\mathbf{H}$, $\mathbf{D}$). It should be noted that the choice of fields on the primal or dual grids are not rigid; in other words, (ρ , $\mathbf{H}$, $\mathbf{D}/\mathbf{J}$) can be defined on the primal grid and (ϕ , $\mathbf{E}$, $\mathbf{B}$) on the dual grid. These relationships are shown in Figs. 2.2 and 2.3. Using Whitney spaces to solve Maxwell's equations has its antecedents in Bossavit's seminal work [20] and those of several others [140, 93, 24, 114, 12]; our presentation is along these lines. As has been shown in these papers, these basis sets and their function spaces are defined as follows:

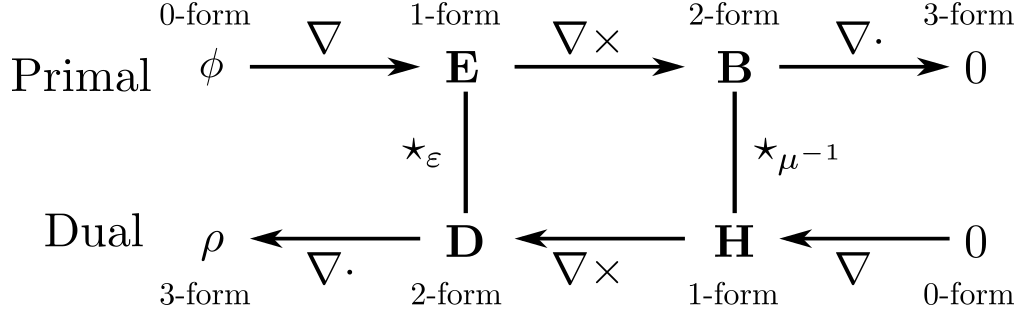


Figure 2.2: Diagram of electromagnetic quantities as differential forms.

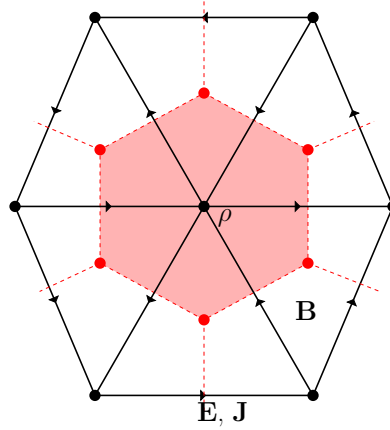


Figure 2.3: Two dimensional diagram of where field and source quantities are defined on a simplicial mesh.

the 0-form defined on nodes, the 1-form defined on edges, the 2-form defined on faces, and the 3-form defined on volumes. In this work, we choose to use the Whitney basis sets that

$$0\text{-form} := W^{(0)} \in H^1 \quad (2.14a)$$

$$1\text{-form} := \mathbf{W}^{(1)}(\mathbf{r}) \in H(\text{curl}) \quad (2.14b)$$

$$2\text{-form} := \mathbf{W}^{(2)}(\mathbf{r}) \in H(\text{div}) \quad (2.14c)$$

$$3\text{-form} := W^{(3)}(\mathbf{r}) \in L^2 \quad (2.14d)$$

The Hodge operator relates the corresponding field and flux quantities using the correct constitutive parameters, as well as provides a mapping between the primal and dual grids [158, 157].

2.3.2.2 Discrete and self consistent Gauss' and Ampere's Laws

In typical solutions to Maxwell equations, there is an implicit assumption that the solution to the two curl equation enforces Gauss' laws together with the equation of continuity. While this is true in the continuous domain, one needs to handle things with care in the discrete domain. Specifically, the basis functions used to represent or measure the fields, fluxes, currents, and charges need to be consistent with each other. Let $\mathcal{L}_{\nabla \circ}$ denote a discrete divergence operator and $\mathcal{L}_{\nabla \times \circ}$ denote a discrete curl operator, whose definitions are dependent on the basis functions. With no loss in generality, let's denote the basis functions, $\mathbf{N}_i(\mathbf{r})$ and $\xi_i(\mathbf{r})$, used to represent and measure the fields and fluxes, and charges, respectively. They belong to the appropriate space of functions depending on which quantity is being measured as determined by (??) and have local support over a simplex or cell. They also have relationships determined by the de-Rham complex shown in figure 2.2. With no loss of generality, let us define the vectors of quantities that are measured by our candidate basis functions. For instance, one can define

$$d_i(t) = \langle \mathbf{N}_i(\mathbf{r}), \epsilon \mathbf{E}(t, \mathbf{r}) \rangle \quad (2.15a)$$

$$(\mathcal{L}_{\nabla \times} \circ \mathbf{h}(t))_i = \langle \mathbf{N}_i(\mathbf{r}), \nabla \times \mu^{-1} \mathbf{B}(t, \mathbf{r}) \rangle \quad (2.15b)$$

$$(\mathcal{L}_{\nabla \circ} \mathbf{d}(t))_i = \langle \xi_i(\mathbf{r}), \nabla \cdot \epsilon \mathbf{E}(t, \mathbf{r}) \rangle \quad (2.15c)$$

$$j_i(t) = \langle \mathbf{N}_i(\mathbf{r}), \mathbf{J}(t, \mathbf{r}) \rangle \quad (2.15d)$$

Next, let us define $\mathbf{d}(t) = [d_1(t), d_2(t), \dots, d_{N_\gamma}(t)]$, $\mathbf{h}(t) = [h_1(t), h_2(t), \dots, h_{N_\alpha}(t)]$, and $\mathbf{j}(t) = [j_1(t), j_2(t), \dots, j_{N_\beta}(t)]$, which can be used to approximate the continuous functions, such as $\mathbf{D}(t, \mathbf{r}) = \sum_{i=1}^{N_\gamma} d_i(t) \mathbf{N}_i(\mathbf{r})$, where N_γ is the number of degrees of freedom; as we will see, depending on the formulation it can either be the number of edges or faces. This definition is the same for N_α and N_β . The degree of freedom vectors may require a Hodge operator to represent the function in the correct space. For solutions to be consistent, the systems of equations should be such that the divergence of Ampere's law yields the

time derivative of Gauss' law, which together with initial conditions will yield Gauss' law. While this is simply stated, there are a number of subtle nuances. In the discrete world, it follows that the same should be valid. Specifically, the spatial basis sets and the time integrator used has to be such that these relationships are satisfied. Note, these conditions must be satisfied exactly because only the curl equations, Faraday's law and Ampere's law, are explicitly solved. Gauss' law must be satisfied indirectly through the correct choice of spatial basis sets and time integration.

As our goal is to ensure the *both* Gauss' laws and the equation of continuity are satisfied, it follows that there has to be a relationship between $\nabla \xi_i(\mathbf{r})$ and $\mathbf{N}_i(\mathbf{r})$. We begin by considering the divergence of discrete Ampere's law; specifically,

$$\partial_t \mathcal{L}_{\nabla} \circ \mathbf{d}(t) = \mathcal{L}_{\nabla} \circ \mathcal{L}_{\nabla \times} \circ \mathbf{h}(t) - \mathcal{L}_{\nabla} \circ \mathbf{j}(t) \quad (2.16)$$

From the above, one can deduce the following:

Condition 1: Consistent spatial basis sets The basis sets should be such that the discrete divergence of the discrete rotation of the magnetic field is zero. In effect, the discrete differential operators should maintain the same properties as their continuous counterpart. To serve as the link between Ampere's law and the continuity equation,

$$\mathcal{L}_{\nabla} \circ \mathcal{L}_{\nabla \times} \circ \mathbf{h}(t) = 0. \quad (2.17)$$

Though the discrete differential operators can be defined using properties of the mesh, they must be consistent with the discretized Faraday's and Gauss' law.

Condition 2: Discrete divergence Let $\xi(\mathbf{r})$ denote functions used to measure the charge on the mesh. Then $\nabla \xi_i(\mathbf{r})$ should span the irrotational component of both $\mathbf{D}(t, \mathbf{r})$ and $\mathbf{J}(t, \mathbf{r})$. In effect, $\text{span} \{ \nabla \xi_i(\mathbf{r}) \} = \mathbf{D}(t, \mathbf{r})$ or $\mathbf{J}(t, \mathbf{r})$ for $\forall t$. In other words, this representation is complete. The need for this condition arises from measuring both

Gauss' law and the equation of continuity. Consider measuring Gauss' law via

$$\begin{aligned}
(\mathcal{L}_{\nabla} \circ \mathbf{d}(t))_i &= \int_{\Omega} d\mathbf{r} \xi_i(\mathbf{r}) \rho(\mathbf{r}) = \int_{\Omega} d\mathbf{r} \xi_i(\mathbf{r}) \nabla \cdot \mathbf{D}(t, \mathbf{r}) \\
\int_{\Omega} d\mathbf{r} \xi_i(\mathbf{r}) \rho(\mathbf{r}) &= - \int_{\Omega} d\mathbf{r} \nabla \xi_i(\mathbf{r}) \cdot \mathbf{D}(t, \mathbf{r}) + \int_{\partial\Omega} d\mathbf{r} \xi_i(\mathbf{r}) \hat{n} \cdot \mathbf{D}(t, \mathbf{r}).
\end{aligned} \tag{2.18}$$

The preceding equation mathematically exemplifies this condition. An almost identical equation can be derived for the equation of continuity. It can be shown boundary terms in vanish interior to the domain and provided the correct boundary condition is imposed on $\hat{n} \cdot \mathbf{D}(t, \mathbf{r})$ on $\partial\Omega$, Gauss' law is implicitly satisfied together with condition 3.

Condition 3: Discrete Time Integration Finally, discrete time stepping used to update the electric flux density in Ampere's equation and the path integral to used to evaluate the total current at any instant of time should be consistent with each other. This will ensure that the solution to Ampere's law agrees with Gauss' law. To gain more insight, we start by noting that when evolving Maxwell's equations over-time, we are in effect integrating the current; however, the time integral of the current is obtained via a path integral in (2.13). It follows, that if one were to take a discrete divergence of Ampere's laws, Condition 1 would yield

$$\partial_t \mathcal{L}_{\nabla} \circ \mathbf{d}(t) = - \mathcal{L}_{\nabla} \circ \mathbf{j}(t) \tag{2.19}$$

Provided Condition 2 is satisfied, it follows that choosing a consistent rule for integrating the charge along the particle path and integrating Ampere's law will ensure conservation of charge.

2.4 Satisfaction of Conditions with Various EM-PIC Methods

Next, we examine three different formulations of EM-PIC; FDTD-PIC, EB-MFEM-PIC, and DH-MFEM-PIC in light of the conditions discussed thus far. While FDTD-PIC is well known, EM-MFEM-PIC and DH-MFEM-PIC place dominant importance on Faraday's and

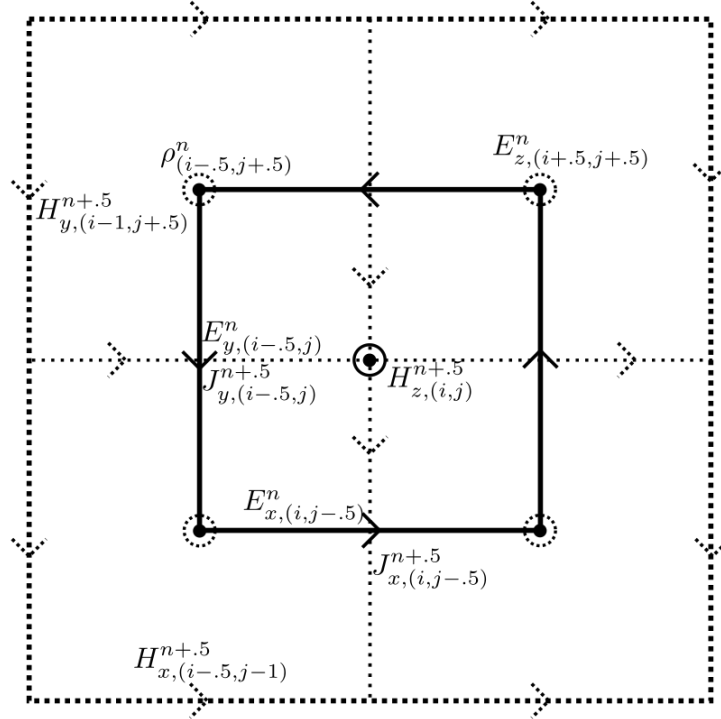


Figure 2.4: FDTD 2D grid. Solid cell is the primal grid. Dotted cells are the dual grid.

Ampere's laws, respectively. As a result, the dominant variables are represented on the primal grid, the others reside on dual grid. In what follows, we seek to show how each formulation satisfies the three conditions.

2.4.1 FDTD-PIC

FDTD-PIC is the combination of the FDTD method [189] with PIC. It is discretized using staggered, structured grids in time and space, as seen in Figure 2.4 for two dimensions. For our discussion, the primal grid contains degrees of freedom for the electric field and magnetic flux density. Likewise, the dual grid has the degrees of freedom defined for the magnetic field and the electric flux density [160]. Particles are mapped to the grid using the 3-forms that measure the charge density. In what follows, we will show that the particle weighting scheme defined by Langdon [91] maps trivially onto the three conditions defined earlier.

2.4.1.1 Satisfaction of Condition 1

The discrete differential operators $\mathcal{L}_{\nabla \times \circ}$ and $\mathcal{L}_{\nabla \cdot \circ}$ on the dual grid are defined as

$$\mathcal{L}_{\nabla \times \circ} = \begin{cases} \pm 1 & \text{if } \hat{n}_j \times \hat{l}_i \text{ points into (out of) the face} \\ 0 & \text{otherwise} \end{cases} \quad (2.20)$$

and

$$\mathcal{L}_{\nabla \cdot \circ} = \begin{cases} \pm 1 & \text{if } \hat{n}_j \text{ points out of (into) cell } c_i \\ 0 & \text{otherwise} \end{cases} \quad (2.21)$$

The operator $\mathcal{L}_{\nabla \times \circ} \in \mathbb{R}^{N_f \times N_e}$, where N_f is the number of faces and N_e is the number of edges. The operator $\mathcal{L}_{\nabla \cdot \circ} \in \mathbb{R}^{N_c \times N_f}$ where N_c is the number of volumes.

Consider an example mesh in Figure 2.5. Assume the edge on the corners of the cell all point out of the page and the normal to the edges point out of the cell. The corresponding curl matrix definition would be

$$[\mathcal{L}_{\nabla \times \circ}] = \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}, \quad (2.22)$$

The divergence matrix would be

$$[\mathcal{L}_{\nabla \cdot \circ}] = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix} \quad (2.23)$$

It is evident that in $\mathcal{L}_{\nabla \cdot \circ} \mathcal{L}_{\nabla \times \circ}$, each entry in the resulting vector is zero, satisfying (2.17).

2.4.1.2 Satisfaction of Condition 2

The basis function $\xi(\mathbf{r})$ in (2.18) is a 3-form, a constant in this formulation. Using the properties of 3-forms, (2.18) reduces to

$$\int_{\Omega} d\mathbf{r} \xi(\mathbf{r}) \nabla \cdot \mathbf{X}(\mathbf{r}) = \int_{\partial\Omega} d\mathbf{r} \hat{n} \cdot \mathbf{X}(\mathbf{r}) \xi(\mathbf{r}). \quad (2.24)$$

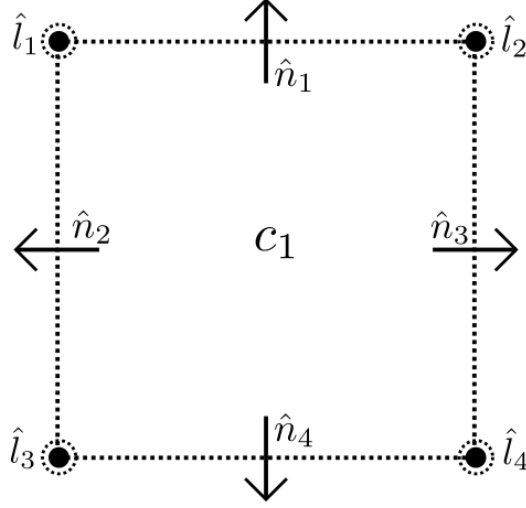


Figure 2.5: Discrete curl and divergence on the dual grid. The curl is defined using the edges $\hat{l}_i$ that come out of the page. The divergence is defined using the face normals $\hat{n}_i$.

Consider the matrix form of $\mathcal{L}_{div} \circ$ based on Figure 2.5

$$\mathcal{L}_{\nabla \cdot \circ} = \begin{bmatrix} 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 & 1 & 0 & 1 \end{bmatrix}. \quad (2.25)$$

A volume integral would be a summation over the cells of a mesh,

$$\sum_{i=1}^{N_v} [\mathcal{L}_{\nabla \cdot \circ}]_{ij} = \begin{bmatrix} 1 & 1 & 1 & 0 & 1 & 1 & 1 \end{bmatrix} \quad (2.26)$$

This would effect the surface integral in (2.24). Therefore, the discrete continuity equation is satisfied exactly and consistency condition is fully satisfied.

2.4.1.3 Satisfaction of Condition 3

Consider (2.24) in conjunction with (2.19). Using a leapfrog time marching scheme, the discrete continuity equation would be

$$[\mathcal{L}_{\nabla \cdot}] \frac{\mathbf{d}^{n+1} - \mathbf{d}^n}{\Delta_t} = -\frac{q}{\Delta_t} [\mathcal{L}_{\nabla \cdot}] \int_{\partial\Omega} d\mathbf{r} \int_{\mathbf{r}^n}^{\mathbf{r}^{n+1}} d\tilde{\mathbf{r}} \hat{\mathbf{n}} \cdot \mathbf{p}(\tilde{\mathbf{r}}), \quad (2.27)$$

where Δ_t is the time step size, $\mathbf{p}(\tilde{\mathbf{r}})$ is the path of the particle. The integral computes the amount of charge that passes through a face. The divergence operator collects the

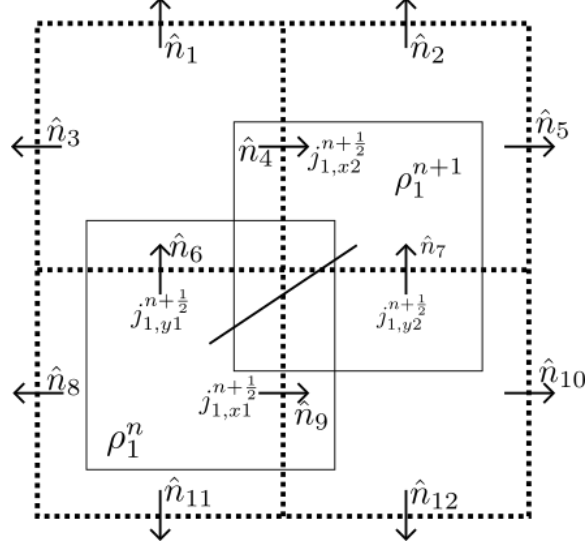


Figure 2.6: FDTD 2D particle current mapping with particles of finite size.

contributions of each face, giving the net change of charge in each cell, as demonstrated in figure 2.6. This is equivalent to the current mapping in [171] for particles with finite shape. If the particle shape is infinitesimally small, it is equivalent to nearest-grid-point particle weighting.

2.4.2 EB-MFEM-PIC Formulation

Next, we analyze EB-MFEM-PIC as defined in [20]. This finite element method can be seen as a generalization of FDTD. Like FDTD, it discretizes Maxwell's equations using a primal-dual grid system, with the field and flux quantities defined in the same manner. However, the grid itself can be unstructured, using non-cubic cells. The formulation for EB-MFEM can be found in appendix 2.8.3.2. We have chosen to demonstrate the validity of the arguments in Section 2.3 using brick elements as it is akin to FDTD-PIC. We defer the discussion on tetrahedral elements to the next section.

2.4.2.1 Satisfaction of Condition 1

The discrete differential operators $\mathcal{L}_{\nabla \times \circ}$ and $\mathcal{L}_{\nabla \cdot \circ}$ are defined on the primal grid as

$$\mathcal{L}_{\nabla \times \circ} = \begin{cases} \pm 1 & \text{if } \hat{n}_j \times \hat{l}_i \text{ points into (out of) the face} \\ 0 & \text{otherwise} \end{cases} \quad (2.28)$$

and

$$\mathcal{L}_{\nabla \cdot \circ} = \begin{cases} \pm 1 & \text{if edge } j \text{ points into (out of) node } i \\ 0 & \text{otherwise} \end{cases} \quad (2.29)$$

The operator $\mathcal{L}_{\nabla \times \circ} \in \mathbb{R}^{N_e \times N_f}$. The operator $\mathcal{L}_{\nabla \cdot \circ} \in \mathbb{R}^{N_n \times N_e}$ where N_n is the number of nodes. Consider the example mesh in Figure 2.7. The corresponding curl matrix definition would be

$$\mathcal{L}_{\nabla \times \circ} = \begin{bmatrix} -1 & 1 & -1 & 1 \end{bmatrix}^T. \quad (2.30)$$

The divergence matrix would be

$$\mathcal{L}_{\nabla \cdot \circ} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{bmatrix} \quad (2.31)$$

It is apparent that each entry in the resulting $\mathcal{L}_{\nabla \cdot \circ} \mathcal{L}_{\nabla \times \circ}$ is zero, satisfying (2.17).

2.4.2.2 Satisfaction of Condition 2

The basis function for the current density spans the gradient of the basis function for the charge density. The divergence operator $\mathcal{L}_{\nabla \cdot \circ}$ sums the edges connected to a node to satisfy (2.18). For PEC boundary conditions, the current density normal to the face is zero, eliminating the surface integral term. This can be seen by summing the rows of (2.31). For non-PEC boundaries, the domain is padded with ghost cells where the boundary nodes are not included. The non-terminating edges then make up the surface integral term when $\mathcal{L}_{\nabla \cdot \circ}$ is applied. Therefore, (2.18) is satisfied.

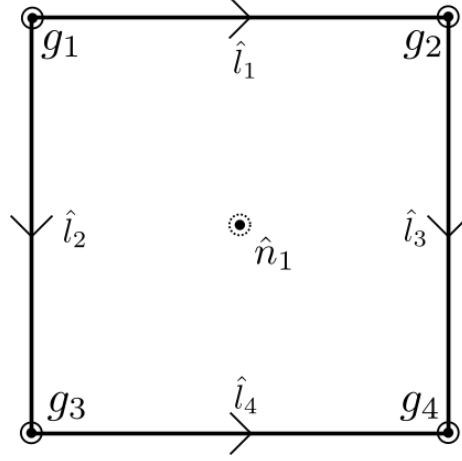


Figure 2.7: FEM 2D curl and divergence mesh. The curl is defined using the edges $\hat{l}_i$ around face center $\hat{n}_i$. The divergence is defined with edges that point into node g_i .

2.4.2.3 Satisfaction of Condition 3

For each cell a particle visits, the corresponding current density is projected onto the edges of that cell. Using (2.18), the discretized continuity equation that satisfies (2.19) is

$$[\mathcal{L}_{\nabla \cdot}] \frac{\mathbf{d}^{n+1} - \mathbf{d}^n}{\Delta_t} = -\frac{q}{\delta_t} [\mathcal{L}_{\nabla \cdot}] \int_{\Omega} d\mathbf{r} \int_{\mathbf{r}^n}^{\mathbf{r}^{n+1}} d\tilde{\mathbf{r}} \nabla W^0 \cdot \mathbf{p}(\tilde{\mathbf{r}}). \quad (2.32)$$

This is equivalent to particle-in-cell area weighting in FDTD and the method used in [51, 130]. Due to the relationship between the 0-form on the primal grid and the 3-form on the dual grid, this is also equivalent to the approach defined in [171] for finite particle shapes.

2.4.3 DH-MFEM-PIC Formulation

The EB-MFEM-PIC formulation defined in 2.4.2 can be reformulated to such that the primal grid has the degrees of freedom associated with the magnetic field and electric flux density. The dual grid contains the degrees of freedom for the electric field and magnetic flux density, still defined using the edges and faces, respectively. The sources are represented on the primal grid using 3-forms for the charge density and 2-forms for the current density. The arguments for this formulation satisfying the three conditions are

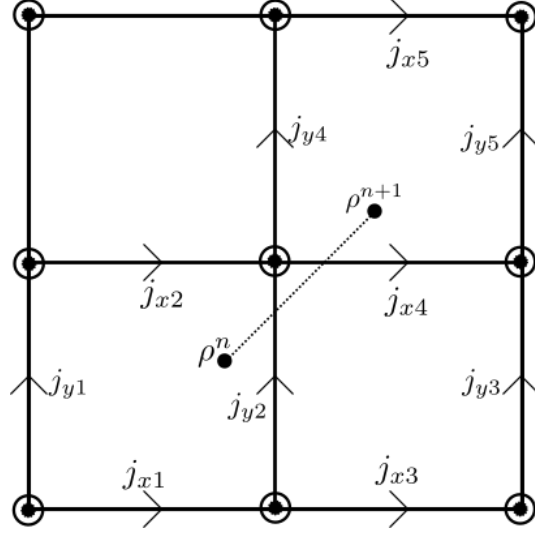


Figure 2.8: FEM 2D particle current mapping with point particles. The particle current is mapped to each edge that encloses a cell along the particle path.

similar to that presented in section 2.4.1. Note, the principal ramification of this approach is that it is a natural framework for modeling sources as both the currents and electric flux density are modeled using the same function space, *and* the fields, currents and charges lie in the primal grid. This is unlike EM-MFEM-PIC formulation where one needs transformations between primal and dual spaces. The ramification of these mappings become more consequential in higher order schemes—a topic that will be visited in a later paper.

2.4.3.1 Satisfaction of Condition 1

The discrete differential operators $\mathcal{L}_{\nabla \times \circ}$ and $\mathcal{L}_{\nabla \cdot \circ}$ are defined on the primal grid, but have the same definitions as (2.20) and (2.21). Consider the example mesh in Figure 2.9. Assume the edge on the corners of the cell all point out of the page and the normal to the edges point out of the cell. The corresponding curl matrix definition for lowest order

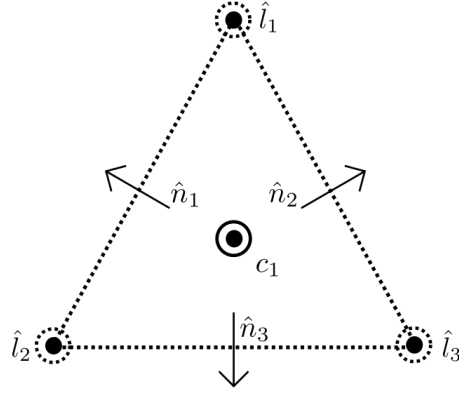


Figure 2.9: Discrete curl mesh on the dual grid. The curl is defined with the outward pointing edge $\hat{l}_i$.

would be

$$[\mathcal{L}_{\nabla \times \circ}] = \begin{bmatrix} -1 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \end{bmatrix}, \quad (2.33)$$

The lowest order divergence matrix would be

$$[\mathcal{L}_{\nabla \cdot \circ}] = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \quad (2.34)$$

Analyzing $\mathcal{L}_{\nabla \cdot \circ} \circ \mathcal{L}_{\nabla \times \circ}$, each entry in the resulting vector is zero, satisfying (2.17).

2.4.3.2 Satisfaction of Condition 2

For lowest order, the continuity equation reduces to (2.24).

Consider the matrix form of $\mathcal{L}_{\nabla \cdot \circ}$ based on figure 2.10

$$\mathcal{L}_{\nabla \cdot \circ} = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & -1 & 1 & 0 \end{bmatrix}. \quad (2.35)$$

A volume integral would be a summation over the cells of a mesh,

$$\sum_{i=1}^{N_v} [\mathcal{L}_{\nabla \cdot \circ}]_{ij} = \begin{bmatrix} 1 & 1 & 0 & 1 & 1 \end{bmatrix} \quad (2.36)$$

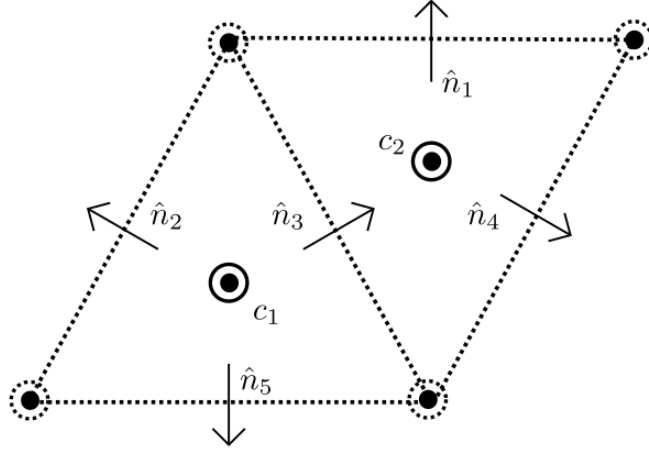


Figure 2.10: FEM divergence mesh. The divergence is defined using face normals $\hat{n}_i$ that point out of cell c_i .

This would effect the surface integral in (2.24). Therefore, the discrete continuity equation is satisfied exactly and consistency condition is fully satisfied.

2.4.3.3 Satisfaction of Condition 3

Again, the satisfaction of condition three relies on the correct definition of current density on the faces of each cell. For consistency of the change of charge density in cells, the amount of charge that passes through the face must be measured exactly. This is equivalent to what is effectively done in [155, 121] through different techniques. Consider the mapping of current defined by the particle in Figure 2.11. Here, though the particle moves at an angle with respect to the face, the current density as seen by the mesh moves in the direction of the face normal. The solver in effect sees a charge density move from cell c_4 to c_3 and the total charge density in c_3 moves to c_1 by time step $n + 1$.

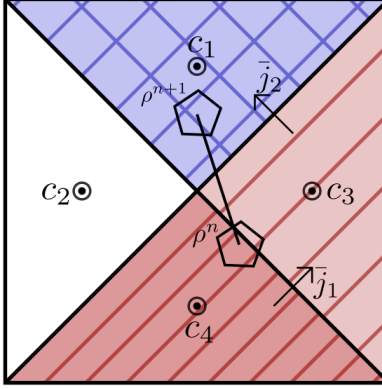


Figure 2.11: FEM particle mapping with finite shape particles. The particle is mapped to cell c_4 and c_3 at first and ends in cell c_1 with current mapped at on the marked faces. The particle shape does not affect the conservation properties of this method.

2.5 Consequences of Inconsistency

In the previous sections, the three rule framework was defined and applied to different formulations of EM-PIC. The references to previous works show how these rules encompasses well known EM-PIC formulations. Next, we will examine ramifications of violating these three rules. By examining potential pitfalls and how it manifests in results, one can more easily diagnose errors in new EM-PIC schemes.

2.5.1 Violation of Condition 1

First, consider violations of the first condition. Failing to satisfy (2.17) can arise from choosing the wrong basis sets to discretize (2.2). One way to do so is to choose basis sets that do not obey the de-Rahm complex. For example, if one solves both Ampere's law and Faraday's law on the same grid, staggered in time. Like in FDTD, we consider representing the electric field and magnetic field; however, this time it is on the same grid. Assume the fields are represented by 1-forms and test (2.2a) and (2.2b) with the same basis functions.

The discretized system is

$$\mathbf{h}^{n+\frac{1}{2}} = \mathbf{h}^{n+\frac{1}{2}} - \Delta_t [\mathcal{L}'_{\nabla \mathbf{x}} \circ] \mathbf{e}^n \quad (2.37a)$$

$$\mathbf{e}^{n+1} = \mathbf{e}^{n+1} + \Delta_t ([\mathcal{L}'_{\nabla \mathbf{x}} \circ] \mathbf{h}^{n+\frac{1}{2}} - \mathbf{j}^{n+\frac{1}{2}}), \quad (2.37b)$$

where $\mathcal{L}'_{\nabla \mathbf{x}} \circ$ is a modified curl operator, as the previously defined operator has the wrong dimensions. If this scheme is done with a structured mesh in FDTD, one would have a higher error as the curl would be represented using forward or backward difference rather than a central difference. Instead of the recurrence scheme found in (2.51b), one would have

$$\begin{aligned} E_{x,(i+\frac{1}{2},j,k)}^{n+1} = & E_{x,(i+\frac{1}{2},j,k)}^n + \frac{\Delta_t}{\varepsilon \Delta_y} (H_{z,(i+\frac{1}{2},j+1,k)}^{n+\frac{1}{2}} - H_{z,(i+\frac{1}{2},j,k)}^{n+\frac{1}{2}}) \\ & - \frac{\Delta_t}{\varepsilon \Delta_z} (H_{y,(i+\frac{1}{2},j,k+1)}^{n+\frac{1}{2}} - H_{y,(i+\frac{1}{2},j,k)}^{n+\frac{1}{2}}) \\ & - \frac{\Delta_t}{\varepsilon} J_{x,(i+\frac{1}{2},j,k)}^{n+1/2} \end{aligned} \quad (2.38)$$

if a forward difference was used.

The effects of this are more clear from an FEM perspective. Consider trying to find modes of a perfect electric conductor rectangular cavity using the generalized eigenvalue problem formed by the time harmonic form of (2.39)

$$\begin{bmatrix} 0 & [\mathcal{L}_{\nabla \mathbf{x}}^* \circ] \\ -[\mathcal{L}_{\nabla \mathbf{x}}^* \circ]^T [\star_{\mu^{-1}}] & 0 \end{bmatrix} \begin{bmatrix} \mathbf{b} \\ \mathbf{e} \end{bmatrix} = \Lambda \begin{bmatrix} [\mathbf{I}] & 0 \\ 0 & [\star_{\varepsilon}] \end{bmatrix} \begin{bmatrix} \mathbf{b} \\ \mathbf{e} \end{bmatrix} \quad (2.39)$$

where the eigenvalues in $\Lambda = j\omega$. The dimensions of the cavity are 0.6 m×0.4 m×1 m. In a consistent scheme, $[\mathcal{L}_{\nabla \mathbf{x}}^* \circ] = [\mathcal{L}_{\nabla \mathbf{x}} \circ]$ and $[\star_{\mu^{-1}}]$ is as defined in (??). However, in the inconsistent scheme we have defined,

$$[\mathcal{L}_{\nabla \mathbf{x}}^* \circ]_{i,j} = \int d\Omega \mathbf{W}_i^{(1)} \cdot \nabla \times \mathbf{W}_j^{(1)} \quad (2.40)$$

and $[\star_{\mu^{-1}}] = [\star_{\varepsilon}]$. When the inconsistent scheme is used, spurious modes are found that do not correspond to the true modes of the cavity as seen in table 2.1. Using this inconsistent scheme could permit incorrect solutions into the field solver, invalidating results.

f_{true}	$f_{\text{consistent}}$	$f_{\text{inconsistent}}$
291.346	290.829	0.280
390.242	389.157	1.036
403.608	402.697	1.841
450.382	449.654	2.451

Table 2.1: First four rectangular cavity modes for consistent and inconsistent FEM solver in MHz

2.5.2 Violation of Condition 2

Next, we consider the repercussions of violating Condition 2. Consider the linear mapping scheme typically found in early PIC literature where the weighting function is defined as

$$W(\mathbf{r} - \mathbf{r}_p(t)) = \prod_{n \in \{x, y, z\}} 1 - \frac{|r_{n,g} - r_{n,p}|}{\Delta_n}. \quad (2.41)$$

When the particle is mapped to the nodes as the charge density, $r_{n,g}$ is the x, y, z -coordinate of the node. When mapped to the edges as the current density, $r_{n,g}$ is the x, y, z -coordinate of the center of the edge. It is well known that this mapping does not satisfy the continuity equation. For example, consider the particle motion in Figure 2.8 where the particle moves from $(.3, .4)$ to $(.7, .6)$. Table 2.2 shows the error in the continuity equation using this mapping. The result is an inconsistency in the solved Ampere's law and measured Gauss' law due to spurious charge seen by the field solver as the next mapping is done. This mapping scheme does not appropriately satisfy (2.18), as the combination of basis functions for the current density at the node is not exactly equal to the gradient of the charge density basis function. Despite being in the same direction, the basis function defined by the linear mapping for the current density is different than the basis functions used to measure the fields. Therefore, the de-Rham complex is not truly satisfied and the spatial link between Gauss' law and Ampere's law is no longer preserved.

	$\partial_t \rho$	$\nabla \cdot \mathbf{J}$	$\partial_t \rho + \nabla \cdot \mathbf{J}$
node 1	-0.100	-0.050	-0.150
node 2	0.300	-0.850	-0.550
node 3	-0.300	0.850	0.550
node 4	0.100	0.050	0.150

Table 2.2: Continuity equation error for linear mapping

	Analytic	1 pt Quad	Error
Edge 1	1.248	1.248	-4.441e-16
Edge 2	0.505	0.505	0.000
Edge 3	0.248	0.248	0.000

Table 2.3: Error of Analytic Integration vs Quadrature Rule for Linear Path

	Q^{n+1}	Q^n	$\frac{Q^{n+1}-Q^n}{\Delta t}$	$\nabla \cdot \mathbf{J}$	$\frac{Q^{n+1}-Q^n}{\Delta t} + \nabla \cdot \mathbf{J}$
Node 1	0.284	0.459	-1.753	1.753	0.000
Node 2	0.550	0.450	1.000	-1.000	-4.440e-16
Node 3	0.166	0.091	0.753	-0.753	0.000

Table 2.4: Continuity Equation Error for Linear Path

2.5.3 Violation of Condition 3

Next, we examine how failing to correctly integrate the spatial integral in (2.19) results in a violation of Gauss' law and the continuity equation due to spurious charge on the grid. Consider the movement of a particle on a linear path that remains in a single cell using a 0-form basis set to measure the charge density. For a linear path, the path integral can be exactly computed either using an analytic scheme [115] or an one point integration rule, as seen in Table 2.3. This translates to machine precision error in the continuity equation in Table 2.4.

Similarly, consider the case when a particle crosses at least one face on its path. When the path is in multiple cells, an error occurs when the path integral is not calculated in each cell, as seen in Table 2.5. This is an inconsistency in (2.19) as though the time integral may be computed correctly, parts of the path integral are missing.

	$\frac{Q^{n+1}-Q^n}{\Delta t} + \nabla \cdot \mathbf{j}_{nc}^{n+1/2}$	$\frac{Q^{n+1}-Q^{n+\alpha}}{\Delta t_2} + \frac{Q^{n+\alpha}-Q^n}{\Delta t_1} + \nabla \cdot \mathbf{j}_{cc}^{n+1/2}$
Node 1	1.008	0.000
Node 2	0.394	-4.441e-16
Node 3	-0.008	2.220e-16
Node 4	-1.394	-4.441e-16

Table 2.5: Continuity Equation Error for Multiple Cells

	Analytic	1 pt Quad	1 pt error	2 pt Quad	2 pt error
Edge 1	1.253	1.250	-0.003	1.253	-6.661e-16
Edge 2	0.500	0.500	0.000	0.500	2.220e-16
Edge 3	0.253	0.250	0.003	0.253	0.000

Table 2.6: Error of Analytic Integration vs Quadrature Rule for Quadratic Path

2.5.4 Results for Consistent DH-MFEM-PIC

Finally, we examine results when all three conditions are satisfied. We have chosen to illustrate these using DH-MFEM-PIC as results for EB-MFEM-PIC are available [130, 115, ?]. First, we consider a particle beam in a 0.1 m PEC cylindrical cavity with a radius of 0.02 m. The particle beam has a voltage of 7.107 kV and current of 0.25A, simulated by inserting ten particles per time step. The starting velocity of the particles entering the tube is 5×10^4 km/s with a beam width of 0.008 m. In this test, when the three conditions are satisfied, the beam will spread as it progresses through the tube with a uniform distribution of particles. Using a DH-based EM-PIC formulation and point particles for particle shape, by following section 2.4.3, a self-consistent charge conserving EM-PIC scheme was created. Point particles are used because without introducing errors, it removes the need to compute the volume of a particle passing through a face, which can be extremely difficult in three dimensions, The error in the continuity equation and Gauss law is found in Figure 2.13, showing that satisfying conditions two and three is possible with a nearest grid point algorithm in FEM. The trend of the spreading beam is compared to that of an EB-MFEM-PIC and a FDTD based EM-PIC formulation in Figure 2.14.

Lastly, we examine the expansion of a plasma ball. A spherical plasma ball is given a Gaussian distribution of ions and electrons in a geometry with first order absorbing

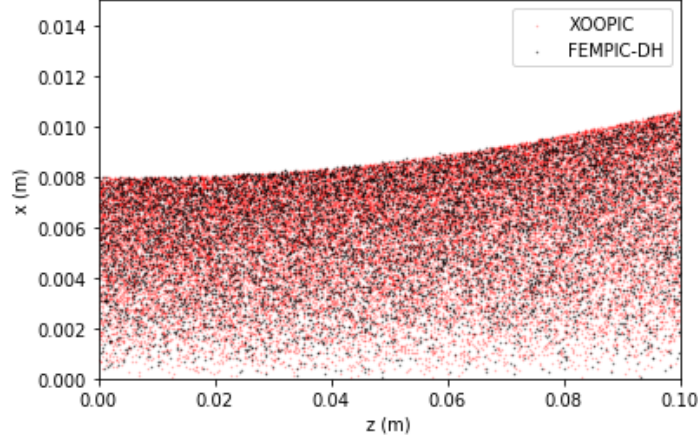


Figure 2.12: Particle beam comparison of **DH-MFEM-PIC** and **FDTD-PIC**.

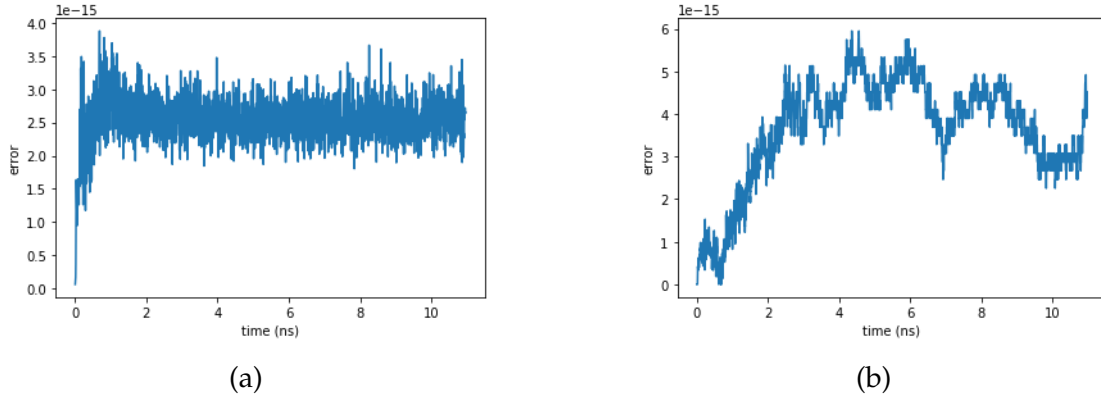


Figure 2.13: Error in the continuity equation (2.13a) and Gauss' law (2.13b) for the particle beam case.

boundary conditions. The experiment was simulated with the DH-FEM formulation with a point particle shape. A combination of Sr^+ ions at 1K and electrons at 100K are placed at a density of 5×10^8 particles per cubic meter such that the system is initially charge neutral. Further details on the experiment setup can be found in [?] and derivations of the analytic results in [86]. As is evident from Figure 2.15, we achieve excellent agreement with the analytic results. Again, because all the conditions are satisfied, the continuity equation and errors in Gauss' law are kept to machine precision.

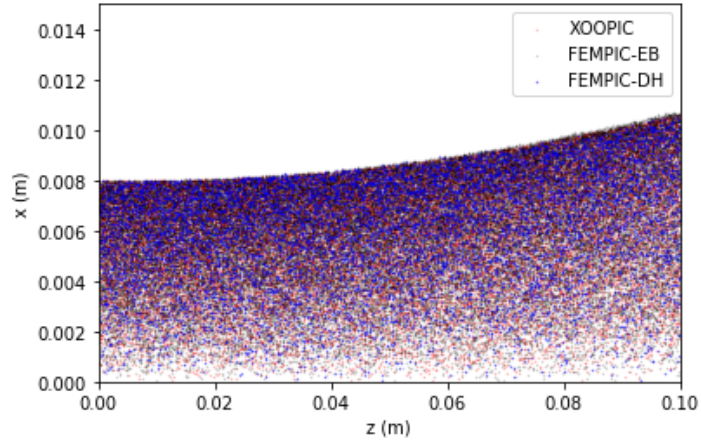


Figure 2.14: Particle Beam for FDTD, *EB*, and *DH* formulation

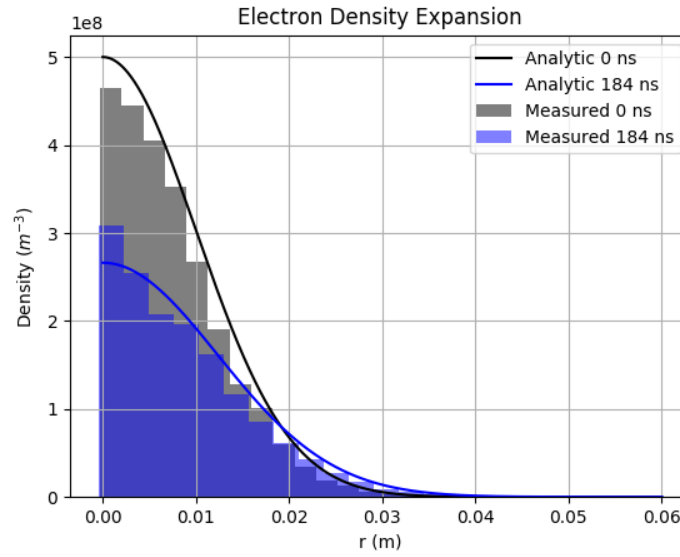


Figure 2.15: Electron density of expanding adiabatic plasma ball using **DH**-MFEM-PIC compared to analytic expected densities.

2.6 Summary and conclusions

In this work, we have presented a framework to define self-consistent EM-PIC schemes. By considering the space of functions used to represent fields, fluxes, and sources, one can ensure that all the relationships between Maxwell's equations are preserved in a consistent manner. This has been demonstrated for FDTD and two formulations of FEM, and shown how it generalizes and relates to well known previous work. The framework is easily related to other field solvers not mentioned directly provided one considers the relationship of the basis functions. Future work will apply this framework to higher order basis functions and particle paths.

2.7 Acknowledgements

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2.8 Appendix

2.8.1 Calculus on Distribution functions

The following must be understood in the sense of distributions. Specifically, we consider derivatives and integral of the delta function. These appear in (2.8) onwards where one represents the spatial variation of PDF using $S(\mathbf{r} - \mathbf{r}_p(t)) = S(\mathbf{r}) \star_s \delta(\mathbf{r} - \mathbf{r}_p(t))$. Calculus on delta function is critical for developing insight into implementing equations of continuity and Gauss' law on the grid. To do so, we start with a transform to $\mathbf{k}$ -space to prove (2.11) and (2.13).

2.8.1.1 Time derivatives

Using $\mathbf{r}_p(t) = \mathbf{r}_{0p} + \int_0^t d\tau \mathbf{v}_p(\tau)$, the time derivative of $\delta(\mathbf{r} - \mathbf{r}_p(t))$ can be written as

$$\begin{aligned}\partial_t \delta(\mathbf{r} - \mathbf{r}_p(t)) &= \partial_t \delta(\mathbf{r} - \mathbf{r}_{0p}) \star \delta\left(\mathbf{r} - \int_0^t d\tau \mathbf{v}_p(\tau)\right) \\ &= \delta(\mathbf{r} - \mathbf{r}_{0p}) \star \partial_t \delta\left(\mathbf{r} - \int_0^t d\tau \mathbf{v}_p(\tau)\right)\end{aligned}\quad (2.42)$$

Next, we exploit

$$\delta(\mathbf{r} - \mathbf{a}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{k} e^{j\mathbf{k} \cdot (\mathbf{r} - \mathbf{a})} \quad (2.43)$$

to yield

$$\begin{aligned}\partial_t \delta\left(\mathbf{r} - \int_0^t d\tau \mathbf{v}_p(\tau)\right) &= \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{k} \partial_t e^{j\mathbf{k} \cdot (\mathbf{r} - \int_0^t d\tau \mathbf{v}_p(\tau))} \\ &= -\nabla \cdot \mathbf{v}_p(t) \delta\left(\mathbf{r} - \int_0^t d\tau \mathbf{v}_p(\tau)\right).\end{aligned}\quad (2.44)$$

Therefore

$$\begin{aligned}\partial_t \delta(\mathbf{r} - \mathbf{r}_p(t)) &= -\delta(\mathbf{r} - \mathbf{r}_{0p}) \star \nabla \cdot \mathbf{v}_p(t) \delta\left(\mathbf{r} - \int_0^t d\tau \mathbf{v}_p(\tau)\right) \\ &= -\nabla \cdot [\mathbf{v}_p(t) \delta(\mathbf{r} - \mathbf{r}_p(t))]\end{aligned}\quad (2.45)$$

2.8.2 Time integrals

Next, starting from the time integral of (2.11) and using the definition of current density in equation (2.9b),

$$\int_0^t d\tau \nabla \cdot \mathbf{v}_p(\tau) S(\mathbf{r} - \mathbf{r}_p(\tau)) = S(\mathbf{r}) \star_s \int_0^t d\tau \nabla \cdot \mathbf{v}_p(\tau) \delta\left(\mathbf{r} - \int_0^\tau d\tau' \mathbf{v}_p(\tau')\right) \quad (2.46)$$

Again, using (2.43) and $\partial_t \tilde{\mathbf{r}}_p(t) = \mathbf{v}_p(t)$,

$$\begin{aligned}&\int_0^t d\tau \nabla \cdot \mathbf{v}_p(\tau) \delta\left(\mathbf{r} - \int_0^\tau d\tau' \mathbf{v}_p(\tau')\right) \\ &= \int_0^t \frac{d\tau}{(2\pi)^3} \nabla \cdot \int_{-\infty}^{\infty} d^3\mathbf{k} \mathbf{v}_p(\tau) e^{j\mathbf{k} \cdot (\mathbf{r} - \int_0^\tau d\tau' \mathbf{v}_p(\tau'))} \\ &= \nabla \cdot \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{k} e^{j\mathbf{k} \cdot \mathbf{r}} \int_0^t d\tau \mathbf{v}_p(\tau) e^{-j\mathbf{k} \cdot \int_0^\tau d\tau' \mathbf{v}_p(\tau')} \\ &= \nabla \cdot \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{k} e^{j\mathbf{k} \cdot \mathbf{r}} \int_{\mathbf{r}_p(0)}^{\mathbf{r}_p(t)} d\tilde{\mathbf{r}}_p e^{-j\mathbf{k} \cdot \tilde{\mathbf{r}}_p}\end{aligned}\quad (2.47)$$

Interchanging the order of the integrals in the above equation results in

$$\int_0^t d\tau \nabla \cdot \mathbf{v}_p(\tau) S(\mathbf{r} - \mathbf{r}_p(\tau)) = \nabla \cdot \int_{\mathbf{r}_p(0)}^{\mathbf{r}_p(t)} d\tilde{\mathbf{r}} S(\mathbf{r} - \tilde{\mathbf{r}}) \quad (2.48)$$

This equation can be used to define the charge density in terms of the particle's path; it can also be used to define the time integral of the current density.

2.8.3 Maxwell Solvers

The following sections are presented purely for completeness and to conform with material presented earlier. We present details of the three Maxwell solvers used here; FDTD, EB-MFEM, and DH-MFEM.

2.8.3.1 FDTD

Define the rooftop function $\Lambda_i(\mathbf{r})$

$$\Lambda_i(\mathbf{r}) = \begin{cases} 1 - \frac{|\hat{i} \cdot \mathbf{r}|}{\Delta_i} & 0 < |\hat{i} \cdot \mathbf{r}| \leq \Delta_i \\ 0 & \text{o.w.} \end{cases} \quad (2.49)$$

where $i = x, y, z$. The basis functions to discretize Maxwell's equations for FDTD are

$$\text{1-form} := \mathbf{u}_i \Lambda_{i+1}(\mathbf{r} - \mathbf{l}_m) \Lambda_{i+2}(\mathbf{r} - \mathbf{l}_m) \quad (2.50a)$$

$$\text{2-form} := \mathbf{u}_i \Lambda_i(\mathbf{r} - \mathbf{f}_m) \quad (2.50b)$$

with $\mathbf{u}_i = \hat{x}, \hat{y}, \hat{z}$, $\mathbf{l}_m$ is the midpoint of each edge, and $\mathbf{f}_m$ is the midpoint of each face. Testing Faraday's law with the normal to cell faces and Ampere's law is with the edge unit vectors yields

$$\begin{aligned} \langle \mathbf{u}_i \delta((\mathbf{r} - \mathbf{f}_m) \cdot \hat{i}), \partial_t \mu \mathbf{H}(t, \mathbf{r}) \rangle &= -\langle \mathbf{u}_i \delta((\mathbf{r} - \mathbf{f}_m) \cdot \hat{i}), \nabla \times \mathbf{E}(t, \mathbf{r}) \rangle \\ \partial_t \mathbf{H}_i(t, \mathbf{f}_m) &= -\mu_0^{-1} \mathbf{u}_i \cdot \nabla \times \mathbf{E}(t, \mathbf{f}_m) \\ &= \mu_0^{-1} \partial_{i+1} \mathbf{E}_{i+2}(t, \mathbf{f}_m) - \mu_0^{-1} \partial_{i+2} \mathbf{E}_{i+1}(t, \mathbf{f}_m) \end{aligned} \quad (2.51a)$$

$$\begin{aligned}
\langle \mathbf{u}_i \delta((\mathbf{r} - \mathbf{f}_m) \cdot \hat{i}), \partial_t \varepsilon \mathbf{E}(t, \mathbf{r}) \rangle &= -\langle \mathbf{u}_i \delta((\mathbf{r} - \mathbf{l}_m) \cdot \hat{i}), \nabla \times \mathbf{H}(t, \mathbf{r}) \rangle \\
&\quad - \langle \mathbf{u}_i \delta((\mathbf{r} - \mathbf{l}_m) \cdot \hat{i}), \mathbf{J}(t, \mathbf{r}) \rangle \\
\partial_t \mathbf{E}_i(\mathbf{l}_m) &= -\varepsilon_0^{-1} \mathbf{u}_i \cdot \nabla \times \mathbf{H}(t, \mathbf{l}_m) - \varepsilon_0^{-1} \mathbf{u}_i \cdot \mathbf{J}(t, \mathbf{l}_m) \\
&= \varepsilon_0^{-1} \partial_{i+1} \mathbf{H}_{i+2}(t, \mathbf{l}_m) - \varepsilon_0^{-1} \partial_{i+2} \mathbf{H}_{i+1}(t, \mathbf{l}_m) - \varepsilon_0^{-1} \mathbf{J}_i(t, \mathbf{l}_m).
\end{aligned} \tag{2.51b}$$

The addition on index i follows cycle $\{x, y, z\}$. This testing is equivalent to the usual presentation of the FDTD recurrence relation. For example, consider $i = x$ in (2.51a) would yield

$$\begin{aligned}
H_{x,(i,j+\frac{1}{2},k+\frac{1}{2})}^{n+\frac{1}{2}} &= H_{x,(i,j+\frac{1}{2},k+\frac{1}{2})}^{n-\frac{1}{2}} - \frac{\Delta t}{\mu \Delta_y} (E_{z,(i,j+1,k+\frac{1}{2})}^n - E_{z,(i,j,k+\frac{1}{2})}^n) \\
&\quad + \frac{\Delta t}{\mu \Delta_z} (E_{y,(i,j+\frac{1}{2},k+1)}^n - E_{y,(i,j+\frac{1}{2},k)}^n).
\end{aligned} \tag{2.52}$$

Likewise, $i = x$ in (2.51b) would yield

$$\begin{aligned}
E_{x,(i+\frac{1}{2},j,k)}^{n+1} &= E_{x,(i+\frac{1}{2},j,k)}^n + \frac{\Delta t}{\varepsilon \Delta_y} (H_{z,(i+\frac{1}{2},j+\frac{1}{2},k)}^{n+\frac{1}{2}} - H_{z,(i+\frac{1}{2},j-\frac{1}{2},k)}^{n+\frac{1}{2}}) \\
&\quad - \frac{\Delta t}{\varepsilon \Delta_z} (H_{y,(i+\frac{1}{2},j,k+\frac{1}{2})}^{n+\frac{1}{2}} - H_{y,(i+\frac{1}{2},j,k-\frac{1}{2})}^{n+\frac{1}{2}}) \\
&\quad - \frac{\Delta t}{\varepsilon} J_{x,(i+\frac{1}{2},j,k)}^{n+1/2}.
\end{aligned} \tag{2.53}$$

2.8.3.2 EB-MFEM Formulation

In this formulation, $\mathbf{E}(t, \mathbf{r}) \approx \sum_{i=1}^{N_e} e_i(t) \mathbf{W}_i^{(1)}(\mathbf{r})$ and $\mathbf{B}(t, \mathbf{r}) \approx \sum_{i=1}^{N_f} b_i(t) \mathbf{W}_i^{(2)}(\mathbf{r})$. Faraday's law is measured with the 2-form basis function and Ampere's law with the 1-form basis function to yield

$$\partial_t \mathbf{b} = [\mathcal{L}_{\nabla \times} \circ] \mathbf{e} \tag{2.54a}$$

$$\partial_t \mathbf{e} = c^2 [\mathcal{L}_{\nabla \times} \circ]^T [\star_{\mu^{-1}}] \mathbf{b} - \varepsilon^{-1} \mathbf{j} \tag{2.54b}$$

assuming the domain is freespace with the speed of light $c = \sqrt{\varepsilon_0 \mu_0}^{-1}$. The Hodge operator matrix is defined as

$$[\star_{\mu^{-1}}]_{ij} = \int_{\Omega} d\Omega \mathbf{W}_i^{(2)}(\mathbf{r}) \cdot \mathbf{W}_j^{(2)}(\mathbf{r}). \tag{2.55}$$

The degrees of freedom for the current are defined as

$$\mathbf{j}_i = \sum_{n=1}^{N_p} \frac{q_n}{\Delta_t} \int_{\mathbf{r}^n}^{\mathbf{r}^{n+1}} d\mathbf{p}_n \cdot \mathbf{W}_i^{(1)}(\mathbf{r}) \quad (2.56)$$

where $\mathbf{p}_n$ is the particle path for the n -th particle.

2.8.3.3 DH-MFEM Formulation

In this formulation, $\mathbf{H}(t, \mathbf{r}) \approx \sum_{i=1}^{N_e} h_i(t) \mathbf{W}_i^{(1)}(\mathbf{r})$ and $\mathbf{D}(t, \mathbf{r}) \approx \sum_{i=1}^{N_f} d_i(t) \mathbf{W}_i^{(2)}(\mathbf{r})$. Ampere's law is measured with the 2-form basis function and Faraday's law with the 1-form basis function to yield

$$\partial_t \mathbf{h} = c^2 [\mathcal{L}_{\nabla \times} \circ] [\star_{\varepsilon^{-1}}] \mathbf{d} \quad (2.57a)$$

$$\partial_t \mathbf{d} = [\mathcal{L}_{\nabla \times} \circ] \mathbf{h} - \mathbf{j}. \quad (2.57b)$$

The Hodge operator matrix is defined as

$$[\star_{\varepsilon^{-1}}]_{ij} = \int_{\Omega} d\Omega \mathbf{W}_i^{(2)}(\mathbf{r}) \cdot \mathbf{W}_j^{(2)}(\mathbf{r}). \quad (2.58)$$

The degrees of freedom for the current are defined as

$$\mathbf{j}_i = \sum_{n=1}^{N_p} \frac{q_n}{\Delta_t} \int_{\mathbf{r}^n}^{\mathbf{r}^{n+1}} d\mathbf{p}_n \hat{n}_i \cdot \mathbf{J}_n(\mathbf{r}) \quad (2.59)$$

where the particle path for the n -th particle and is only evaluated on the surface.

CHAPTER 3

HIGHER ORDER CHARGE CONSERVING ELECTROMAGNETIC FINITE ELEMENT PARTICLE IN CELL METHOD

3.1 Introduction

Modeling novel beam-wave interaction devices, such as accelerators, vacuum electronics, and directed energy devices [?, ?, ?] relies on robust numerical tools capable of self-consistent analysis of the interaction of a plasma with electromagnetic fields. This is typically done using an electromagnetic particle-in-cell (EM-PIC) method to evolve a given plasma distribution in time and space [16]. It consists of a method that discretizes both the Newton's equations of motion and a Maxwell's field solver. The coupling between the two is effected through the Lorentz force due to the electric field and magnetic flux density. Given the range of applications, there has been extensive interest in developing PIC solvers; a majority of those used in field are based on finite difference time domain (FDTD) methods [109]. The simplicity of the formulation, ease of particle position updates, and readily available parallelization algorithms make this approach an attractive workhorse for PIC. In what follows, we will use the a concatenation of abbreviations to denote regime and method to solve PIC. For instance, EM-FDTD PIC denotes an electromagnetic PIC using FDTD.

While EM-FDTD PIC has a number of advantages, there has been significant recent effort to explore the advantages offered by finite element methods to solving PIC problems. To a large part, this is driven by success of this methodology in microwave and millimeter frequency regimes wherein the success of this method has been demonstrated in analysis and design of complex topologies and electrically large objects. The foray of FEM into PIC is not without challenges, the principal of which is charge conservation. To understand this, note that in evolving the fields, we only solve the two curl equations (Faraday's and

Ampere's laws) and need a framework wherein Gauss' law are satisfied as well. This implies that discretization in space *and* time should be such that these laws are satisfied. Ref. [43] rigorously develops the conditions that should be satisfied, and demonstrates how current EM-PIC formulations satisfy these conditions. For instance, the spatial and temporal basis sets used in an explicit FDTD time-stepping scheme, together with an appropriate integration of the path, satisfies these constraints. Developing such a method for FEM was a long standing challenge.

This was solved recently; see pioneering papers by [154, 130, 116, 129]. The methods introduced here were based on explicit updates of field solution and particle position, and on the proper representation of quantities on the underlying discrete mesh. In the same vein, a Poisson bracket approach that utilizes Whitney forms defined by B-spline FEM formulations [?] to define a structure-preserving EM-PIC scheme [?, ?], with several of these methods using higher order basis sets. Note, in manner akin to FDTD, one solves all of Maxwell's equations. In an explicit setting, this approach avoids exciting null spaces (and corruption of Gauss' law due to these null spaces) [?, ?, ?].

But restriction of field solve to an explicit field update has challenges; it is only conditionally stable and the smallest time step is governed by the finest feature in the model and *not* the physics. Overcoming this bottleneck has a well known remedy. Indeed, Newmark-Beta methods are unconditionally stable and the constraint on time comes from the physics that one needs to capture. But implicit field solve implies the need to rethink PIC solves such that the Gauss' laws are satisfied. A problem that is unstated is that implicit solves introduce a null space; for Maxwell solvers, this null space is of the form $\nabla\phi(\mathbf{r})$ and for the wave equation, this null space is of the form $t\nabla\phi(\mathbf{r})$. It is apparent that the null space will corrupt the satisfaction Gauss' laws in addition to other challenges. This problem was solved recently [128, 127]. Specifically, imposition of Coulomb Gauge using a quasi-Helmholtz decomposition (in simply connected systems) in [127] enables satisfying Gauss' law to machine precision for *both* the Maxwell solver and the wave equations. This

implies that the infrastructure that is already in place to solve the vector wave equation can readily be used for PIC analysis.

As we build this line of progress, the next ingredient that is missing is higher order basis sets for field, current and particle representation within a PIC framework. Hierarchical and interpolatory basis functions are known for FEM field solvers [?, ?, ?]. For smoothly varying geometries, higher order bases provide more accurate fields while utilizing fewer degrees of freedom. Furthermore, these higher order formulations satisfy the relationships of the *de-Rahm* complex [48, 22, 9, 178]. Developing a higher order EM-FEMPIC framework will be the key contribution of this paper. Specifically, we will present an unconditionally stable, exact current mapping FEM EM-PIC scheme that uses higher order basis functions on tetrahedral meshes.

The rest of this paper is organized as follows: In Section 4.2 provide a brief problem statement. Next, in Section 3.3, we define the spatial and temporal discretization of the problem. Section 3.3.2 describes the current mapping scheme used to conserve charge regardless of the time marching scheme. In Section 4.4, we present results that demonstrate the use of the higher order FEM-PIC scheme. Finally, we conclude this paper in Section 4.5 outlining future directions of research.

3.2 Problem Statement

Consider a region of free space Ω containing charged species that is bounded by $\partial\Omega$. For simplicity we consider only a single species. The permittivity and permeability of free space are denoted as ϵ_0 and μ_0 , and the speed of light denoted using $c = 1/\sqrt{\mu_0\epsilon_0}$. There also exists a time-varying electromagnetic field due to moving charges and potentially an impressed electromagnetic field. The distribution of the charge species can be represented by a phase space distribution function (PSDF) $f(t, \mathbf{r}, \mathbf{v})$ that satisfies the Vlasov equation

$$\begin{aligned} \partial_t f(t, \mathbf{r}, \mathbf{v}) + \mathbf{v} \cdot \nabla f(t, \mathbf{r}, \mathbf{v}) + \\ \frac{q}{m} [\mathbf{E}(t, \mathbf{r}) + \mathbf{v} \times \mathbf{B}(t, \mathbf{r})] \cdot \nabla_v f(t, \mathbf{r}, \mathbf{v}) = 0. \end{aligned} \tag{3.1}$$

Next, will describe how the equations to be solved and how the problem is discretized in space and time.

3.3 Overview of Discrete Solutions

To solve the above equations, we start with defining charge and current density in terms of the PSDF, $\rho(t, \mathbf{r}) = q \int_{\Omega} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}$ and $\mathbf{J}(t, \mathbf{r}) = q \int_{\Omega} \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}$. Using a particle approximation using N_p samples with shape functions $S(\mathbf{r})$, one obtains

$$\rho(t, \mathbf{r}) = q \sum_{p=1}^{N_p} S(\mathbf{r} - \mathbf{r}_p(t)) \quad (3.2a)$$

$$\mathbf{J}(t, \mathbf{r}) = q \sum_{p=1}^{N_p} \mathbf{v}_p(t) S(\mathbf{r} - \mathbf{r}_p(t)) \quad (3.2b)$$

where $\mathbf{r}_p(t)$ and $\mathbf{v}_p(t)$ are the position and velocity of particle p . In this work the shape functions are chose to eb Dirac delta functions, though generalization to other shape functions is possible [43]. The particular choice shape function is immaterial to the results of this paper. The electromagnetic fields, $\mathbf{E}(t, \mathbf{r})$ and $\mathbf{B}(t, \mathbf{r})$, are solutions to Maxwell's curl equations

$$-\frac{\partial \mathbf{B}(t, \mathbf{r})}{\partial t} = \nabla \times \mathbf{E}(t, \mathbf{r}) \quad (3.3a)$$

$$\frac{\partial \mathbf{D}(t, \mathbf{r})}{\partial t} = \nabla \times \mathbf{H}(t, \mathbf{r}) - \mathbf{J}(t, \mathbf{r}) \quad (3.3b)$$

and satisfy Gauss' laws

$$\nabla \cdot \mathbf{B}(t, \mathbf{r}) = 0 \quad (3.4a)$$

$$\nabla \cdot \mathbf{D}(t, \mathbf{r}) = \rho(t, \mathbf{r}). \quad (3.4b)$$

The fields are also subject to boundary conditions which are either Dirichlet, Neumann, or impedance boundary conditions on $\partial\Omega_D$, $\partial\Omega_N$, or $\partial\Omega_I$ which bound the domain as

$$\hat{n} \times \mathbf{E}(t, \mathbf{r}) = \mathbf{\Psi}_D(t, \mathbf{r}) \text{ on } \partial\Omega_D, \quad (3.5a)$$

$$\hat{n} \times \mathbf{H}(t, \mathbf{r}) = \mathbf{\Psi}_N(t, \mathbf{r}) \text{ on } \partial\Omega_N, \quad (3.5b)$$

$$\hat{n} \times \frac{\mathbf{B}(t, \mathbf{r})}{\mu} - \gamma \hat{n} \times \hat{n} \times \mathbf{E}(t, \mathbf{r}) = \Psi_I(t, \mathbf{r}) \text{ on } \partial\Omega_I. \quad (3.5c)$$

The fields, which are defined with respect to the free space background medium, are related to the fluxes through constitutive relations

$$\mathbf{D}(t, \mathbf{r}) = \varepsilon_0 \mathbf{E}(t, \mathbf{r}) \quad (3.6a)$$

$$\mathbf{H}(t, \mathbf{r}) = \mu_0^{-1} \mathbf{B}(t, \mathbf{r}). \quad (3.6b)$$

The source definitions are used to evolve the particle positions using Newton's equations of motion and Lorentz force, viz., $\mathbf{F}(t, \mathbf{r}) = q(t, \mathbf{r})(\mathbf{E}(t, \mathbf{r}) + \mathbf{v}(t, \mathbf{r}) \times \mathbf{B}(t, \mathbf{r}))$. The simulation follows the usual PIC cycle: particles are mapped to a discretized space to solve for the electric field and magnetic flux density, which are in turn used to push the particles, defining a new current and particle positions, restarting the cycle. Though the PSDF is sampled with particles, the total description of the electromagnetic problem is continuous, and must be discretized in space and time.

3.3.1 Discretization in Space

Assume that the domain Ω is represented using a collection of finite elements $\mathcal{K} = \{\mathcal{N}, \mathcal{E}, \mathcal{F}, \mathcal{T}\}$ defined using N_n nodes, N_e edges, N_f faces and N_t tetrahedron. Each tetrahedron contains basis functions to represent fields, fluxes, and sources that follow the *de-Rham* sequence as seen in Fig. 3.1[?, ?]. This sequence preserves the differential relations between the quantities of interest, such that the curl of a field is a flux, the divergence of a flux is a charge. The Hodge star operator $\star$ maps a field to a flux on a dual mesh. It is well known that Whitney basis functions can be used to represent the electric field and magnetic flux [113, 83, 130].

For a k th order interpolatory basis functions, the electric field is represented using N_1 higher order Whitney edge basis functions, $\mathbf{E}(t, \mathbf{r}) = \sum_{i=1}^{N_1} e_i(t) \mathbf{W}_i^{(1)}(\mathbf{r})$, where there are $6(k+1)$ degrees of freedom associated with edges, $4k(k+1)$ degrees of freedom associated with faces, and $k(k^2-1)/2$ associated with the cell volumes. The magnetic flux density is

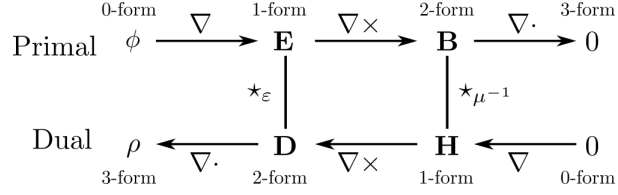


Figure 3.1: Relationship of fields and fluxes with respect to the de-Rham complex.

represented using N_2 Whitney face basis function, $\mathbf{B}(t, \mathbf{r}) = \sum_{i=1}^{N_2} b_i(t) \mathbf{W}_i^{(2)}(\mathbf{r})$ where there are $(k+1)(k+2)/2$ degrees of freedom associated with faces and $k(k+1)(k+2)/2$ associated with the cell volumes. A more complete description of these basis functions is provided in the Appendix.

We have chosen to define the problem such that Faraday's law (3.3a), $\mathbf{E}(t, \mathbf{r})$, and $\mathbf{B}(t, \mathbf{r})$ are defined on the primal grid. Therefore, Ampere's law (3.3b), $\mathbf{H}(t, \mathbf{r})$, $\mathbf{D}(t, \mathbf{r})$, as well as $\mathbf{J}(t, \mathbf{r})$, and $\rho(t, \mathbf{r})$ are defined in the dual space on the corresponding dual grid. This means that while the electric field and magnetic flux can be directly represented using a Whitney basis on the primal mesh, the sources $\rho(t, \mathbf{r})$, $\mathbf{J}(t, \mathbf{r})$ cannot. On structured grids it is straightforward to define dual basis function spaces to represent dual quantities, however, on an unstructured FEM mesh the dual fields are only indirectly accessible via Hodge operators. Therefore the source distribution $\rho(t, \mathbf{r})$ cannot be directly represented, and is instead measured with higher order nodal basis functions on the primal mesh, which are defined in the Appendix. The current density $\mathbf{J}(t, \mathbf{r})$, which lies in the same space as $\mathbf{D}(t, \mathbf{r})$, is measured by the the electric field basis, the higher order Whitney edge functions.

Before we proceed with prescribing the discrete framework, consider an auxillary function

$$\mathbf{G}(t, \mathbf{r}) = \int_0^t \mathbf{J}(\tau, \mathbf{r}) d\tau \quad (3.7)$$

such that Ampere's law is rewritten as

$$\frac{\partial \mathbf{D}(t, \mathbf{r})}{\partial t} = \nabla \times \mathbf{H}(t, \mathbf{r}) - \frac{\partial \mathbf{G}(t, \mathbf{r})}{\partial t}. \quad (3.8)$$

Using (3.8) and Faraday's law and spatial basis functions defined earlier, one may write the

discrete system as

$$\underbrace{\begin{bmatrix} [\star_{\mu^{-1}}] & 0 \\ 0 & [\star_{\epsilon_0}] \end{bmatrix}}_{\bar{\bar{M}}} \begin{bmatrix} \partial_t \bar{B}(t) \\ \partial_t \bar{E}(t) \end{bmatrix} + \underbrace{\begin{bmatrix} 0 & [\tilde{\nabla} \times] \\ -[\tilde{\nabla} \times]^T & [\star_I] \end{bmatrix}}_{\bar{\bar{S}}} \begin{bmatrix} \bar{B}(t) \\ \bar{E}(t) \end{bmatrix} = \underbrace{\begin{bmatrix} 0 \\ -\frac{\partial_t \bar{G}(t)}{\epsilon} \end{bmatrix}}_{\bar{\bar{F}}} \quad (3.9)$$

where the degree of freedom vectors $\bar{E}(t) = [e_1(t), e_2(t), \dots, e_{N_e}(t)]$, $\bar{B}(t) = [b_1(t), b_2(t), \dots, b_{N_f}(t)]$, and $\bar{G}(t) = [g_1(t), g_2(t), \dots, g_{N_e}(t)]$ with $g_i(t) = \langle \mathbf{W}_i^{(1)}(\mathbf{r}), \mathbf{G}(t, \mathbf{r}) \rangle$. The coupled system matrix is composed of discrete Hodge matrix operators

$$[\star_{\epsilon}]_{i,j} = \langle \mathbf{W}_i^{(1)}(\mathbf{r}), \epsilon \cdot \mathbf{W}_j^{(1)}(\mathbf{r}) \rangle \quad (3.10)$$

$$[\star_{\mu^{-1}}]_{i,j} = \langle \mathbf{W}_i^{(2)}(\mathbf{r}), \mu^{-1} \cdot \mathbf{W}_j^{(2)}(\mathbf{r}) \rangle, \quad (3.11)$$

the surface impedance matrix

$$[\star_I]_{i,j} = \langle \hat{n}_i \times \mathbf{W}_i^{(1)}(\mathbf{r}), \mu^{-1} \hat{n}_j \times \mathbf{W}_j^{(1)}(\mathbf{r}) \rangle_{\partial\Omega} \quad (3.12)$$

and a discrete curl matrix

$$[\tilde{\nabla} \times]_{i,j} = \langle \mathbf{W}_i^{(2)}, \nabla \times \mathbf{W}_j^{(1)}(\mathbf{r}) \rangle. \quad (3.13)$$

The operator $\langle \cdot, \cdot \rangle$ and $\langle \cdot, \cdot \rangle_{\partial\Omega}$ define a volume and surface integral, respectively, over the support of the basis functions, which is either a tetrahedron or face. The curl matrix $[\tilde{\nabla} \times]$ includes the metric information, unlike the definition usually obtained through discrete exterior calculus $[\nabla \times]$, which has entries of only 0, +1, or -1. For lowest order $k = 1$, this definition can be obtained as

$$[\nabla \times] = [\star_{\mu^{-1}}]^{-1} [M_c]; \quad (3.14)$$

however, the simplicity of defining the matrix by inspection is lost for $k > 1$.

3.3.2 Evolution of Particle Path and Current Mapping

The fields are evolved in time using an unconditionally stable Newmark-beta time marching scheme [42]. This allows larger time steps than would be afforded by a leapfrog method. In this framework, the current mapping (or evolution of charge) has to be consistent with that used for evolution of fields. Unfortunately, a naive approach to incorporate the particle current as the forcing function will violate conservation of charge. The method presented in [128] is agnostic to any time stepping method used for a field solve, and overcomes this bottleneck. In this paper, a similar method is used, but adapted to a higher order basis function in space. Using the definition of the particle current density in (3.7), the Newmark-beta time marching scheme is defined as

$$\begin{aligned}
(\gamma \bar{\bar{M}} + \beta \Delta_t \bar{\bar{S}}) \bar{\bar{X}}^{n+1} - \gamma \Delta_t \bar{\bar{S}} \bar{\bar{X}}^n + (\gamma \bar{\bar{M}} + \beta \Delta_t \bar{\bar{S}}_M) \bar{\bar{X}}^{n-1} \\
+ \gamma \Delta_t \bar{\bar{F}}^{n+1} + \gamma \Delta_t \bar{\bar{F}}^{n-1} = 0
\end{aligned} \tag{3.15}$$

where $\bar{\bar{X}}^m = [\bar{B}^T(t_m) \ \bar{E}^T(t_m)]$ and $\bar{\bar{F}}^m = [0 \quad -\varepsilon^{-1} \bar{G}^T(t_m)]$. The degree of freedom vector $\bar{G} = [g_1(t), g_2(t), \dots, g_{N_e}(t)]$ with $g_i(t) = \langle \mathbf{W}_i^{(1)}, \mathbf{G}(t, \mathbf{r}) \rangle$. The parameters γ and β are used to change the stability of the scheme, often choosing $\gamma = .5$ and $\beta = .25$. To define the forcing function $\bar{\bar{F}}$, it is necessary to use an integration rule appropriate for the product of the higher order edge basis function and the particle path, which may also be a higher order polynomial. A key point that should be noted is the de-linking of the time stepping algorithm used for particle push and field updates. Consistency is ensured by proper inclusion in the right hand side of (4.3). Note, that this assumes non-relativistic motion. In this work, a fourth order Adams-Bashforth push is used, making the particle path a fourth order Lagrange polynomial.

3.3.3 Satisfaction of Gauss's Magnetic Law

While the above equation can be used, as shown [127] one would need to impose a Coulomb gauge to ensure that the null spaces do not corrupt the solution. The level

of the null space that is excited depends on the accuracy of the solution at every time step; which in turn, is related to how well the initial conditions are remembered in a time marching system. While [127] used a topological framework, here we investigate an alternate approach. Our goal is more modest and targeted. We seek to examine particle motion due to impressed magnetic lenses, we want to ensure the discrete representation of impressed magnetic flux density is divergence free when represented using Whitney basis. To that end, consider reconstructing an impressed magnetic flux density $\mathbf{B}^i(t, \mathbf{r})$ which satisfies (3.4a). The usual approach to obtain the coefficients to approximate $\mathbf{B}^i(t, \mathbf{r})$ would be to use Galerkin testing with the divergence-conforming basis set

$$[\star_{\mu^{-1}}]\mathbf{b} = \mathbf{f} \quad (3.16)$$

where $\mathbf{f}_i = \langle \mathbf{W}_i^{(2)}(\mathbf{r}), \mathbf{B}^i(t, \mathbf{r}) \rangle$. However, this construction of $\tilde{\mathbf{B}}^i(t, \mathbf{r})$ will not satisfy Gauss's law unless $\tilde{\mathbf{B}}^i(t, \mathbf{r}) = \mathbf{B}^i(t, \mathbf{r})$. This is accomplished by solving an optimization problem where Gauss's magnetic law is the constraint.

$$\begin{bmatrix} [\star_{\mu^{-1}}] & [\nabla \cdot]^T \\ [\nabla \cdot] & 0 \end{bmatrix} \begin{bmatrix} \mathbf{b} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathcal{B} \\ 0 \end{bmatrix} \quad (3.17)$$

For the lowest order spatial basis functions, the discrete divergence operator $[\nabla \cdot]$ can be written by inspection. The discrete divergence operator for higher orders, like the discrete curl operator, cannot be written as easily. It can be written as

$$[\nabla \cdot] = [\star_3]^{-1}[\tilde{\nabla} \cdot] \quad (3.18)$$

where

$$[\star_3]_{ij} = \langle W_i^{(3)}(\mathbf{r}), W_j^{(3)}(\mathbf{r}) \rangle \quad (3.19)$$

and

$$[\tilde{\nabla} \cdot]_{ij} = \langle W_i^{(3)}(\mathbf{r}), \nabla \cdot \mathbf{W}_j^{(2)}(\mathbf{r}) \rangle \quad (3.20)$$

Table 3.1: Satisfaction of Gauss' Magnetic Law for Linear Field

m	err in B	err in $\nabla \cdot \mathbf{B}$	err in B	err in $\nabla \cdot \mathbf{B}$
1	1.0604×10^{-1}	2.9681×10^{-5}	1.1367×10^{-1}	4.5062×10^{-19}
2	1.1049×10^{-15}	6.1606×10^{-19}	1.2201×10^{-15}	4.4173×10^{-19}
3	3.8299×10^{-15}	1.9566×10^{-18}	9.8539×10^{-15}	3.9481×10^{-18}

Table 3.2: Satisfaction of Gauss' Magnetic Law for Sinusoidal Field

m	err in B	err in $\nabla \cdot \mathbf{B}$	err in B	err in $\nabla \cdot \mathbf{B}$
1	1.3198×10^{-2}	1.6310×10^{-5}	1.5048×10^{-2}	1.1404×10^{-18}
2	6.1965×10^{-4}	3.1300×10^{-7}	5.8211×10^{-4}	1.2061×10^{-18}
3	6.3122×10^{-6}	2.7822×10^{-9}	7.0793×10^{-6}	1.0762×10^{-17}

with $W^{(3)}(\mathbf{r})$ as the higher order volumetric basis function, which is defined in the Appendix. This allows the reconstructed field, regardless of the error in the representation of the original function, to still satisfy (3.4a).

Consider the tests done in Table 3.1 and 3.2. In this test, a divergence free function was reconstructed in a volume $50 \text{ cm} \times 15 \text{ cm} \times 20 \text{ cm}$, for several orders of spatial basis functions. In Table 3.1, the function $\mathbf{B}(\mathbf{r}) = y\hat{x} + x\hat{y}$ can be reconstructed exactly with second order and higher basis functions. Therefore, once the function was modeled correctly to machine precision, the divergence free nature of the reconstructed field is seen in both the constrained and non-constrained formulation. However, in Table 3.2, the function was $\mathbf{B}(\mathbf{r}) = \sin(y)\hat{x} + \cos(x)\hat{y}$, which cannot be represented exactly by a finite set of polynomials. Despite having similar accuracy, only the constrained formulation satisfies (3.4a). It is evident that the formulation has the desired properties with respect to representation of fields. As alluded to earlier, we will use this only for representing only the impressed field. A topological approach, akin to [127], is being developed and will be presented in later papers.

3.4 Results

In this section, we present several numerical tests using higher order FEM-PIC. Particle free results are provided here to demonstrate correctness of our implementation. We

demonstrate that the higher order basis functions presented satisfies the continuity equation and Gauss' law for a number of cases using the stated particle mapping scheme.

3.4.1 Higher Order Cost

Here we present the error in computed fields with respect to number of unknowns and basis function order. The relative error in a field propagating through a region of free space is shown in Fig. 3.2. The region is $0.25 \text{ m} \times 0.2 \text{ m} \times 0.5 \text{ m}$ in size. The normally incident electric field is defined as

$$\bar{E}(\bar{r}, t) = \hat{y} \cos(2\pi f_0 \tau) e^{-(\tau - 8\sigma)^2 / 2\sigma^2} (\text{V/m}), \quad (3.21)$$

where where $\tau = t - \bar{r} \cdot \hat{z}/c$, $\sigma = 3/[2(f_{\max} - f_0)]$ with the center $f_0 =$ and maximum frequency denoted $f_{\max} = 195 \text{ MHz}$. The relative error is defined as

$$\text{relative error} = \frac{\|\mathbf{E}_i^{(r)} - \mathbf{E}_i^{(a)}\|_2}{\|\mathbf{E}^{(a)}\|_2} \quad (3.22)$$

. It take several orders of magnitude more unknowns for a first order basis function to reach the same level of accuracy as a second order basis function. The trade off is the condition number of the system increases by roughly an order of magnitude as the order increases which effects the rate at which an iterative solver will converge. Therefore, consideration can be taken in balancing the size of the problem and simulation time for a given error.

3.4.2 Higher Order Particle Motion

The first example with particles is the orbit of a single particle around a nucleus. This test demonstrates when higher order bases give more accurate particle trajectories. At a certain distance, a particle with initial velocity perpendicular to the radial electric field will result in a circular orbit in a plane. In this test, a particle with initial velocity $\mathbf{v} = 3 \times 10^6 \hat{\phi} \text{ m/s}$ is set .25m from the centroid of a cylindrical ring geometry. The geometry has an inner radius of .2m and outer radius of .3m. Five meshes were generated to compare refinement

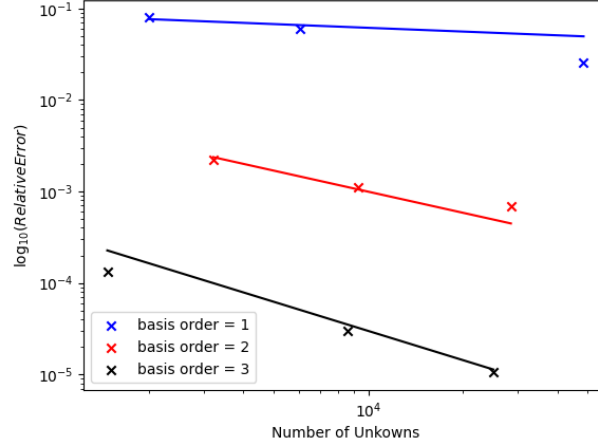


Figure 3.2: Relative Error in $\mathbf{E}_{t,r}$ for field propagating through free space.

in the edge length to basis function order. The electric field due to a nucleus with a charge of $Q_n = 1.423nC$ is reconstructed using the higher order interpolatory Whitney edge basis set and used to push the electron in the geometry. The analytic definition of the electric field is

$$\mathbf{E}(\mathbf{r}) = \frac{Q_n \hat{\mathbf{r}}}{4\pi\epsilon\mathbf{r} \cdot \mathbf{r}} \quad (3.23)$$

which, unlike the constant magnetic field used for cyclotron motion experiments, can be improved by using higher order spatial basis functions. The experiment was run for 6000 time steps with $\Delta_t = 0.4ns$, which corresponds to approximately 4 cycles. The effect of the higher order basis functions can be seen in 3.3 and 3.4 where the relative error is defined in (3.22).

For both the $\hat{z}$ and $\hat{\rho}$ components of the electric field, the error in the fields converges. The improvement of the field error translates to an improvement of the particle trajectory. In 3.5, the relative error is shown for the $\hat{z}$ component of the particle position. A key takeaway is that using a higher order basis function leads to more accurate particle trajectories than simply refining the mesh.

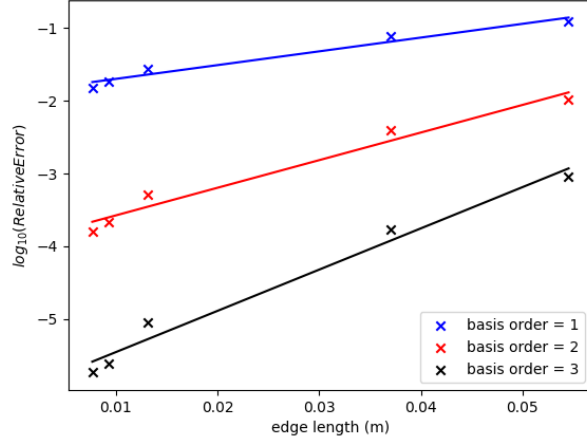


Figure 3.3: Relative Error in E_ρ for orbital motion

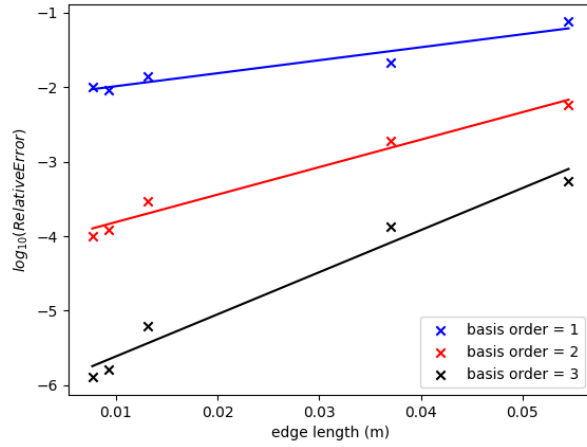


Figure 3.4: Relative Error in E_z for orbital motion.

3.4.3 Plasma Ball

In this example, we simulate an adiabatic expansion of a plasma ball. This example has both approximate analytic solutions [87] as well as experimental data [89]. A Gaussian distribution of 12000 Sr^+ ions and electrons is placed at the center of a spherical geometry that is enclosed with a first order absorbing boundary condition. The initial temperature of Sr^+ ions is 1K and electrons are 100K placed at a density of 5×10^8 particles per cubic meter such that the particles are and will remain sufficiently away from the boundary.

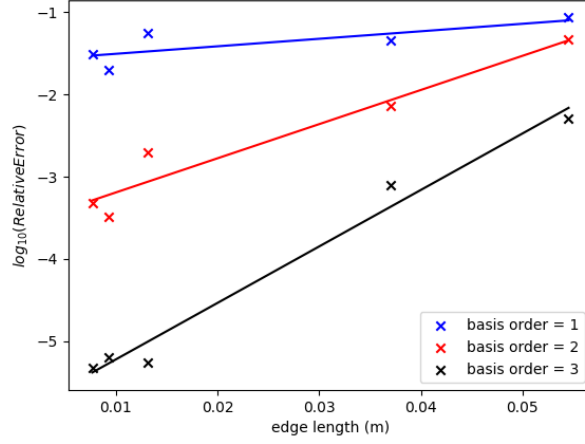


Figure 3.5: Relative Error in $\mathbf{r}$ for orbital motion.

Here, we use three geometries; the first with a radius of 6 cm with an average edge length of 1.02 cm, the second 12 cm with average edge length of 2.04 cm, and the third 18 cm with average edge length of 3.06 cm. The experiment was run with first and second order basis functions, with a comparison to the analytic solution in Table 3.3. Though there is good agreement between all of the experimental and analytic data, there is not a clear improvement as order increases. This is due to the fields being well behaved enough in this example that they are approximated well enough by the first order basis functions.

3.4.4 Expanding Particle Beam

In this test, we demonstrate an expanding plasma beam in the PEC cavity. This test is a standard test to confirm charge conservation as errors will accumulate and cause striations in the beam. Additionally, quasi-analytic solutions and comparisons to this method and other discretization schemes can be found in [138]. Macroparticles are injected into the cavity at an initial velocity and are allowed to repel each other as they progress down the cavity. The parameters used in this experiment are included in Table 3.4.

Key here is that the higher order basis functions are defined such that the differential relations between the basis functions for the electric field and magnetic flux are preserved.

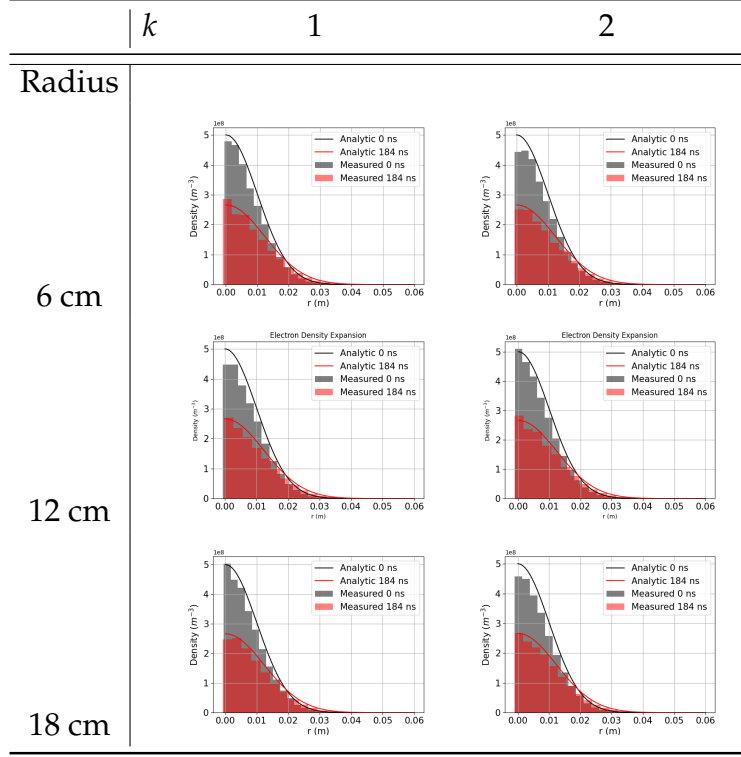


Table 3.3: Plasma Ball expansion for different basis function orders and geometry radii

Table 3.4: Expanding Particle Beam Parameters

Parameter	Value
Cavity Radius	20 mm
Cavity Length	100 mm
Boundary Conditions	PEC
v_0	$1.02 \cdot 10^7$ m/s
v_0/c	0.16678
beam radius r_b	8.00 mm
Number particles per time step	10
species	electrons
Turn on time	2 ns
beam current	5 mA
macro-particle size	103921.12
min edge length	3.89 mm
max edge length	13.5 mm
Δ_t	33.3 ps

First, consider the error in the measured charge density as defined by (3.22) shown in 3.6. Here, the error is small and saturates as the total number of particles in the cavity stabilizes. The increase of error as the basis function order increases can be attributed to

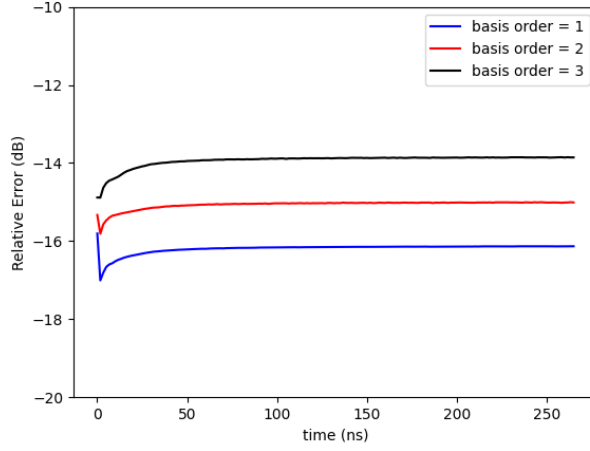


Figure 3.6: Relative Error of $\tilde{\rho}(t, \mathbf{r})$ vs $-\nabla \cdot \mathbf{G}(t, \mathbf{r})$ for particle beam.

Table 3.5: Error in impressed Quadrupole Fields

basis order 1		basis order 2		basis order 3	
N_2	error	N_2	error	N_2	error
140629	9.835×10^{-2}	89502	1.143×10^{-2}	28488	1.726×10^{-2}
597623	3.8299×10^{-2}	343812	3.803×10^{-3}	103876	3.9481×10^{-3}
		637050	2.424×10^{-3}	240270	6.932×10^{-4}

the increase of the condition number of the mass matrix that is inverted to compute the divergence of the integrated current. The error between the divergence of the electric flux and integrated current is shown in 3.7. The error is near machine precision, demonstrating the higher order divergence operator acting on the curl of the magnetic field does go to zero. Lastly, different time marching schemes can be taken by varying the values of γ and β in (4.4) using first order spatial basis functions. The error in Gauss' law for three different time marching schemes is shown in 3.8, where average acceleration has $\gamma = .5, \beta = .25$, backward difference has $\gamma = 1.5, \beta = 1$, and galerkin has $\gamma = 1.5, \beta = .8$. The error remains at machine precision as expected. In total, this shows that the representation of the particle in the simulation is correct and that Gauss' law is satisfied.

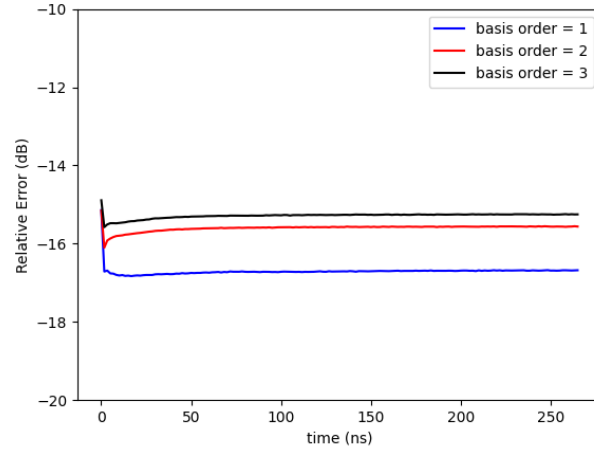


Figure 3.7: Relative Error of $[\nabla \cdot] \mathbf{D}(t, \mathbf{r})$ vs $-[\nabla] \mathbf{G}(t, \mathbf{r})$ for particle beam.

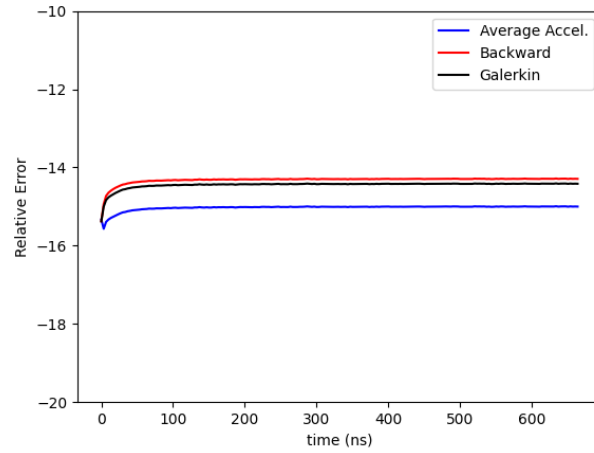


Figure 3.8: Relative Error of $[\nabla \cdot] \mathbf{D}(t, \mathbf{r})$ vs $-[\nabla] \mathbf{G}(t, \mathbf{r})$ for particle beam with different time marching schemes.

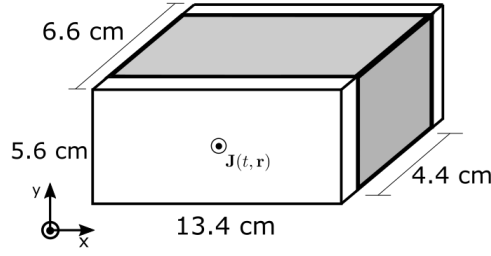


Figure 3.9: Schematic for perfect electrical conducting box with Pafonsky quadrupole (shaded).

3.4.5 Pafonsky Quadrupole

In this example, the Panofsky quadrupole used in [?] is modeled. This example uses higher order basis functions to get more accurate impressed fields using fewer degrees of freedom than a lower order method. From Table 3.5, a mesh with more than several million degrees of freedom would be needed to obtain a result with similar error in the impressed fields. This would significantly effect the time needed to simulate the result. The quadrupole is 13.4 cm in width, 5.6cm in height, and .044 cm in height, shown in Fig. 3.9. We define a rectangular PEC cavity with the quadrupole .011cm from the xy-plane. The fields due to the quadrupole are calculated by evaluating Bio-Savart's law using the defined current density. It would be too expensive to recalculate the fields as particles pass through the system, therefore the coefficients needed to reconstruct the fields are obtained through (3.17), which also enforces (3.4a). Particles are emitted from the xy-plane at $z = 0$, passing through the fields generated by the quadrupole. The beam is emitted such that the beam will focus in the y -dimension and defocus in the x -dimension. The iterative solver tolerance for both the fields and the divergence enforcement was set to $1e-5$. A snapshot of the particle positions at 35.7 ns is shown in Fig 3.10 and 3.11, where the background magnetic flux density $\mathbf{B}_y(t, \mathbf{r})$ and $\mathbf{B}_x(t, \mathbf{r})$ are plotted, respectively. The particle beam smoothly expands in the x -dimension and compresses in the y -dimension which is a sign that charge is being conserved correctly.

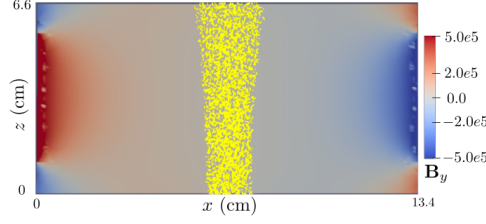


Figure 3.10: Particle beam traveling in $x - z$ plane in Pafonsky quadrapole with background $\mathbf{B}_y(t, \mathbf{r})$.

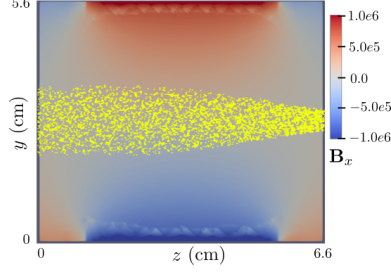


Figure 3.11: Particle beam traveling in $y - z$ plane in Pafonsky quadrapole with background $\mathbf{B}_x(t, \mathbf{r})$.

3.5 Summary

In this work, we have presented a higher order, exact current mapped FEM-based EM-PIC with unconditionally stable time marching. When higher order fields dominate the physics being modeled, higher order basis functions can reduce the number of degrees of freedom needed to model it while also getting more accurate fields. A method was also provided to ensure that Gauss' magnetic law is satisfied, which can occur when time marching schemes other than leap frog are used. Future work will create quasi-Helmholtz decomposition for higher order basis sets which will further increase the efficiency of using higher order basis while also allowing fields obtained by the vector wave equation to be used. Even with the use of higher order basis, there is a limit to the size of problem that can fit on a single node. To handle this challenge, domain decomposition approaches for Maxwell solvers will be developed.

3.6 Appendix

In this appendix, we define the higher order interpolatory basis functions. The basis functions are formed by multiplying the lowest order Whitney elements by an interpolatory Lagrange polynomial. We use the definition by Silvester [?]

$$P_i(\lambda) = \begin{cases} \frac{1}{i!} \prod_{m=0}^{i-1} (k\lambda - m), & 1 \leq i \leq k \\ 1, & i = 0 \end{cases} \quad (3.24)$$

and the shifted Silvester Polynomial

$$\hat{P}_i(\lambda) = \begin{cases} \frac{1}{(i-1)!} \prod_{m=1}^{i-1} (k\lambda - m), & 2 \leq i \leq k+1 \\ 1, & i = 1 \end{cases} \quad (3.25)$$

3.6.1 Node Basis Function

The k -th order nodal basis function $W_s^{(0)}(\mathbf{r}) \in H^1$ is defined as

$$W_i^{(0)}(\mathbf{r}) = Q^{(0)} \tilde{W}_i(\mathbf{r}) \quad (3.26)$$

where

$$\tilde{W}_s^{(0)}(\mathbf{r}) = \lambda_s \quad (3.27)$$

and

$$Q^{(0)} = \hat{P}_s(\lambda_s) P_t(\lambda_t) P_u(\lambda_u) P_v(\lambda_v). \quad (3.28)$$

There are a total of $(k+1)(k+2)(k+3)/6$ degrees of freedom in each tetrahedron with 4 associated with nodes, $k-1$ for each edge, $(k-1)(k-2)$ for each face, and $k(k-1)(k-2)/6$ internal to each tetrahedron.

3.6.2 Whitney Edge Basis Function

The k -th order edge basis function $\mathbf{W}_s^{(1)}(\mathbf{r}) \in H(\nabla \times)$ is defined as

$$\mathbf{W}_s^{(1)}(\mathbf{r}) = Q^{(1)} \tilde{\mathbf{W}}_{st}^{(1)}(\mathbf{r}) \quad (3.29)$$

where

$$\tilde{\mathbf{W}}_s^{(1)}(\mathbf{r}) = \lambda_s \nabla \lambda_t - \lambda_t \nabla \lambda_s \quad (3.30)$$

and

$$Q^{(1)} = \hat{P}_s(\lambda_s) \hat{P}_t(\lambda_t) P_u(\lambda_u) P_v(\lambda_v). \quad (3.31)$$

There are a total of $k(k+2)(k+3)/2$ degrees of freedom in each tetrahedron with k associated with each edge, $k(k-1)/2$ with each face, and $k(k-1)(k-2)/6$ internal to each tetrahedron.

3.6.3 Whitney Face Basis Function

The k -th order face basis function $\mathbf{W}_s^{(2)}(\mathbf{r}) \in H(\nabla \cdot)$ is defined as

$$\mathbf{W}_s^{(2)}(\mathbf{r}) = Q^{(2)} \tilde{\mathbf{W}}_s^{(2)}(\mathbf{r}) \quad (3.32)$$

where

$$\tilde{\mathbf{W}}_s^{(2)}(\mathbf{r}) = \lambda_s \nabla \lambda_t \times \nabla \lambda_u + \lambda_t \nabla \lambda_u \times \nabla \lambda_v + \lambda_u \nabla \lambda_s \times \nabla \lambda_t \quad (3.33)$$

and

$$Q^{(2)} = \hat{P}_s(\lambda_s) \hat{P}_t(\lambda_t) \hat{P}_u(\lambda_u) P_v(\lambda_v). \quad (3.34)$$

There are a total of $k(k+1)(k+3)/2$ degrees of freedom in each tetrahedron with $k(k+1)/2$ with each face and $k(k-1)(k+1)/6$ internal to each tetrahedron.

3.6.4 Volume Basis Function

The k -th order volume basis function $\tilde{W}^{(3)}(\mathbf{r}) \in L^2$ is defined as

$$W_s^{(3)}(\mathbf{r}) = Q^{(3)} \tilde{W}^{(3)}(\mathbf{r}) \quad (3.35)$$

where

$$\begin{aligned} \tilde{W}^{(3)}(\mathbf{r}) = & \lambda_s \nabla \lambda_t \cdot \nabla \lambda_u \times \lambda_v + \lambda_t \nabla \lambda_u \cdot \nabla \lambda_v \times \lambda_s \\ & + \lambda_u \nabla \lambda_v \cdot \nabla \lambda_s \times \lambda_t + \lambda_v \nabla \lambda_s \cdot \nabla \lambda_t \times \lambda_u \end{aligned} \quad (3.36)$$

and

$$Q^{(3)} = \hat{P}_s(\lambda_s)\hat{P}_t(\lambda_t)\hat{P}_u(\lambda_u)\hat{P}_v(\lambda_v). \quad (3.37)$$

The function is associated with tetrahedra with $k(k + 1)(k + 2)/6$ unknowns in each tetrahedron, all of which are internal to the cell.

CHAPTER 4

DOMAIN DECOMPOSITION FRAMEWORK FOR MAXWELL FINITE ELEMENT SOLVERS AND APPLICATION TO PIC

4.1 Introduction

The design of novel accelerator and vacuum devices require computational tools capable of simulating self-consistent interactions between plasma and electromagnetic fields [149, 2, 107, 49]. This is commonly done by evolving a particle distribution in time due to the Lorentz force defined by an electric field and magnetic flux density; this includes both external/impressed and those generated by the acceleration of charged species. The predominant approach is the finite difference time domain based particle in cell method (EM-FDTD PIC) [16]. This method has seen decades of use and advancement, primarily due its ease of use and efficiency, as the fields can be determined from a simple recurrence formula rather than matrix inversion. Furthermore, parallel implementations and fast techniques have enabled EM-FDTD PIC to simulate large problems [146, 167, 61, 133]. However, there has been interest in exploring alternatives to EM-FDTD PIC. To a large extent, this is motivated by the higher order fidelity that one can obtain in terms of both geometry as well as physics.

In response to this need, the past decade has seen extensive effort to create an electromagnetic particle in cell method based around the finite element method (EM-FEMPIC); see [109, 130] and papers therein. It has been shown that by choosing proper basis sets for the fields and currents, it is possible to obtain charge conserving EM-FEMPIC schemes through exact current mapping [117, 129, 130]. Unfortunately, these methods use explicit time stepping with first order basis functions to represent both the fields, particles, currents, and time. More recent work has utilized in higher order spatial basis better represent fields, but the error in representation is still constrained by the representation for time [69];

note, the moniker “structure-preserving” is used when referring to a method that uses Whitney basis/ensures that the *de-Rham* relations hold. The downside of using explicit time stepping, it is *conditionally stable*, and the time step to ensure stability is determined by the smallest feature size. Obviously, this is a challenge when analyzing plasma in geometrically complex in structures.

More recent work provided a general framework for charge conservation to be satisfied, irrespective of time stepping scheme [43]. A practical demonstration of satisfaction of conservation laws for implicit unconditionally stable finite element scheme for Maxwell equation was shown for a set of test problems in [128]. It was also shown in this paper, that the proposed methodology was valid for a wave equation FEM solver as well. Unfortunately, it is well known that there exist a null space that grows as $t\nabla\phi(\mathbf{r})$ for the wave equation solvers and a null space that varies as $\nabla\phi(\mathbf{r})$ for implicit Maxwell solvers, where $\phi(\mathbf{r})$ is a scalar field. While it may be possible to control the magnitude of the null space excited in Maxwell solvers, the one for the wave equation unfortunately rears its head with time. The development of a discrete Coulomb gauge in [127] shows how one may obtain a method that satisfies Gauss’ laws for *both* wave equation and Maxwell equation solvers. Despite this progress, a fundamental bottleneck remains. All EM-FEMPIC methods are more expensive than EM-FDTD PIC methods.

The reason is for the efficiency of FDTD schemes fairly simple; there is no inversion thanks to the structure of the method [161]. Unfortunately, FEM methods typically involve inversion of matrices. As is well known, a direct inversion would cost $O(N_{dof}^3)$ per time step where N_{dof} is the number of degrees of freedom. Alternatively, one typically uses an iterative solver whose cost scales as $O(N_{iter}N_{dof})$, where N_{iter} is the number of iterations which depends on the error threshold. As a result, one takes recourse to preconditioners. But it has been shown that the most computationally effective approach has been to use finite element tearing and integration [56, 54]. A bulk of the effort has been applying this technique to amortize cost of wave equations and largely in the Fourier domain

[97, 96, 185, 181], with some scant papers in the time domain [4, 122].

The underlying principle for developing a domain decomposition scheme is a finite element tearing and interconnecting (FETI) framework. Here, domain is partitioned into multiple regions/subdomains. For each subdomain, the unknowns are divided into interior and boundary quantities. The quantities on the boundary are shared between multiple subdomains, and are related via appropriate transmission conditions. Via manipulations, one only solves for unknowns on the boundary of subdomains which is far fewer than the overall number of unknowns. All interior unknowns can be related to the ones on the boundary. Note, this differs from the domain decomposition approaches currently used for FDTD, which takes a Schwarz approach which uses overlapping subdomains, requiring iteration of each subdomain to get a converged solution[90].

Thus the main contribution of this paper are as follows: (a) we derive two FETI schemes for time domain Maxwell equation solvers, (b) these methods are then used within an unconditionally stable EM-FEMPIC framework using an exact current mapping scheme, and (c) we present a number of results that demonstrate the efficacy of the proposed technique.

The rest of this paper is organized as follows. Section 4.2 will define the problem setup. Section 4.2.1 will briefly review particle mapping approach used followed by the field discretization in space and time in Section 4.2.2. Section 4.3 will define the two domain decomposition formulations. Results using both of these methods will be presented in Section 4.4 followed by conclusions and future work in Section 4.5.

4.2 Preliminaries

Let a region $\Omega \in \mathbb{R}^3$ be bounded by surface $\partial\Omega$ contain at least one charged species. The charges are represented by a phase space distribution function (PSDF) that is subject

to the Maxwell-Vlasov equation

$$\begin{aligned} \partial_t f(t, \mathbf{r}, \mathbf{v}) + \mathbf{v} \cdot \nabla f(t, \mathbf{r}, \mathbf{v}) + \\ \frac{q}{m} [\mathbf{E}(t, \mathbf{r}) + \mathbf{v} \times \mathbf{B}(t, \mathbf{r})] \cdot \nabla_v f(t, \mathbf{r}, \mathbf{v}) = 0. \end{aligned} \quad (4.1)$$

The electric field $\mathbf{E}(t, \mathbf{r})$ and magnetic flux density $\mathbf{B}(t, \mathbf{r})$ are obtained through the mixed finite element method, which discretizes Faraday's law and Ampere's law. The PSDF is evolved through the PIC cycle, which consists of:

1. Gathering the particles onto the mesh to be mapped into the field solve,
2. Solving for the fields due to the current from the particle motion,
3. Interpolating the fields at the particle positions,
4. Pushing the particles to new positions.

The following subsections will describe how Maxwell's equations are discretized in space and time, and how the particles are mapped into the field solver.

4.2.1 Current Mapping

The charge and current density is defined using using the conventional definition using the PSDF, $\rho(t, \mathbf{r}) = q \int_{\Omega} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}$ and $\mathbf{J}_{\rho}(t, \mathbf{r}) = q \int_{\Omega} \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}$. The PSDF is approximated by using N_p samples, or particles, with shape $S(\mathbf{r})$ such that the charge and current density are defined as $\rho(t, \mathbf{r}) = q \sum_{p=1}^{N_p} S(\mathbf{r} - \mathbf{r}_p(t))$ and $\mathbf{J}_{\rho}(t, \mathbf{r}) = q \sum_{p=1}^{N_p} \mathbf{v}_p(t) S(\mathbf{r} - \mathbf{r}_p(t))$ where $\mathbf{r}_p(t)$ and $\mathbf{v}_p(t)$ are the position and velocity of particle p . In this work, the shape function are delta functions, though other shape functions are also valid and can be used to improve noise quality. The proper function to measure the charge density is the 0-form and the 1-form for the current density. Different schemes to evolve Newton's equations can be used to preserve certain quantities like phase. In this work, to maintain accuracy of

the time evolution at larger time step sizes, the Adams-Bashforth scheme is used. Lastly, the time integral of the current density

$$\mathbf{G}(t, \mathbf{r}) = \int_0^t d\tau \mathbf{J}_\rho(\tau, \mathbf{r}) \quad (4.2)$$

is used to allow the particle current to evolve consistently with the fields. Otherwise, there is a disconnect between the continuity equation and Gauss' law.

4.2.2 Field discretization

4.2.2.1 Spatial Discretization

The FEM formulation used in this work is the mixed finite element method. The basis functions used are the 1-form $\mathbf{W}^{(1)}(\mathbf{r}) \in H(curl; \Omega)$ which allows for tangential continuity of fields, and the 2-form $\mathbf{W}^{(2)}(\mathbf{r}) \in H(div; \Omega)$ which allows for normal continuity of fluxes. The reconstructed fields used to accelerate the particles are defined as $\mathbf{E}(t, \mathbf{r}) = \sum_{i=1}^{N_e} e_i(t) \mathbf{W}^{(1)}(\mathbf{r})$ and $\mathbf{B}(t, \mathbf{r}) = \sum_{i=1}^{N_f} b_i(t) \mathbf{W}^{(2)}(\mathbf{r})$ where N_e are the number of edges and N_f are the number of faces. Testing Faraday's law with the 2-form and Ampere's law with the 1-form leads to the semidiscrete Maxwell system

$$\underbrace{\begin{bmatrix} [\star_{\mu^{-1}}] & 0 \\ 0[\star_{\epsilon_0}] \end{bmatrix}}_{\bar{\bar{A}}_1} \underbrace{\begin{bmatrix} \partial_t \bar{\bar{B}} \\ \partial_t \bar{\bar{E}} \end{bmatrix}}_{\bar{\bar{A}}_0} + \underbrace{\begin{bmatrix} 0 & [\tilde{\mathbf{V}}\mathbf{x}] \\ -c^2[\tilde{\mathbf{V}}\mathbf{x}]^T & c[\star_I] \end{bmatrix}}_{\bar{\bar{A}}_0} \underbrace{\begin{bmatrix} \bar{\bar{B}} \\ \bar{\bar{E}} \end{bmatrix}}_{\bar{\bar{F}}} = \underbrace{\begin{bmatrix} 0 \\ \bar{\bar{L}} \\ \bar{\bar{\epsilon}} \end{bmatrix}}_{\bar{\bar{F}}} \quad (4.3)$$

where the degree of freedom vectors $\bar{\bar{E}} = [e_1(t), e_2(t), \dots, e_{N_e}(t)]$, $\bar{\bar{B}} = [b_1(t), b_2(t), \dots, b_{N_f}(t)]$, and $\bar{\bar{L}} = [l_1(t), l_2(t), \dots, l_{N_e}(t)]$ with $l_i(t) = \langle \mathbf{W}_i^{(1)}(\mathbf{r}), \mathbf{J}_s(t, \mathbf{r}) - \partial_t \mathbf{G}(t, \mathbf{r}) \rangle$. The surface currents $\mathbf{J}_s(t, \mathbf{r})$ exist on $\partial\Omega$ due to a Neumann or robin boundary condition. The integrated particle current is chosen to satisfy charge conservation for arbitrary time marching schemes.

4.2.2.2 Time Discretization

This work utilizes the Newmark- β time marching scheme to evolve the fields in time. This scheme uses parameters γ and β , which creates an unconditionally stable time

marching scheme when $\gamma = .5$ and $\beta = .25$. Other choices can lead to different stability conditions. The parameter choices effect the definition of a temporal basis function $N(t)$ that is tested by function $W(t)$ [193]. When (4.3) is discretized with Newmark- β with $\gamma = 0.5$ and $\beta = 0.25$, the fully discretized system becomes

$$\begin{aligned}
& (0.5\bar{\bar{A}}_1 + 0.25\Delta_t\bar{\bar{A}}_0)\bar{X}^{n+1} - .5\Delta_t\bar{\bar{A}}_0\bar{X}^n \\
& + (0.5\bar{\bar{A}}_1 + .25\Delta_t\bar{\bar{A}}_0)\bar{X}^{n-1} + 0.5\Delta_t\tilde{G}^{n+1} + 0.5\Delta_t\tilde{G}^{n-1} \\
& + 0.25\Delta_t\tilde{F}^{n+1} - 0.5\Delta_t\tilde{F}^n + 0.25\tilde{F}^{n-1} = 0.
\end{aligned} \tag{4.4}$$

Here, $\bar{X}^m = [\bar{B}^m \ \bar{E}^m]^T$, $\tilde{G}^m = [0\epsilon^{-1}\bar{G}]^{m,T}$, and $\tilde{F}^m = [0\epsilon^{-1}\bar{J}_s^m]$ at time step m . Because $\bar{J}_s$ is on the surface, it does not contribute to Gauss' law and therefore does not break charge conservation.

4.3 Domain Decomposition

Consider the region Ω depicted in 4.5a that is divided into N_v non-overlapping subdomains where subdomain Ω_i and Ω_j are separated by boundary Γ_{ij} . The junction of more than two volumes is a "corner" denoted by Γ_c . In each subdomain Ω_i , (4.4) is defined and is assumed to be a self contained "primal" problem that has fictitious excitations from "dual" unknowns. The dual unknowns, the Lagrange multipliers denoted by Λ , effect either Neumann or robin boundary conditions such that the equivalence theorem can be applied for each Ω_i with respect to Ω using the external currents on $\partial\Omega_i$, the fictitious boundary current from Λ , and the particle current in Ω_i . By solving for the dual unknowns and a small subset of the primal unknowns, the overall computational cost of solving the original monolithic system in (4.4) is reduced.

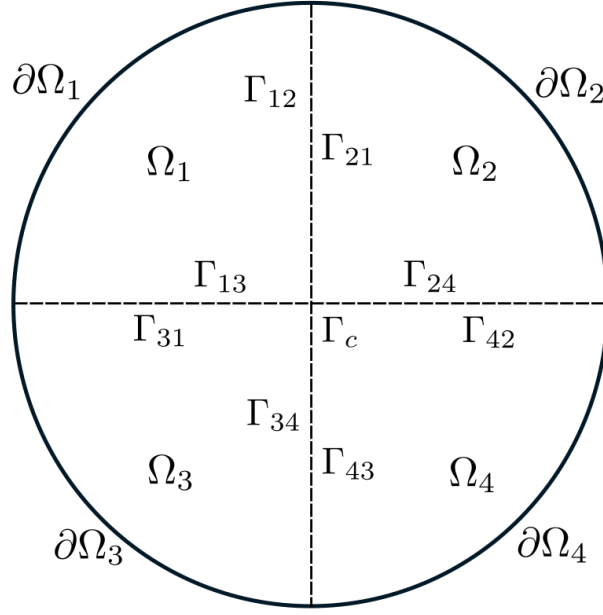


Figure 4.1: Region Ω partitioned into N_v subdomains.

4.3.1 MFEM-DP 1

The first formulation presented uses a Neumann-like boundary condition to enforce the continuity conditions of the fields at the interior boundaries,

$$\hat{n} \times \mathbf{E}_i(t, \mathbf{r}) = \hat{n} \times \mathbf{E}_j(t, \mathbf{r}) \quad \mathbf{r} \in \Gamma_{ij} \quad (4.5a)$$

$$\hat{n} \cdot \mathbf{B}_i(t, \mathbf{r}) = \hat{n} \cdot \mathbf{B}_j(t, \mathbf{r}) \quad \mathbf{r} \in \Gamma_{ij}. \quad (4.5b)$$

This is accomplished by ensuring $\mathbf{x}_i^n = \mathbf{x}_j^n|_{\Gamma_{ij}}$ and defining

$$\hat{n} \times \mathbf{H}_i(t, \mathbf{r}) = \Lambda(t, \mathbf{r}) \quad \mathbf{r} \in \Gamma_{ij}. \quad (4.6)$$

The system of equations to be solved in each sub-region

$$\left(0.5\bar{\bar{A}}_1 + 0.25\Delta_t\bar{\bar{A}}_0\right) \bar{X}^{n+1} = \mathcal{L} - \Lambda \in \Omega_i \quad (4.7)$$

where

$$\begin{aligned} \mathcal{L} = & 0.5\Delta_t\bar{\bar{A}}_0\bar{X}^n \\ & - \left(0.5\bar{\bar{A}}_1 + .25\Delta_t\bar{\bar{A}}_0\right) \bar{X}^{n-1} - 0.5\Delta_t\tilde{G}^{n+1} - 0.5\Delta_t\tilde{G}^{n-1} \\ & - 0.25\Delta_t\tilde{F}^{n+1} + 0.5\Delta_t\tilde{F}^n - 0.25\tilde{F}^{n-1}. \end{aligned} \quad (4.8)$$

This Lagrange multiplier is only Neumann-like because the time history of Lagrange multiplier is not kept, unlike the other currents in the system. Let the unknowns defined on Γ_c be denoted by the subscript c and all other unknowns in Ω_i denoted by subscript r , such that (4.7) can be written as

$$\begin{bmatrix} \bar{\bar{A}}_{rr}^{(i)} & \bar{\bar{A}}_{rc}^{(i)} \\ \bar{\bar{A}}_{cr}^{(i)} & \bar{\bar{A}}_{cc}^{(i)} \end{bmatrix} \begin{bmatrix} \bar{X}_r^{(i),n+1} \\ \bar{X}_c^{(i),n+1} \end{bmatrix} = \begin{bmatrix} \mathcal{L}_r^{(i)} \\ \mathcal{L}_c^{(i)} \end{bmatrix} - \begin{bmatrix} \bar{\Lambda}_r^{(i)} \\ \bar{\Lambda}_c^{(i)} \end{bmatrix} \in \Omega_i \quad (4.9)$$

where $\bar{\bar{A}} = .5\bar{\bar{A}}_1 + .25\Delta_t\bar{\bar{A}}_0$. The first set of equations can be rewritten as

$$\bar{X}_r^{(i),n+1} = \bar{\bar{A}}_{rr}^{(i),-1} (\mathcal{L}_r^{(i)} - \bar{\bar{A}}_{rc}^{(i),-1} \bar{X}_c^{(i),n+1} - \bar{\Lambda}_r^{(i)}) \quad (4.10)$$

which can be substituted into the second set of equations

$$\begin{aligned} \left(\bar{\bar{A}}_{cc}^{(i)} - \bar{\bar{A}}_{cr}^{(i),-1} \bar{\bar{A}}_{rr}^{(i),-1} \bar{\bar{A}}_{rc}^{(i)} \right) \bar{X}_c^{(i),n+1} &= \mathcal{L}_c^{(i)} \\ &- \bar{\bar{A}}_{cr}^{(i)} \bar{\bar{A}}_{rr}^{(i),-1} \left(\mathcal{L}_r^{(i)} - \bar{\Lambda}_r^{(i)} \right) - \bar{\Lambda}_c^{(i)}. \end{aligned} \quad (4.11)$$

Define a signed Boolean matrix $\bar{\bar{B}}_r^{(i)}$ that maps unknowns in Ω_i , excluding those on Γ_c , to a set of unique global unknowns defined on $\cup \Gamma_{ij}$. By defining $\sum_{i=1}^{N_v} \bar{\bar{B}}_r^{(i)} \bar{x}^{(i)} = 0$, it enforces (4.5a) and (4.5b). Furthermore, the transpose $\bar{\bar{B}}_r^{(i),T}$ forms a map from the global set of boundary unknowns to those of a particular volume. A similar unsigned Boolean matrix can be defined for unknowns that lie on Γ_c within Ω_i , $\bar{\bar{B}}_c$, which maps to a set of unique global unknowns. Using $\bar{\bar{B}}_r$ on (4.10) and summing over all volumes results in

$$\bar{\bar{K}}_{rr} \Lambda_r = \bar{\mathcal{L}}_r - \bar{\bar{K}}_{rc} \bar{X}_c \quad (4.12)$$

where

$$\bar{\bar{K}}_{rr} = \sum_{i=1}^{N_v} \bar{\bar{B}}_r \bar{\bar{A}}_{rr}^{(i)} \bar{\bar{B}}_r^{(i),T} \quad (4.13a)$$

$$\bar{\bar{K}}_{rc} = \sum_{i=1}^{N_v} \bar{\bar{B}}_r \bar{\bar{A}}_{rr}^{(i)} \bar{\bar{A}}_{rc}^{(i)} \bar{\bar{B}}_c^{(i),T} \quad (4.13b)$$

$$\bar{\mathcal{L}}_r = \sum_{i=1}^{N_v} \bar{\bar{B}}_r^{(i)} \bar{\bar{A}}_{rr}^{(i),-1} \mathcal{L}_r^{(i)} \quad (4.13c)$$

and $\bar{X}_c$ the degree of freedom vector for corner unknowns.

The boundary condition (4.5a) is enforced at the corners of Ω_i by defining $\sum_{i=1}^{N_v} \bar{B}_c^{(i),T} \lambda_c^{(i)} = 0$. Using that definition, (4.11) becomes

$$\bar{K}_{cc} \bar{X}_c^{n+1} = \bar{\mathcal{L}}_c + \bar{K}_{cr} \Lambda_r. \quad (4.14)$$

where

$$\bar{K}_{cc} = \sum_{i=1}^{N_v} \bar{B}_c^{(i)} (\bar{A}_{cc}^{(i)} - \bar{A}_{cr}^{(i),-1} \bar{A}_{rr}^{(i),-1} \bar{A}_{rc}^{(i),-1}) \bar{B}_c^{(i),T} \quad (4.15a)$$

$$\bar{K}_{cr} = \sum_{i=1}^{N_v} \bar{B}_c^{(i)} \bar{A}_{cr}^{(i)} \bar{A}_{rr}^{(i),-1} \bar{B}_r^{(i),T} \quad (4.15b)$$

$$\bar{\mathcal{L}}_c = \sum_{i=1}^{N_v} \bar{B}_c^{(i)} (\mathcal{L}_c^{(i)} - \bar{A}_{cr}^{(i)} \bar{A}_{rr}^{(i),-1} \mathcal{L}_r^{(i)}). \quad (4.15c)$$

Comparable to vector wave equation domain decomposition formulations, $\bar{K}_{cc}$ is sparse and generally much smaller than $\bar{K}_{rr}$. Therefore, if solving the boundary problem directly, it is possible to define

$$\bar{X}_c^{n+1} = \bar{K}_{cc}^{-1} (\bar{\mathcal{L}}_c + \bar{K}_{cr} \Lambda_r) \quad (4.16)$$

and then use substitution into (4.12) to yield

$$\bar{\mathcal{K}}_{rr} \Lambda_r = \bar{\mathcal{L}}_r - \bar{K}_{rc} \bar{K}_{cc}^{-1} \bar{\mathcal{L}}_c \quad (4.17)$$

where $\bar{\mathcal{K}}_{rr} = (\bar{K}_{rr} + \bar{K}_{rc} \bar{K}_{cc}^{-1} \bar{K}_{cr})$. If using an iterative solver, (4.12) and (4.14) can be solved as a coupled system instead.

4.3.2 MFETI-DP2

In the previous formulation, a unique Lagrange multiplier was defined for each edge and face on Γ . This formulation enforces field continuity through a Neumann-like boundary condition. Another way of enforcing field continuity would be to use a robin boundary condition. The boundaries between Ω_i and Ω_j , Γ_{ij} and Γ_{ji} , are distinct and have a unique

Lagrange multiplier defined for each subdomain. Instead of (4.6), the boundary condition on the Lagrange multipliers becomes

$$\Lambda^{(i)}(t, \mathbf{r}) = \hat{n}_i \times \mathbf{H}(t, \mathbf{r}) - \eta^{-1} \hat{n}_i \times \hat{n}_i \times \mathbf{E}(t, \mathbf{r}) \in \Gamma_{ij}. \quad (4.18)$$

The edges on Γ_{ij} , as well as the interior unknowns and unknowns on $\partial\Omega_i$ are included in a vector $\bar{X}_I^{(i)}$. The Lagrange multipliers for the corner edges remain the same, with a unique Lagrange multiplier for each feature. The faces on an Γ_{ij} are grouped together with the corner edges, which we will denote as $\bar{X}_N$. The system of equations solved in each subdomain is

$$\begin{bmatrix} \bar{A}_{II}^{(i)} & \bar{A}_{IN}^{(i)} \\ \bar{A}_{NI}^{(i)} & \bar{A}_{NN}^{(i)} \end{bmatrix} \begin{bmatrix} \bar{X}_I^{(i),n+1} \\ \bar{X}_N^{(i),n+1} \end{bmatrix} = \begin{bmatrix} \mathcal{R}_I^{(i)} \\ \mathcal{R}_N^{(i)} \end{bmatrix} - \begin{bmatrix} .5\Delta_t \bar{\Lambda}_I^{(i),n+1} \\ \bar{\Lambda}_N^{(i)} \end{bmatrix} \in \Omega_i \quad (4.19)$$

where given

$$\begin{aligned} \mathcal{R} &= .5\Delta_t \bar{\bar{A}}_0 \bar{X}^n \\ &- (.5\bar{\bar{A}}_1 + .25\Delta_t \bar{\bar{A}}_0) \bar{X}^{n-1} - .5\Delta_t \tilde{G}^{n+1} - .5\Delta_t \tilde{G}^{n-1} \\ &- .25\Delta_t \tilde{F}^{n+1} + .5\Delta_t \tilde{F}^n - .25\tilde{F}^{n-1} - .5\Delta_t \Lambda^n + .25\Lambda^{n-1}, \end{aligned} \quad (4.20)$$

$\mathcal{R}_I^{(i)}$ contains $\mathcal{R}$ associated with interior unknowns, external unknowns, and unknowns of edges on Γ_{ij} and $\mathcal{R}_N^{(i)}$ contain the remaining unknowns in subdomain Ω_i . To derive the set of equations to solve for the dual unknowns, first consider the summation of (4.18) for two volumes

$$\Lambda^{(i)}(t, \mathbf{r}) + \Lambda^{(j)}(t, \mathbf{r}) + (Y_i + Y_j) \hat{n}_i \times \hat{n}_i \times \mathbf{E}(t, \mathbf{r}). \quad (4.21)$$

Define an unsigned Boolean matrix such that $\bar{\bar{B}}_I^{(i)} \bar{X}_I = \bar{e}_I^{(i)}$, the unknowns for the electric field on Γ_{ij} . Also, define the map from the boundary edges on Γ_{ij} to its counterpart on Γ_{ji} , $\bar{T}_{ij}$. Testing (4.21) with curl-conforming basis functions $\mathbf{W}^e$, generalizing the case to any number of subdomains, and using $\bar{\bar{B}}_I^{(i)}$ and $\bar{T}_{ji}$ restrict and map the unknowns of Ω_j to Ω_i yields

$$\Lambda^{(i)} + \sum_{j \in \sigma(i)} \bar{T}_{ij} (\Lambda^{(j)} - (Y_i + Y_j) \bar{\bar{M}}_T^{(j)} \bar{\bar{B}}_I^{(j)} \bar{X}_I^{(j)}) = 0 \quad (4.22)$$

where $\sigma(i)$ are all subdomains Ω_j which share a boundary with Ω_i and the matrix $\bar{\bar{M}}_T^{(i)} \langle \hat{n} \times \mathbf{W}^e, \hat{n} \times \mathbf{W}^e \rangle|_{\Gamma_{ij}}$.

Rewrite the first set of equations in (4.19) as

$$\bar{X}_I^{(i),n+1} = \bar{\bar{A}}_{II}^{(i),-1} (\mathcal{R}_I^{(i)} - .5\Delta_t \bar{\Lambda}_I^{(i),n+1} - \bar{\bar{A}}_{IN}^{(i)} \bar{X}_N^{(i),n+1}) \quad (4.23)$$

Now, (4.23) can be plugged into (4.22) to yield

$$\begin{aligned} \Lambda^{(i)} + \sum_{j \in \sigma(i)} T_{ij} (\bar{I}^{(j)} - (Y_i + Y_j) \bar{\bar{M}}_T^{(j)} \bar{\bar{B}}_I^{(j)} \bar{\bar{A}}_{II}^{(j),-1} \bar{\bar{B}}_I^{(j),T}) \Lambda^{(j)} \\ = \sum_{j \in \sigma(i)} T_{ij} \bar{\bar{B}}_I^{(j)} \bar{\bar{A}}_{II}^{(j),-1} (\bar{\bar{A}}_{IN}^{(j)} \bar{\bar{B}}_N^{(j)} \bar{X}_N - \mathcal{R}_I). \end{aligned} \quad (4.24)$$

In order to complete the definition of the equation to solve for Λ_I over $\cup \Gamma_{ij}$, we first define the equation for $\bar{X}_N$, the unknowns associated with faces on Γ_{ij} and edges on Γ_c .

The derivation of the equation to solve for $\bar{X}_N$ follows a similar path as $\bar{X}_c$ from MFET-DP1. First, substitute (4.23) into the second set of equations in (4.22) to yield

$$\begin{aligned} (\bar{\bar{A}}_{NN}^{(i)} - \bar{\bar{A}}_{NI}^{(i),-1} \bar{\bar{A}}_{II}^{(i),-1} \bar{\bar{A}}_{IN}^{(i)}) \bar{X}_N^{(i),n+1} = \mathcal{L}_N^{(i)} \\ - \bar{\bar{A}}_{NI}^{(i)} \bar{\bar{A}}_{II}^{(i),-1} (\mathcal{L}_I^{(i)} - \bar{\Lambda}_I^{(i)}) - \bar{\Lambda}_N^{(i)}. \end{aligned} \quad (4.25)$$

The Boolean matrix $\bar{\bar{B}}_N^{(i)}$ is defined as

$$\bar{\bar{B}}_N^{(i)} = \begin{bmatrix} \bar{\bar{B}}_{r,f}^{(i)} & 0 \\ 0 & \bar{\bar{B}}_c^{(i)} \end{bmatrix} \quad (4.26)$$

to enforce (4.5b) for the faces on Ω_i and (4.5a) edges on corners where $\bar{\bar{B}}_{r,f}^{(i)}$ is the portion of $\bar{\bar{B}}_r^{(i)}$ that acts on the face degrees of freedom. Using a similar process as (4.14), the equation for

$$\bar{\bar{K}}_{NN} \bar{X}_N^{n+1} = \bar{\mathcal{R}}_N + \bar{\bar{K}}_{NI} \Lambda_I. \quad (4.27)$$

where

$$\bar{\bar{K}}_{NN} = \sum_{i=1}^{N_v} \bar{\bar{B}}_N^{(i)} (\bar{\bar{A}}_{NN}^{(i)} - \bar{\bar{A}}_{NI}^{(i)} \bar{\bar{A}}_{II}^{(i),-1} \bar{\bar{A}}_{IN}^{(i),-1}) \bar{\bar{B}}_N^{(i),T} \quad (4.28a)$$

$$\bar{\bar{K}}_{NI} = \sum_{i=1}^{N_v} \bar{\bar{B}}_N^{(i)} \bar{\bar{A}}_{NI}^{(i)} \bar{\bar{A}}_{II}^{(i),-1} \bar{\bar{B}}_I^{(i),T} \bar{\bar{B}}_L^{(i),T} \quad (4.28b)$$

$$\bar{\mathcal{R}}_N = \sum_{i=1}^{N_v} \bar{\bar{B}}_N^{(i)} (\mathcal{R}_N^{(i)} - \bar{\bar{A}}_{NI}^{(i)} \bar{\bar{A}}_{II}^{(i),-1} \mathcal{R}_I^{(i)}). \quad (4.28c)$$

The global system of equations for the edge Lagrange multipliers Define a Boolean matrix $\bar{\bar{B}}_L^{(i)}$ that maps the local Lagrange multipliers to a global vector. The Boolean matrix is applied to (4.24) and discretized in time to define the equation

$$\bar{\bar{K}}_{II} \Lambda_I = \bar{\mathcal{R}}_I - \bar{\bar{K}}_{IN} \bar{N}_N^{n+1} \quad (4.29)$$

where

$$\begin{aligned} \bar{\bar{K}}_{II} = \underline{I} + \sum_{i=1}^{N_v} \underline{B}_L^{(i)} \\ \sum_{j \in \sigma(i)} \bar{\bar{T}}_{ij} (\bar{\bar{I}}^{(j)} - \underline{M}_T^{(j)} \bar{\bar{B}}_I^{(j)} \bar{\bar{A}}_{II}^{(j),-1} \bar{\bar{B}}_I^{(j),T} \underline{B}_L^{(j),T} \end{aligned} \quad (4.30a)$$

$$\bar{\bar{K}}_{IN} = - \sum_{i=1}^{N_v} \underline{B}_L^{(i)} \sum_{j \in \sigma(i)} \underline{T}_{ji} \underline{M}_T^{(j)} \underline{B}_I^{(j)} \bar{\bar{A}}_{II}^{(j),-1} \bar{\bar{A}}_{IN} \underline{B}_N^{(j),T} \quad (4.30b)$$

$$\bar{\mathcal{R}}_I = - \sum_{i=1}^{N_v} \underline{B}_L^{(i)} \sum_{j \in \sigma(i)} \underline{T}_{ji} \bar{\bar{M}}_T \underline{B}_I^{(j)} \bar{\bar{A}}_{II}^{(j),-1} \mathcal{R}_I^{(i)} \quad (4.30c)$$

It can be solved as a coupled system with (4.27) or in a Schur complement system similar to (4.17) using

$$\bar{\bar{\mathcal{K}}}_{II} \Lambda_I = \bar{\mathcal{L}}_I - \bar{\bar{K}}_{IN} \bar{\bar{K}}_{NN}^{-1} \bar{\mathcal{L}}_N. \quad (4.31)$$

where $\bar{\bar{\mathcal{K}}}_{II} = \left(\bar{\bar{K}}_{II} - \bar{\bar{K}}_{IN} \bar{\bar{K}}_{NN}^{-1} \bar{\bar{K}}_{NI} \right)$. However, $\bar{\bar{K}}_{NN}$ is much larger than its MFETI-DP1 counterpart $\bar{\bar{K}}_{cc}$ and will take more time and memory to compute and store its inverse.

4.3.3 Discussion

The proposed domain decomposition formulations reduces the cost of solving for the fields by defining a set of equations on fictitious interior boundaries of the true problem.

Table 4.1: Average number of unknowns per volume and ratio of interior to boundary unknowns for different decompositions of Ω_{rect} .

N_v	MFETI-DP1		MFETI-DP2	
	avg unk.	$\frac{\text{int. unk.}}{\text{bnd. unk.}}$	avg unk.	$\frac{\text{int. unk.}}{\text{bnd. unk.}}$
2	1815	N/A	1755	6.75
5	776	1.71	705	1.00
10	404	0.60	351	0.34
25	170	0.15	133	0.08
50	89	0.05	60	0.03

The definitions of these equations uses small matrix inverses, and therefore are generally not sparse. Furthermore, those matrix inverses have to be stored in memory. At the very least, one matrix inverse for each subdomain is needed, making the memory storage more than solving for the original system. However, it is expected that for direct inverses, inverting either the coupled equations of (4.12) and (4.14) or (4.29) and (4.27) would be more efficient than solving the original problem. If storing the inverse of the matrix associated with Γ_c is possible, (4.17) and (4.31) are even smaller in size. The following discussion uses a sample problem to further probe properties of MFETI-DP1 and MFETI-DP2.

Define Ω_{rect} as a rectangular region in free space with dimension $.25 \text{ m} \times .2 \text{ m} \times .3 \text{ m}$ discretized with average edge length of 5.5 cm. The region is split into subdomains in several configurations listed in Table 4.1 so that MFETI-DP1 and MFETI-DP2 can be applied. Figure 4.3 shows the condition number of the matrix formed by the coupled equations (4.12) and (4.14) for MFETI-DP1, (4.29) and (4.27) for MFETI-DP2, as well as the Schur complement forms $\bar{\bar{\mathcal{K}}}_{rr}$ and $\bar{\bar{\mathcal{K}}}_{II}$ with different numbers of subdivisions compared to the condition number of the monolithic system matrix $\bar{\bar{A}}$. Solving the coupled equations results in condition number that are generally at or worse than the monolithic solve. Using the Schur complement results in condition numbers comparable to the monolithic solve for MFETI-DP1 and several orders of magnitude smaller for MFETI-DP2.

In the case of iterative solvers, MFETI-DP1 and MFETI-DP2 are shown to converge faster than the monolithic solve. Consider the case when Ω_{rect} is illuminated by an incident

field defined by

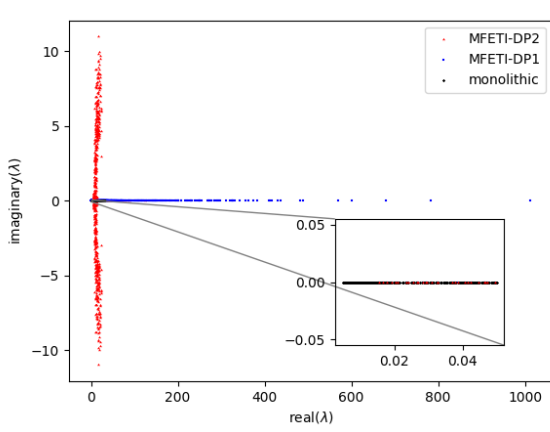
$$\bar{E}(\bar{r}, t) = \hat{y} \cos(2\pi f_0 \tau) e^{-(\tau-8\sigma)^2/2\sigma^2} \text{ (V/m)}. \quad (4.32)$$

The bandwidth of the modulated Gaussian is $\sigma = 3(\pi f_{bw})$, where the bandwidth $f_{bw} = f_{max} - f_0$ with maximum frequency $f_{max} = 500\text{MHz}$ and center frequency $f_0 = 300\text{MHz}$. The time step size is 0.333 ns which is ten times larger than what could be taken by a similar FDTD solver or leapfrog method for MFEM. Figure 4.4 shows the iteration counts for the coupled solves for MFETI-DP1 and MFETI-DP2 compared to the monolithic solve using GMRES with a tolerance of 10^{-6} and restarted after 20 iterations when Ω_{rect} is illuminated by an incident field. With a diagonal preconditioner, both domain decomposition approaches perform better than the monolithic solve, with MFETI-DP2 performing best overall.

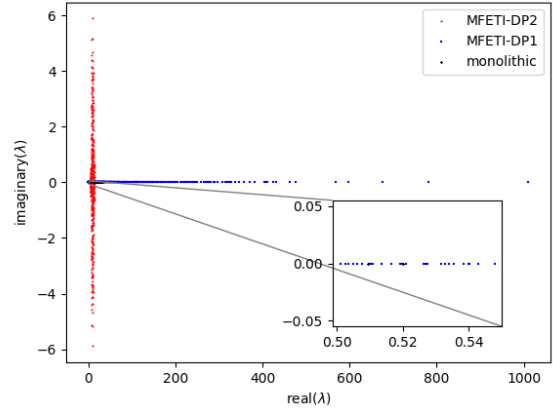
Finally, the eigenspectra of the different formulations are compared, which impact the stability of the time marching scheme. For the time marching scheme used in this work to be stable, the matrix used to evolve the system in time must have eigenvalues $\text{Re}(\lambda) \geq 0$ for the system to be unconditionally stable. Figure 4.2 shows that for solving both the coupled system and using the Schur complement approach, the domain decomposition methods will be stable. From the insert in the figures, the effect of using the schur complement shifts the eigenvalues of $\bar{\mathcal{K}}_{rr}$ and $\bar{\mathcal{K}}_{II}$ away from the imaginary axis, though MFETI-DP2 is shifted further away than MFETI-DP1.

4.4 Results

In this section, we present numerical results that show how the proposed algorithms perform compared to a non-DDM approach. Additionally, we will demonstrate that as the fields are equivalent, the overall trajectory of the particles are the same.



(a) MFETI-DP matrix eigenvalues.



(b) MFETI-DP matrix eigenvalues using Schur complement.

Figure 4.2: System matrix eigenvalues.

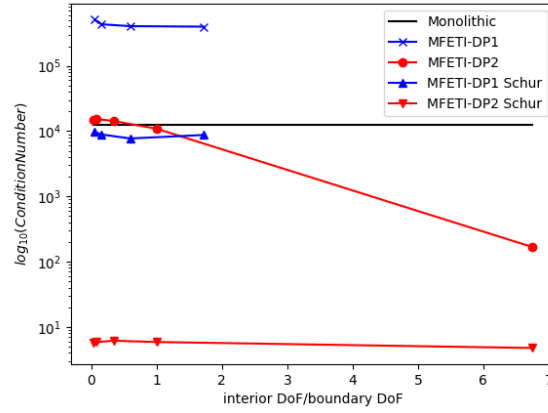


Figure 4.3: Condition number of system matrix.

4.4.1 Field Comparison

The first example shows performance of the methods and difference in the fields. In this example, a $0.25m \times 0.2m \times 1m$ box is illuminated an incident field defined by

$$\bar{E}(\vec{r}, t) = \hat{y} \cos(2\pi f_0 \tau) e^{-(\tau - 8\sigma)^2 / 2\sigma^2} \text{ (V/m)}. \quad (4.33)$$

The bandwidth of the modulated Gaussian is $\sigma = 3(\pi f_{bw})$, where the bandwidth $f_{bw} = f_{max} - f_0$ with maximum frequency $f_{max} = 595\text{MHz}$ and center frequency $f_0 = 295\text{MHz}$. The time step size $\delta_t = (150f_0)^{-1}$ and the experiment is run for 1500 time steps. The

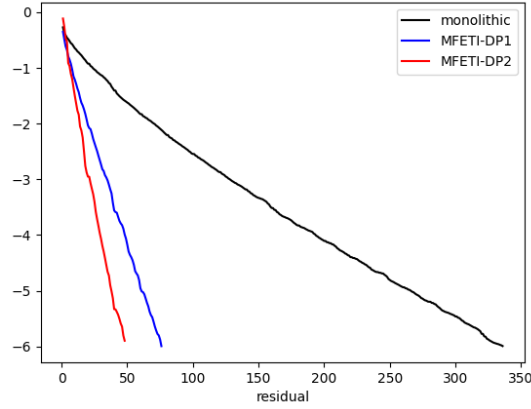
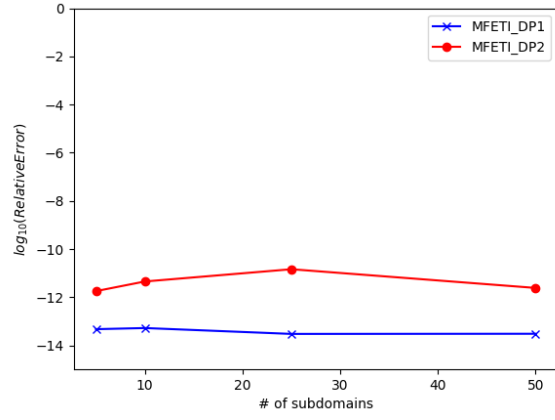


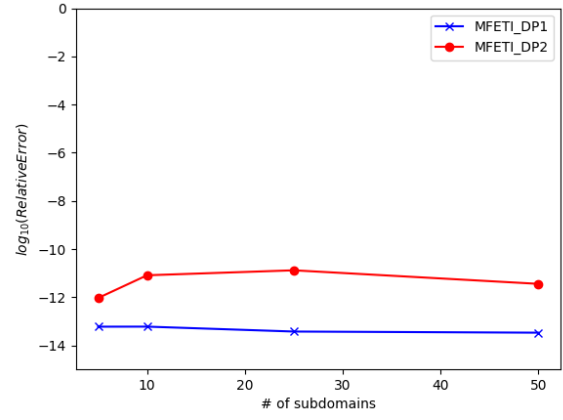
Figure 4.4: Convergence of history of GMRES for monolithic, MFETI-DP1, and MFETI-DP2.

boundary conditions on the external boundaries are robin boundary conditions. Three approaches are compared: monolithic (no DDM), MFETI-DP1, and MFETI-DP2 using three levels of discretization with average edge lengths of $h_1 = 5.20\text{cm}$, $h_2 = 3.63\text{cm}$, and $h_3 = 2.59\text{cm}$. The DDM meshes were split using METIS, such that no volumes have a regular shape. Figure 4.5, shows that the fields obtained through domain decomposition for edge lengths h_1 , h_2 , and h_3 respectively. Regardless of the number of subdivisions, the methods remain accurate to near machine precision with respect to the monolithic solve. This implies that using either domain decomposition formulation would cause the same acceleration on particles as the fields are the same.

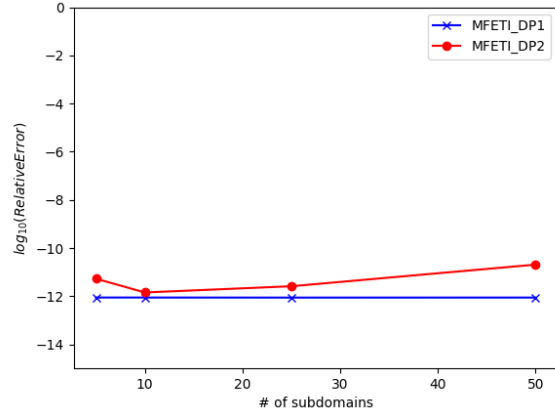
The next result demonstrates the effect of MFETI-DP on simulation time. As seen in Figure 4.6, both formulations are faster than the original monolithic solve for any number of subdivisions. However, there is an optimal ratio of interior volume unknowns to boundary unknowns for the fastest runtime. For each case, there is a crossover point at which further subdividing Ω incurs a cost in solving the boundary problem that is greater than the savings by reducing the unknowns in each volume.



(a) Geometry with average edge length h_1 .



(b) Geometry with average edge length h_2 .

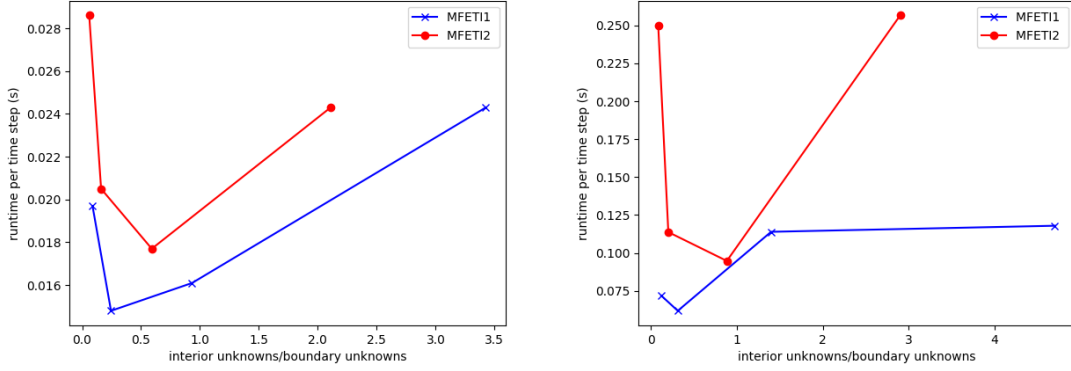


(c) Geometry with average edge length h_3 .

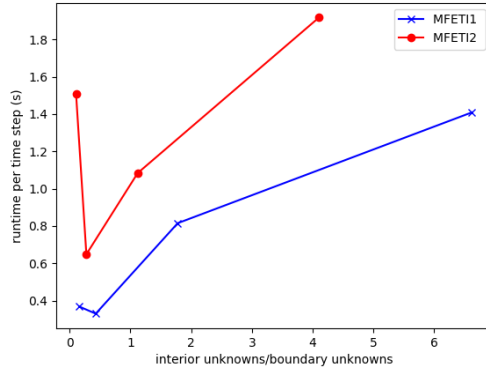
Figure 4.5: Relative error in electric field for MFETI-DP.

Table 4.2: Ratio of interior to boundary unknowns for different decompositions for particle beam test.

N_v	MFETI-DP1		MFETI-DP2	
	$\frac{\text{int. unk}}{\text{bnd. unk}}$	runtime (s)	$\frac{\text{int. unk}}{\text{bnd. unk}}$	runtime (s)
5	3.000	571.4	1.893	694.1
10	0.955	614.8	0.652	711.9
25	0.257	466.7	0.181	488.6
50	0.094	562.5	0.077	507.6



(a) Geometry with average edge length h_1 . (b) Geometry with average edge length h_2 .



(c) Geometry with average edge length h_3 .

Figure 4.6: Timing data for MFETI-DP.

4.4.2 Particle Beam

The next two examples demonstrate MFETI-DP1 and MFETI-DP2 with particles. In these experiments, the fields that are obtained through domain decomposition are used to push the particles, which are not subject to any decomposition scheme. The first example is a particle beam traveling through a cylindrical PEC cavity. This case is a standard test to show charge conservation as errors readily appear as striations in the particle distribution. Furthermore, approximate solutions can be used to further verify the result. The first test is done on a cavity that is 10 cm in length and 0.02 cm in radius discretized with an average edge length of 5 mm resulting in roughly 21K unknowns. The ten particles at each time step enter at the bottom face of the cavity with a radius of 8 mm. The beam voltage and

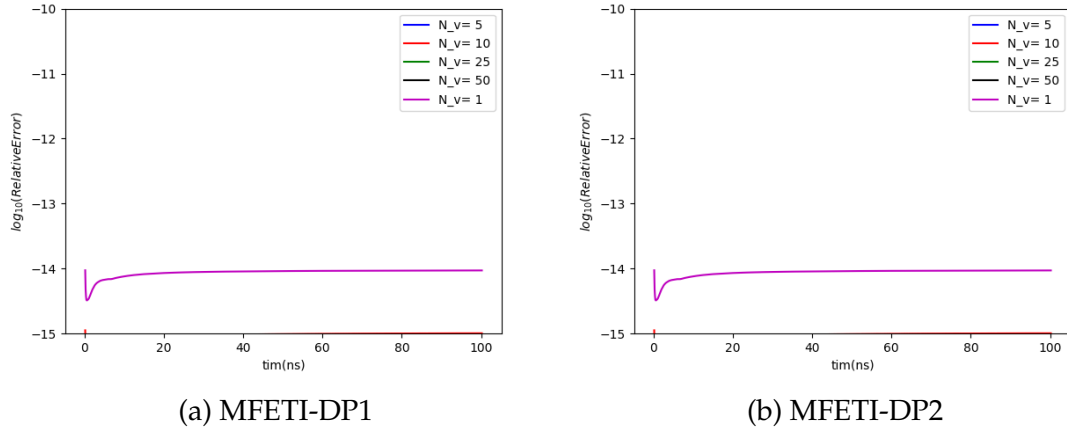
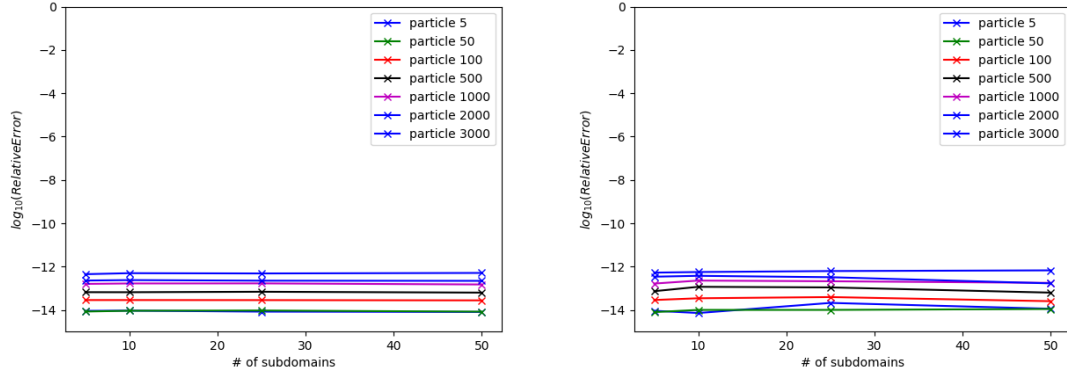


Figure 4.7: Error in Gauss' law for particle beam.

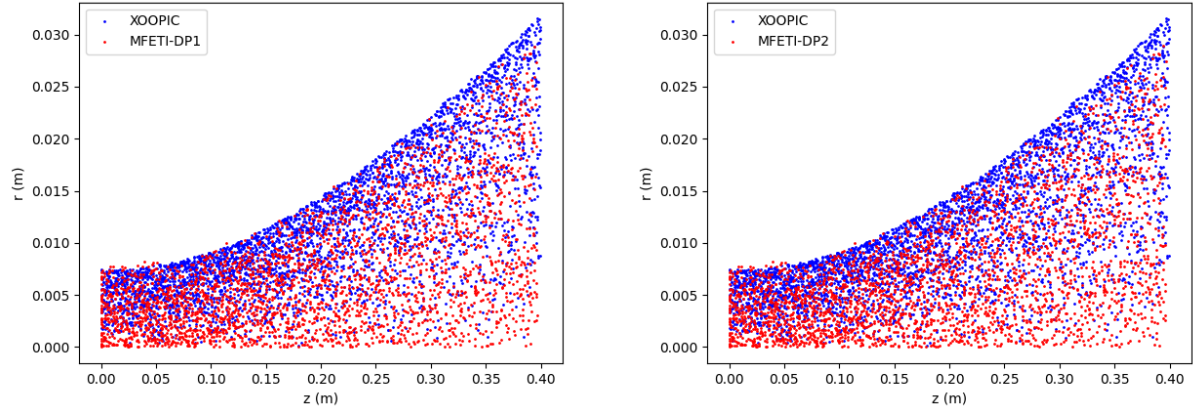
current are 500 V and 50 mA respectively, causing the an initial velocity 1.326×10^4 km/s. The geometry was subdivided in four configurations, the details of which are listed in Table 4.2. The experiment was run for 1000 time steps at a time step size of 1 ns, which for the monolithic case took 1,342 seconds. As shown in figure 4.7, all the simulations maintained charge conservation over the course of the run. There is no notable difference in the simulations, regardless of the number of subdivisions used. Seven particles were tracked over the course of the run to track the particle trajectories with the domain decomposition. Because the fields are virtually equivalent, the particle trajectories are consistent across the different geometries. Figure 4.8 shows the error in the tracked particles' path with respect to the path in the monolithic solve.

The next result was a particle beam in a larger PEC cavity. In this case, the PEC cylinder was 40 cm in length and 10 cm in radius. The geometry has an average edge length of 7.38 mm and a total of 218,059 unknowns. The beam voltage and current are 3.2 kV and 50 mA respectively, resulting in an initial velocity of 3.35×10^4 km/s. The experiment was run for both MFETI-DP1 and MFETI-DP2 using the iterative solver GMRES using a tolerance of 10^{-6} . The particle distribution is compared to a well-validated axisymmetric EM-FDTD PIC code, XOOPIC [170] and shows good agreement in Figure 4.9.



(a) Difference in particle path for MFETI-DP1. (b) Difference in particle path for MFETI-DP2.

Figure 4.8: Error in tracked particle positions.



(a) XOOPIC vs MFETI-DP1.

(b) XOOPIC vs MFETI-DP2.

Figure 4.9: Particle beam expansion for enlarged PEC cavity.

4.4.3 Plasma Ball

The last example presented is the case of an adiabatic expansion of a plasma ball. This example takes a considerable number of degrees of freedom to resolve the debye length and allow the particles to expand for an extended period of time. However, this can be made more tractable by using either domain decomposition schemes and unconditionally stable time marching to evolve the system with larger time steps than a similar EM-FDTD PIC formulation would allow. Additionally, this experiment has analytic solutions [87] that can be used for validation. A charge neutral, Gaussian distribution of 24000 particles is set at

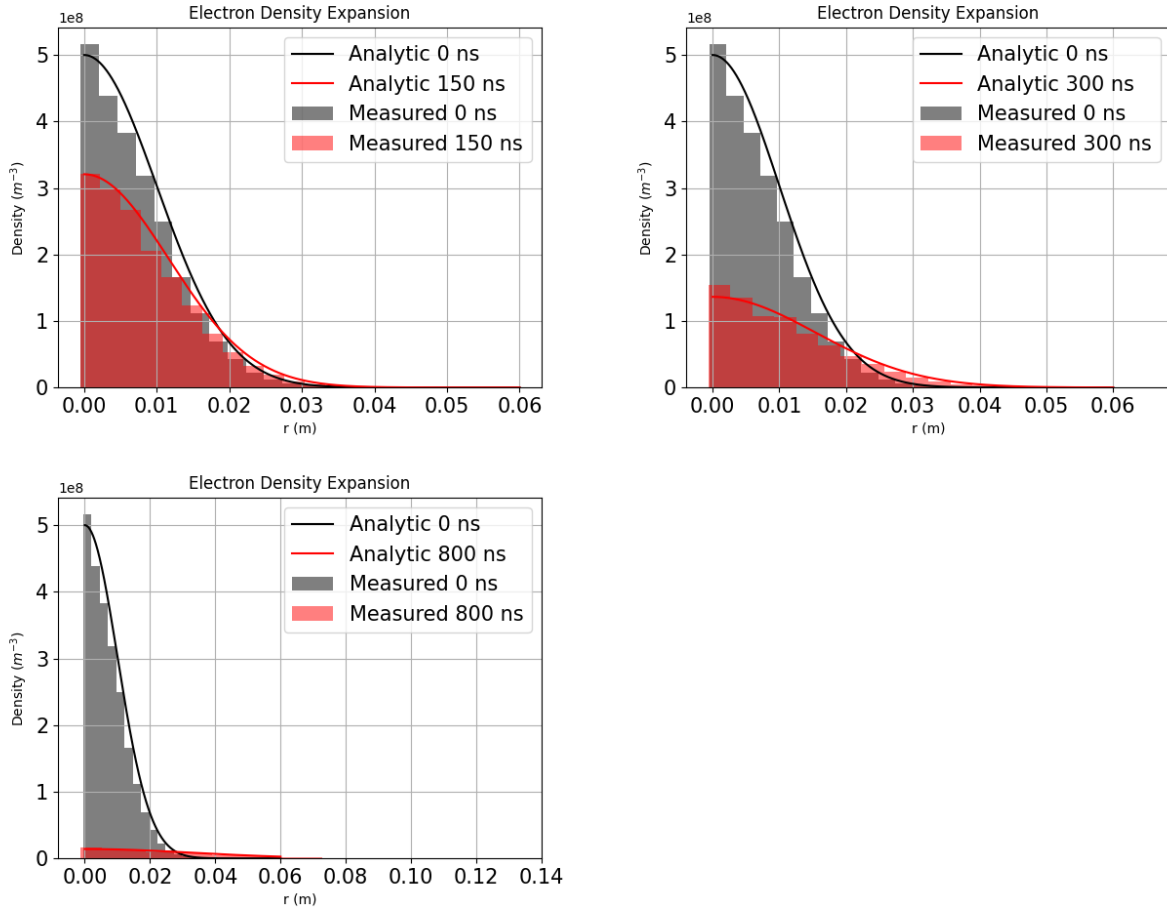


Figure 4.10: Adiabatic plasma ball expansion after 150, 300, and 800 ns.

the center of a spherical region 24 cm in diameter. The Sr^+ ions are at 1K and the electrons are at 100K with a density of 5×10^8 particles per cubic meter. The outer boundary has an impedance boundary condition and the boundary is sufficiently far from the particles that none leave during the simulation. The average edge length is 1 cm with a total of 681,214 unknowns. Figure 4.10 shows good agreement of the particle distribution with the analytic result at 150 ns, 300 ns, and 800 ns.

4.5 Summary

In this work, we presented two formulations for domain decomposition using non-overlapping subdomains for the mixed finite element method. The methods were used to create a MFETI-PIC scheme which allows for computing the fields due to particle motion

for larger problems. For sufficiently large problems, this results in time savings without loss of accuracy. All the results shown were computed on a single node; however, the method can be made parallel to take full advantage of high performance computing resources. Doing so suggest creating a domain decomposition framework for particle mapping and pushing consistent with the field solver.

Future work will focus on creating a qausi-helmholtz decomposition for the FETI-framework. This ensures that the nullspace of the field solver does not corrupt the satisfaction of charge conservation. This is a key issue for using the time domain vector wave equation approach which has a nullspace that grows linearly in time. The combination of domain decomposition and qausi-Helmholtz decomposition will allow for solving even larger problems as the number of degrees of freedom is reduced to those associated with edges, rather than have both edges and faces as presented here.

CHAPTER 5

CONCLUSION AND FUTURE WORK

The focus of this work is to define what is needed to create a charge conserving EM-FEMPIC schemes that are accurate and efficiently simulate large problems. These capabilities are needed to simulate real problems in a reasonable time frame.

The mathematics needed to conserve charge in an electromagnetic finite element particle-in-cell method were examined first. The rubrics provide a rationale behind the particular choice of basis functions in this work and the literature, as well as the needed insight to use other time marching schemes while satisfying all of Maxwell's equations. A connection was drawn between three Maxwell solver approaches: FDTD, EB-MFEM, and DH-MFEM. The insight in this chapter has been applied throughout this thesis, as well as in related works. Counterexamples were provided to show the consequences of failing to follow the rubrics. Examples also showed that the DH-based method yields results comparable to FDTD and EB-based EM-FEMPIC schemes.

Next, a charge conserving higher order EM-FEMPIC scheme was demonstrated. Whitney basis functions for nodes, edges, faces, and volumes were used to ensure both of Gauss' laws were satisfied. This is possible because they satisfy the de-Rham complex. The number of degrees of freedom needed to obtain a certain level of accuracy was shown to be reduced for higher order approaches. The results showed that the increased accuracy of the fields improved the accuracy of the particle trajectories.

Finally, two domain decomposition methods for Maxwell solvers were presented and applied to EM-FEMPIC. The two methods followed the finite element tearing and interconnect approach, utilizing both Neumann and Robin boundary conditions for the interior boundaries. The fields obtained by both approaches were shown to give the same fields as solving the system without the fictitious divisions. It was also demonstrated that both approaches decreased simulation time compared to the standard monolithic

approach. Results with particles showed that introducing the domain decomposition did not affect the satisfaction of Gauss' laws. Furthermore, as the fields obtained were the same as the original method, the particle trajectories remained unchanged while obtained in a shorter period of time.

Several challenges and advances remain with the work presented within this thesis. First, the techniques applied in the latter chapters for EB-based Maxwell solvers can be similarly applied for DH-based solvers. More work can be done to better understand the benefits and drawbacks between the two approaches. The impact of different particle shape functions on the methods presented in this work also remains an open topic. Though it does not affect charge conservation, other factors such as noise would be impacted which may influence the performance of designed devices.

However, the bulk of future work is built upon expanding on the domain decomposition techniques presented. The nullspaces of the proposed approaches should be studied more in depth. Furthermore, it inherently creates a multiply connected system that would benefit from an appropriate quasi-Helmholtz decomposition. Not only would it ensure that Gauss' law is satisfied exactly and not corrupted by any nullspace, it also enables using the vector wave equation as a field solver. This would further reduce the computational cost as the system of equations would no longer need to solve for the magnetic flux and it could be obtained through a forward calculation instead. Other preconditioning schemes and direct methods for domain decomposition are also highly desirable.

APPENDICES

APPENDIX A

UNCONDITIONALLY STABLE TIME STEPPING METHOD FOR MIXED FINITE ELEMENT MAXWELL SOLVERS

A.1 Introduction

Efficient solutions to Maxwell's equations is of significant interest to problems in fields ranging from microwave engineering to optics to radar to remote sensing to plasma physics [84, 145, 59, 92, 136]. As a result, it has seen extensive development over the past four decades. So much so that there exist reliable commercial simulators that are trusted for design and analysis; to wit, most microwave engineering and antenna design is carried out on a laptop before being fabricated and tested. Despite these advances, there are a number of open problems and challenges, largely brought on by our desire to improve the fidelity of simulation for increasingly complex geometric and material layouts. Adding temporal dimension to the analysis increases the challenges as well. The methods used for solution to Maxwell's equations are based either on differential or integral equations; this paper will focus on the former.

Over the years, differential equation based methods have become the mainstay of computational electromagnetic tools; starting with the classical Yee-algorithm for direct discretization of Maxwell's equations [189] to finite element methods (FEMs) [29, 93]. A number of challenges had to be overcome to make FEMs robust and viable for use in design and analysis of systems [114, 83]. Over the years, research on FEM has focused on developing methods so as to increase the accuracy and reduce computational costs; these include higher order interpolatory basis functions [71], higher order hierarchical basis sets [70], and domain decomposition methods [94]. These techniques have largely been applied to solving the vector wave equation in the frequency domain. In the time

domain, the temporal discretization follows a Newmark-Beta prescription [66, 144]. With the right choice of parameters, it has been shown that this prescription is unconditionally stable. The time step size is not intimately tied to the smallest mesh feature, but chosen to capture the physics to a prescribed order. However, the solutions to the vector wave equation are prone to inaccuracies arising from a non-trivial null space that corresponds to a function of the form $t\nabla\phi(\vec{r})$, where $\phi(\vec{r})$ is a scalar function of space.

There has been an effort to use finite elements to directly solve Maxwell's equations [20, 85, 182], *albeit* less so than vector wave formulations. These methods follow the prescription of the Yee-algorithm. Faraday's and Ampere's law are staggered in time leading to a leap frog time stepping. As a result, they do not have a time-growing null space, are conditionally stable, and energy conserving. Unfortunately, the time step size depends on the size of the features of the mesh and materials defined within it. The resulting time step sizes are very small, significantly more so than needed to represent content at the highest frequency. This is in contrast to the state of the art of solving the vector wave equation.

It would be ideal if one could render TD-MFEM provably unconditionally stable (it would enable reaping the advances made for vector wave equation FEM solvers). Earlier work has analyzed the stability for leapfrog time stepping in TD-MFEM [142]. Likewise, unconditionally stable time stepping schemes have been used in TD-MFEM, but without any rigorous analysis to prove stability [3]. In this work, we will prove that using Newmark-Beta method for TD-MFEM can produce unconditionally stable time stepping schemes that are up to second order accurate in time. With the correct choice in parameters, the time stepping schemes are shown to be energy conserving and non-dissipative. Furthermore, these properties hold for higher-order spatial basis functions used to discretize TD-MFEM. Thus, the specific contributions of this work are (i) a general framework for creating time stepping schemes of up to second order for the TD-MFEM of arbitrary spatial order, (ii) proof of stability for different boundary conditions and error analysis for the time stepping

scheme, (iii) analysis of the null space of the discrete system, and (iv) numerical results that verifying the analytic proofs.

The rest of the paper is organized as follows: Section A.2 describes the general problem. Section A.3 presents the spatial and temporal discretization of Maxwell's equations. The section contrasts the Newmark-Beta method to the leapfrog method and provides stability and error analysis of the Newmark-Beta method applied to the MFEM. Section A.4 presents several numerical results verifying properties discussed in previous sections and the overall efficacy of the method. Finally, conclusion and other remarks are provided in Section A.5.

A.2 Problem Statement

Consider the volume $\Omega \in \mathbb{R}^3$ bounded by Γ shown in figure A.1. In this domain, assume the region has homogeneous, isotropic, and time-independent constitutive parameters, denoted by ε (F/m) for the permittivity and μ (H/m) for the permeability. Assume that

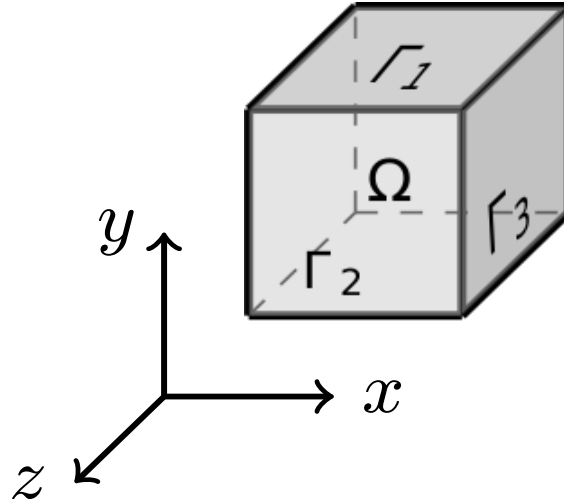


Figure A.1: Sample Volume Ω with Different Boundary Conditions

the volume is source free, being free of impressed charges or currents. The magnetic field $\vec{H}(\vec{r}, t)$ (A/m) and electric flux density $\vec{D}(\vec{r}, t)$ (C/m²) are defined in terms of the magnetic flux density $\vec{B}(\vec{r}, t)$ (Wb/m²) and electric field $\vec{E}(\vec{r}, t)$ (V/m), respectively, through

the constitutive parameters such that

$$\bar{H}(\bar{r}, t) = \mu^{-1} \bar{B}(\bar{r}, t) \quad (\text{A.1a})$$

$$\bar{D}(\bar{r}, t) = \varepsilon \bar{E}(\bar{r}, t). \quad (\text{A.1b})$$

The electric field and magnetic flux density are governed by Maxwell's equations

$$\begin{aligned} \frac{\partial \bar{B}(\bar{r}, t)}{\partial t} &= -\nabla \times \bar{E}(\bar{r}, t) \\ \frac{\partial \varepsilon \bar{E}(\bar{r}, t)}{\partial t} &= \nabla \times \frac{\bar{B}(\bar{r}, t)}{\mu} \\ \nabla \cdot (\varepsilon \bar{E}(\bar{r}, t)) &= 0 \\ \nabla \cdot \bar{B}(\bar{r}, t) &= 0. \end{aligned} \quad (\text{A.2})$$

The boundary Γ may be partitioned into several subdomains, Γ_i , such that $\Gamma := \cup_i \Gamma_i$. Each Γ_i has a boundary condition, either Dirichlet (Γ_D), Neumann (Γ_N), or impedance (Γ_I) [83].

The boundary conditions are defined as

$$\hat{n} \times \bar{E}(\bar{r}, t) = \Psi_D(\bar{r}, t) \quad \text{on } \Gamma_D \quad (\text{A.3a})$$

$$\hat{n} \times \frac{\bar{B}(\bar{r}, t)}{\mu} = \Psi_N(\bar{r}, t) \quad \text{on } \Gamma_N \quad (\text{A.3b})$$

$$\hat{n} \times \frac{\bar{B}(\bar{r}, t)}{\mu} - Y \hat{n} \times \hat{n} \times \bar{E}(\bar{r}, t) = \Psi_I(\bar{r}, t) \quad \text{on } \Gamma_I \quad (\text{A.3c})$$

where $Y = \sqrt{\varepsilon/\mu}$ (Ω) is the surface admittance. The functions $\Psi_D(\bar{r}, t)$, $\Psi_N(\bar{r}, t)$, and $\Psi_I(\bar{r}, t)$ represent some arbitrary function that is defined by the user. Additionally, we assume initial conditions on the fields, $\bar{E}(\mathbf{r}, 0)$ and $\bar{B}(\mathbf{r}, 0)$, satisfy (A.2).

A.3 MFEM Formulation

A.3.1 Variational Formulation

Solutions to (A.2) are found by creating variational equations with appropriate function spaces. The suitable function space for the electric field is the Hilbert space

$$H(curl; \Omega) = \{\bar{u} \in \bar{L}^2(\Omega); \nabla \times \bar{u} \in \bar{L}^2(\Omega)\}, \quad (\text{A.4})$$

which ensures that the tangential component of the field are continuous across tetrahedral faces. Likewise, the Hilbert space

$$H(div; \Omega) = \{\bar{u} \in \bar{L}^2(\Omega); \nabla \cdot \bar{u} \in L^2(\Omega)\} \quad (\text{A.5})$$

is used for the magnetic flux density, which permits functions that have normal continuity across tetrahedral faces. The Whitney edge basis function and Whitney face basis function reside in $H(curl; \Omega)$ and $H(div; \Omega)$, respectively, and can be used to discretize the fields [20]. The variational equations are formed by taking inner products of Faraday's law with the Whitney face basis function $\bar{B}^*$ and Ampere's law with the Whitney edge basis function $\bar{E}^*$ such that

$$\int d\Omega \frac{1}{\mu} \frac{\partial}{\partial t} \bar{B} \cdot \bar{B}^* = - \int d\Omega \frac{1}{\mu} \nabla \times \bar{E} \cdot \bar{B}^*, \quad (\text{A.6a})$$

$$\int d\Omega \varepsilon \frac{\partial}{\partial t} \bar{E} \cdot \bar{E}^* = \int d\Omega \nabla \times \frac{1}{\mu} \bar{B} \cdot \bar{E}^*. \quad (\text{A.6b})$$

A.3.2 Spatial Discretization

The spatial discretization is obtained by applying Galerkin's method to the variational equations. As previously stated, Whitney edge and face elements as seen in [20] define the lowest order representation of $\bar{E}^*$ and $\bar{B}^*$. The electric field is represented using Whitney edge elements and the magnetic flux using Whitney face elements such that

$$\bar{E}(\bar{r}, t) = \sum_{i=1}^{N_e} e_i(t) \bar{W}_i^1(\bar{r}), \quad \bar{B}(\bar{r}, t) = \sum_{i=1}^{N_f} b_i(t) \bar{W}_i^2(\bar{r}), \quad (\text{A.7})$$

where N_e is the number of edges and N_f is the number of faces. It is natural to use higher order basis function for more accuracy. We use the interpolatory higher order basis functions defined in [71] for Whitney edge elements and for Whitney face elements defined in [70]. We define vectors $\bar{e} = [e_1(t), e_2(t), \dots, e_{N_e}(t)]^T$ and $\bar{b} = [b_1(t), b_2(t), \dots, b_{N_f}(t)]^T$ that have the degrees of freedom $e_i(t)$ and $b_i(t)$ as elements. Using the defined expansion for the field and flux quantities, applying the Galerkin method to (A.6) yields the semi-discrete

Maxwell's equations

$$\begin{aligned}\frac{\partial \mathbf{M}_{\mu^{-1}} \bar{b}}{dt} &= -\mathbf{M}_c \bar{e} \\ \frac{\partial \mathbf{M}_\varepsilon \bar{e}}{dt} &= \mathbf{M}_c^T \bar{b} - \mathbf{M}_I \bar{e} + \bar{j}_N + \bar{j}_I.\end{aligned}\tag{A.8}$$

Here matrices are defined as

$$[\mathbf{M}_\varepsilon]_{i,j} = \int_{\Omega} d\Omega \varepsilon \bar{W}_i^1(\bar{r}) \cdot \bar{W}_j^1(\bar{r}),\tag{A.9a}$$

$$[\mathbf{M}_{\mu^{-1}}]_{i,j} = \int_{\Omega} d\Omega \frac{1}{\mu} \bar{W}_i^2(\bar{r}) \cdot \bar{W}_j^2(\bar{r}),\tag{A.9b}$$

$$[\mathbf{M}_c]_{i,j} = \int_{\Omega} d\Omega \frac{1}{\mu} \bar{W}_i^2(\bar{r}) \cdot \nabla \times \bar{W}_j^1(\bar{r}),\tag{A.9c}$$

$$[\mathbf{M}_c^T]_{i,j} = \int_{\Omega} d\Omega \frac{1}{\mu} \bar{W}_j^2(\bar{r}) \cdot \nabla \times \bar{W}_i^1(\bar{r}),\tag{A.9d}$$

$$[\mathbf{M}_I]_{i,j} = \int_{\Gamma_I} d\Gamma_Y \hat{n} \times \bar{W}_i^1(\bar{r}) \cdot \hat{n} \times \bar{W}_j^1(\bar{r}).\tag{A.9e}$$

The elements of the coefficient vectors $\bar{j}_N$ and $\bar{j}_I$ defined as

$$\begin{aligned}[\bar{j}_N]_i(t) &= \int_{\Gamma_N} d\Gamma_N \bar{W}_i^1(\bar{r}) \cdot \Psi_N(\bar{r}, t) \\ [\bar{j}_I]_i(t) &= \int_{\Gamma_I} d\Gamma_I \bar{W}_i^1(\bar{r}) \cdot \Psi_I(\bar{r}, t)\end{aligned}\tag{A.10}$$

and represent the boundary current due to Neumann and impedance boundary conditions.

Another interpretation of the TD-MFEM is through discrete exterior calculus. The Galerkin discrete Hodge matrices $\mathbf{M}_\varepsilon$ and $\mathbf{M}_{\mu^{-1}}$ are defined as [157]. The discrete curl operator $\mathbf{D}_c$ is defined as

$$\mathbf{D}_c = \frac{1}{\mu} \mathbf{M}_{\mu^{-1}}^{-1} \mathbf{M}_c.\tag{A.11}$$

The discrete curl operator and its transpose for the lowest order maps edges of a tetrahedron to the faces it bounds, as well as preserves the direction of the curl on that face [158]. This follows from the concept of the exterior derivative in the generalized Stokes theorem from exterior calculus. Equation (A.11) holds for all orders, however only has a simple mapping of faces to edges for the lowest order.

A.3.3 Temporal Discretization

The semi-discrete Maxwell's equations, derived in the previous section, are fully discretized by choosing an appropriate temporal discretization. Discretization schemes exist that solve the electric field and magnetic flux density concurrently or in a staggered fashion. In a staggered scheme, the solutions to Faraday's law and Ampere's law lie at different time steps, which allows a different time stepping method for each equation. A concurrent time stepping scheme couples the equations into a single system, written in the form

$$\begin{bmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{M}_\epsilon \end{bmatrix} \begin{bmatrix} \partial_t \bar{b} \\ \partial_t \bar{e} \end{bmatrix} + \begin{bmatrix} 0 & \mathbf{D}_c \\ -\mathbf{D}_c^T \mathbf{M}_{\mu^{-1}} & \mathbf{M}_I \end{bmatrix} \begin{bmatrix} \bar{b} \\ \bar{e} \end{bmatrix} = \begin{bmatrix} 0 \\ \bar{j}_N + \bar{j}_I \end{bmatrix}, \quad (\text{A.12})$$

where $\mathbf{I}$ is the identity matrix. The single time derivative allows for the choice of a single time stepping scheme and implies the solved quantities lie at the same time step. The following subsections discuss the leapfrog method (for sake of completeness) and the Newmark-Beta method and their applications to finding solutions to the semi-discrete Maxwell's equations. Note, that time step sizes for leapfrog ($\Delta_{t,LF}$) and Newmark-Beta ($\Delta_{t,N\beta}$) will be different.

A.3.3.1 Leapfrog Method

In the leapfrog method, the time derivatives in Faraday's law and Ampere's law are discretized using central finite differences staggered at half-time step intervals. Applying this to (A.8) yields

$$\bar{b}^{n+\frac{1}{2}} = \bar{b}^{n-\frac{1}{2}} - \Delta_{t,LF} \mathbf{D}_c \bar{e}^n \quad (\text{A.13a})$$

$$(\mathbf{M}_\epsilon + \mathbf{M}_I) \bar{e}^{n+1} = \mathbf{M}_\epsilon \bar{e}^n + \Delta_{t,LF} \mathbf{D}_c^T \mathbf{M}_{\mu^{-1}} \bar{b}^{n+\frac{1}{2}} + \Delta_{t,LF} (\bar{j}_N^{n+\frac{1}{2}} + \bar{j}_I^{n+\frac{1}{2}}). \quad (\text{A.13b})$$

The time stepping scheme consists of an explicit update in Faraday's law and a matrix inversion in Ampere's law as the Galerkin Hodge matrix is sparse, but not diagonal. It is

conditionally stable [65, 176] provided time step size satisfies

$$\Delta_{t,LF} \leq \frac{2}{\sqrt{\rho(\mathbf{M}_\epsilon^{-1} \mathbf{D}_c^T \mathbf{M}_{\mu^{-1}} \mathbf{D}_c)}}. \quad (\text{A.14})$$

When the time step size satisfies the stability requirement, the time stepping scheme also conserves energy. The mesh that discretizes the volume Ω determines the maximum time step size. The spectral radius of the matrices tends to grow as elements in the mesh shrink, limiting the time step size in relation to the maximum frequency the mesh could resolve.

A.3.3.2 Spectral radius

One drawback of this time-stepping scheme is that its stability is tied to the discretization of the mesh and the dielectric and magnetic material within Ω . As the electrical size of the elements shrink, so does the maximum time step size, regardless of coarser features of the mesh.

Table A.1: Leapfrog maximum time-step vs mesh edge lengths

λ_{max}	$c\Delta_{t,LF}$	h_{max}	h_{avg}	h_{min}
1.0587E+03	6.1468E-02	5.0000E-01	3.2400E-01	1.9376E-01
2.5661E+03	3.9481E-02	3.2773E-01	2.1477E-01	1.3689E-01
6.4293E+03	2.4943E-02	2.2165E-01	1.4365E-01	7.8437E-02
9.8165E+03	2.0186E-02	1.6865E-01	1.0925E-01	5.7826E-02
1.2769E+02	1.7699E-01	1.4142E+00	1.0424E+00	8.5782E-01
2.3979E+02	1.2916E-01	1.5326E+00	8.8836E-01	4.2409E-01
1.4249E+03	5.2983E-02	1.4142E+00	5.6001E-01	1.8142E-01
1.1535E+04	1.8622E-02	1.4142E+00	2.2648E-01	6.2023E-02

In Table A.1, the relationship between the edge lengths h , spectral radius λ_{max} , and time step sizes $\Delta_{t,LF}$ for the leapfrog scheme are presented. The spectral radius increases as the edge lengths shrink, resulting in a smaller maximum time step. Instead, it is preferred that time step is dictated by the bandwidth of the signals present in the simulation. In the results, it will show that the spatial errors tend to dominate error far more than temporal error, especially for the lowest order spatial basis functions.

A.3.3.3 Newmark-Beta

The Newmark-Beta method is a concurrent time stepping method to solve second order differential equations [125, 183], and is a popular method of choice for solving TD-FEM. To begin, the first order differential equation from (A.12) is recast as a second order differential equation,

$$\mathbf{A}_2 \partial_t^2 \bar{\mathbf{u}} + \mathbf{A}_1 \partial_t \bar{\mathbf{u}} + \mathbf{A}_0 \bar{\mathbf{u}} + \bar{\mathbf{f}} = 0, \quad (\text{A.15})$$

where

$$\bar{\mathbf{u}} = \begin{bmatrix} \bar{\mathbf{b}} \\ \bar{\mathbf{e}} \end{bmatrix}, \quad \bar{\mathbf{f}} = \begin{bmatrix} 0 \\ -(\bar{\mathbf{j}}_I + \bar{\mathbf{j}}_N) \end{bmatrix}, \quad (\text{A.16})$$

$$\mathbf{A}_2 = 0, \quad \mathbf{A}_1 = \begin{bmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{M}_\varepsilon \end{bmatrix}, \quad \mathbf{A}_0 = \begin{bmatrix} 0 & \mathbf{D}_c \\ -\mathbf{D}_c^T \mathbf{M}_\mu^{-1} & \mathbf{M}_I \end{bmatrix}.$$

Applying a 1-dimensional finite element method in time and identifying particular weights in the formulation results in a three-step recurrence relation that uses two parameters to yield different accuracy and stability properties [191]. The three-step recurrence relation for (A.16) is defined as

$$\begin{aligned} & [\gamma \mathbf{A}_1 + \beta \Delta_{t,N\beta} \mathbf{A}_0] \bar{\mathbf{u}}^{n+1} \\ & + [(1 - 2\gamma) \mathbf{A}_1 + (\frac{1}{2} + \gamma - 2\beta) \Delta_{t,N\beta} \mathbf{A}_0] \bar{\mathbf{u}}^n \\ & + [(\gamma - 1) \mathbf{A}_1 + (\frac{1}{2} - \gamma + \beta) \Delta_{t,N\beta} \mathbf{A}_0] \bar{\mathbf{u}}^{n-1} \\ & + (\beta \Delta_{t,N\beta}) \bar{\mathbf{f}}^{n+1} + (\frac{1}{2} + \gamma - 2\beta) \Delta_{t,N\beta} \bar{\mathbf{f}}^n + (\frac{1}{2} - \gamma + \beta) \Delta_{t,N\beta} \bar{\mathbf{f}}^{n-1} = 0 \end{aligned} \quad (\text{A.17})$$

which has the degrees of freedom for the electric field and magnetic flux density at the same timestep. The parameters γ and β affect the accuracy and stability properties. The following sections prove and demonstrate that with appropriate choice of parameters, the TD-MFEM system with Dirichlet, Neumann, and impedance boundary conditions is not only unconditionally stable, but also energy conserving.

A.3.4 Stability Analysis

In order to determine the stability of the Newmark-Beta time-stepping scheme, the zero-input response of the system is examined using a z-transform. For the system to be stable, the roots of the z-transformed scheme must lie on or within the unit circle in the complex plane. The spectral theorem is used on (A.17) such that the matrix $\mathbf{A}_1^{-1}\mathbf{A}_0$ is replaced by its eigenvalue λ [83, 192]. Taking the z-transform yields the quadratic equation

$$\begin{aligned} & \left([\gamma + \beta\Delta_{t,N\beta}\lambda]z^2 + [(1 - 2\gamma) + (\frac{1}{2} + \gamma - 2\beta)\Delta_{t,N\beta}\lambda]z \right. \\ & \left. + [(\gamma - 1) + (\frac{1}{2} - \gamma + \beta)\Delta_{t,N\beta}\lambda] \right) \bar{u}(z) = 0 \end{aligned} \quad (\text{A.18})$$

with zeros

$$z = \frac{1 - 2\gamma + (1/2 + \gamma - 2\beta)\Delta_{t,N\beta}\lambda}{2\gamma + 2\beta\Delta_{t,N\beta}\lambda} \pm \frac{\sqrt{1 + (1 - 2\gamma)\Delta_{t,N\beta}\lambda + [(1/2 + \gamma)^2 - 4\beta](\Delta_{t,N\beta}\lambda)^2}}{2\gamma + 2\beta\Delta_{t,N\beta}\lambda}. \quad (\text{A.19})$$

The parameters γ and β must be chosen to have the desired accuracy and stability characteristics for a given time step of size $\Delta_{t,N\beta}$. For a time stepping scheme to be unconditionally stable, $|z| \leq 1$ for all $\Delta_{t,N\beta}$. This leaves the characterization of the eigenvalue λ of the coupled Maxwell system, which will be shown to have a nonnegative real part.

A.3.4.1 Eigenanalysis of System with Dirichlet and Impedance Boundary Conditions

The zeros of the stability equation values depend on the parameters γ and β , the time step size $\Delta_{t,N\beta}$, and the eigenvalues of the matrix system. First, consider a system with no impedance boundary conditions. The coupled Maxwell system can be analyzed by forming the generalized eigenvalue system

$$\mathbf{A}_1^{-1}\mathbf{A}_0 \begin{bmatrix} \bar{b} \\ \bar{e} \end{bmatrix} = \begin{bmatrix} 0 & \mathbf{D}_c \\ -\mathbf{M}_\varepsilon^{-1}\mathbf{D}_c^T\mathbf{M}_{\mu^{-1}} & 0 \end{bmatrix} \begin{bmatrix} \bar{b} \\ \bar{e} \end{bmatrix} = \lambda \begin{bmatrix} \bar{b} \\ \bar{e} \end{bmatrix}, \quad (\text{A.20})$$

which leads to

$$\mathbf{D}_c \bar{e} = \lambda \bar{b}, \quad (\text{A.21a})$$

$$-\mathbf{M}_\varepsilon^{-1}\mathbf{D}_c^T\mathbf{M}_{\mu^{-1}}\bar{\mathbf{b}} = \lambda\bar{\mathbf{e}}. \quad (\text{A.21b})$$

It follows that

$$\mathbf{D}_c\mathbf{M}_\varepsilon^{-1}\mathbf{D}_c^T\mathbf{M}_{\mu^{-1}}\bar{\mathbf{b}} = -\lambda^2\bar{\mathbf{b}} = \Lambda\bar{\mathbf{b}} \quad (\text{A.22a})$$

$$\mathbf{M}_\varepsilon^{-1}\mathbf{D}_c^T\mathbf{M}_{\mu^{-1}}\mathbf{D}_c\bar{\mathbf{e}} = -\lambda^2\bar{\mathbf{e}} = \Lambda\bar{\mathbf{e}}. \quad (\text{A.22b})$$

The eigenvalues λ of the system matrix $\mathbf{A}_1^{-1}\mathbf{A}_0$ are purely imaginary when there are no impedance boundary conditions. This fact can be used to simplify (A.19) to find values γ and β that will result in a stable time stepping scheme.

The eigenvalues of the system change when impedance boundary conditions are imposed. The eigenvalues of $\mathbf{A}_1^{-1}\mathbf{A}_0$ have nonnegative real parts with impedance boundary conditions. First, the matrices in (A.16) are redefined in a more general form,

$$\mathbf{A}_1 = \begin{bmatrix} \mathbf{M}_{\mu^{-1}} & 0 \\ 0 & \mathbf{M}_\varepsilon \end{bmatrix}, \quad \mathbf{A}_0 = \begin{bmatrix} 0 & \mu_0^{-1}\mathbf{M}_c \\ -\mu_0^{-1}\mathbf{M}_c^T & \mathbf{M}_I \end{bmatrix} \quad (\text{A.23})$$

where the basis functions can be of any order. To determine the behaviour of $\mathbf{A}_1^{-1}\mathbf{A}_0$, we create a similar matrix $\mathbf{A}_s = \mathbf{F}\mathbf{A}_s\mathbf{F}^{-1}$, where $\mathbf{F} = \mathbf{A}_1^{-1}$, leading to

$$\mathbf{A}_s = \begin{bmatrix} 0 & -\mu_0^{-1}\mathbf{M}_{\mu^{-1}}^{\frac{-1}{2}}\mathbf{M}_c\mathbf{M}_\varepsilon^{\frac{-1}{2}} \\ \mu_0^{-1}\mathbf{M}_\varepsilon^{\frac{-1}{2}}\mathbf{M}_c^T\mathbf{M}_{\mu^{-1}}^{\frac{-1}{2}} & \mathbf{M}_\varepsilon^{\frac{-1}{2}}\mathbf{M}_I\mathbf{M}_\varepsilon^{\frac{-1}{2}} \end{bmatrix}. \quad (\text{A.24})$$

This matrix is a non-symmetric saddle point matrix, whose properties are discussed in Theorem 3.6 in [13]. The matrix $\mathbf{A}_s$ can be proven to be positive semi-definite because the matrix $\mathbf{M}_I$ is positive semi-definite. Therefore, the eigenvalues of $\mathbf{A}_s$, and by the properties of similar matrices $\mathbf{A}_1^{-1}\mathbf{A}_0$, have nonnegative real parts. This is demonstrated for the zeroth and second order vector basis function for both Dirichlet and impedance boundary conditions in figure A.2. The eigenvalues for the Dirichlet case lie on the imaginary axis, while the impedance boundary condition case is symmetric about the real axis in right half plane. Knowing that the eigenvalues have nonnegative real parts, it is possible to find general regions of stability and conditions for which the Newmark-Beta time-stepping scheme is nondissipative. The scheme is unconditionally stable for $\gamma \geq 0.5$ and $\beta \geq \gamma/2$.

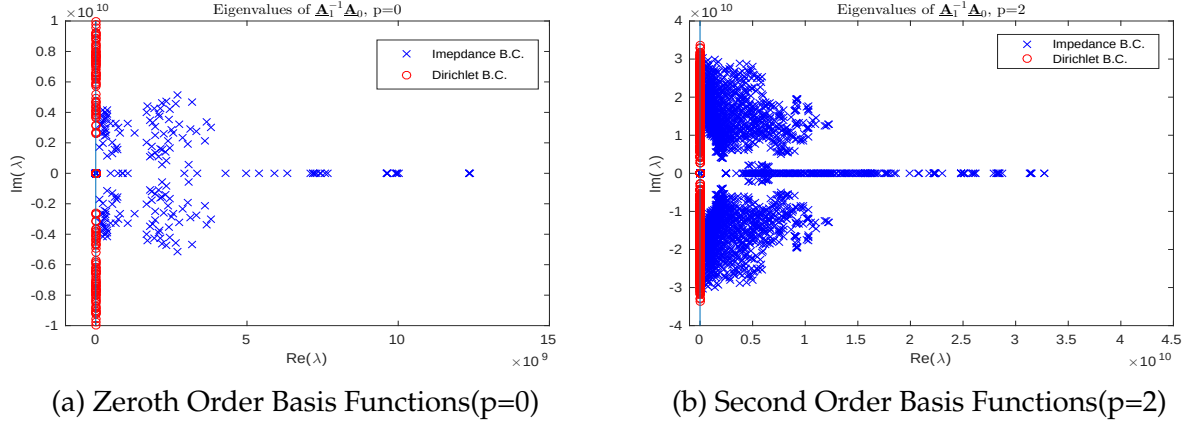


Figure A.2: Eigenvalues of $\mathbf{A}_1^{-1} \mathbf{A}_0$

When $\gamma = 0.5$, $\beta \geq 0.25$, $|z| = 1$ for all the possible eigenvalues of $\mathbf{A}_1^{-1} \mathbf{A}_0$, (A.17) forms a nondissipative time-stepping scheme, which is essential in many applications. When $\gamma = 0.5$ and $\beta = 0.25$ or $\beta = 0.5$, we obtain a Crank-Nicholson scheme, which is known to be unconditionally stable and second order. Other choices of γ and β lead to dissipative, yet still stable time stepping schemes.

A.4 Results

In this Section, we demonstrate numerically the utility of using the Newmark-Beta time stepping scheme with TD-MFEM. In particular, the resulting time stepping scheme is unconditionally stable while maintaining the convergence and accuracy properties of the more common leapfrog method.

A.4.1 Field Convergence

To numerically demonstrate convergence, a TEM plane wave is simulated propagating in free space normally incident through a $0.5 \text{ m} \times 0.5 \text{ m} \times 0.5 \text{ m}$ cube. The electric field is defined as

$$\vec{E}(\vec{r}, t) = \hat{y} \cos(2\pi f_0(t - \vec{r} \cdot \hat{z}/c - 8\sigma)) e^{-(t - \vec{r} \cdot \hat{z}/c - 8\sigma)^2 / 2\sigma^2} \text{ (V/m)}, \quad (\text{A.25})$$

where $\sigma = 3/[2(f_{\max} - f_0)]$ with the center and maximum frequency denoted as f_0 and $f_{\max}$, respectively. The relative error is defined as

$$\text{Relative Error} = \frac{\|\int d\Omega(\bar{\phi}_{exp}(\bar{r}, t) - \bar{\phi}_{ana}(\bar{r}, t))\|_2}{\|\int d\Omega\bar{\phi}_{ana}(\bar{r}, t)\|_2} \quad (\text{A.26})$$

where $\bar{\phi}(\bar{r}, t)$ can be either the electric field or magnetic flux density. The speed of propagation is the speed of light $c = 1/\sqrt{\epsilon\mu} = 1/\sqrt{\epsilon_0\mu_0}$ (m/s). Dirichlet boundary conditions as defined in (A.3) are used on each face of the volume, where $\bar{E}(\bar{r}, t)$ is defined in (A.25) and $\bar{B}(\bar{r}, t)$ follows from Maxwell's equations.

For the spatial convergence tests, the center frequency is 11 MHz, maximum frequency 21 MHz. Figure A.3 shows the convergence properties of the fields with respect to space and basis function order. The convergence rate is the same between the two time stepping schemes, with similar errors as well. This is expected as the spatial discretization is the same. It is also noted that increasing the order of the basis function yields a greater improvement in accuracy than simply decreasing the element sizes.

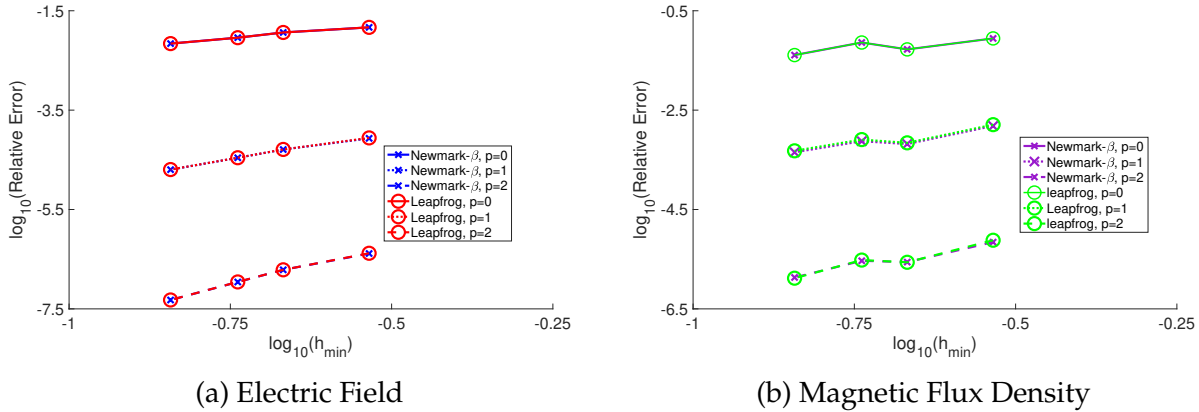


Figure A.3: Space Convergence

Figure A.4 shows the relative error in the electric field and magnetic flux as the time step size is changed using the Newmark-Beta time stepping scheme with $\gamma = .5$ and $\beta = .25$ for different orders of vector basis functions. The domain Ω is a 0.5 m $\times$ 0.5 m $\times$ 0.5 m cube partitioned into 439 tetrahedra with an average edge length $h_{\text{avg}} = 143.7$ mm. As the

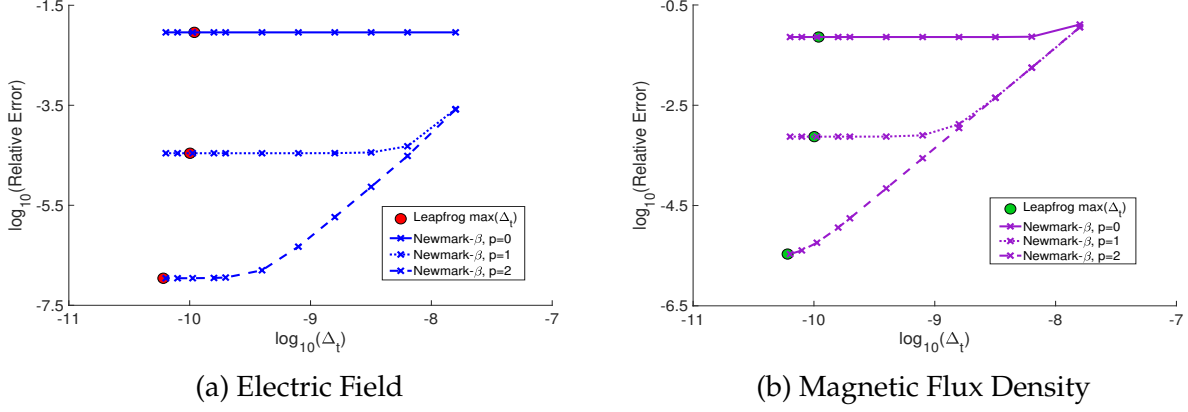


Figure A.4: Time Convergence

order of the Newmark-Beta time stepping scheme is the same as the Leapfrog scheme, it behaves similarly as the Newmark-Beta , but only for time step sizes smaller than the maximum time step size that is marked. Increasing the order of basis functions results in a smaller maximum time step size, whereas the unconditionally stable method allows for much larger time step sizes while maintaining the advantages of using higher order basis functions.

A.4.2 Computational Cost Comparison

In the previous section, the spatial and temporal convergence of the Newmark-Beta time stepping scheme was compared to the leapfrog method. Here we compare the cost of using the Newmark-Beta time marching scheme. The leapfrog method requires requires matrix inversion for (A.13b). The Newmark-Beta method in (A.17) requires matrix inversion as well. The matrices in both (A.13b) and (A.17) are sparse, having $\mathcal{O}(N_e)$ and $\mathcal{O}(N_e + N_f)$ nonzero elements, respectively. For practical problems, direct inversion is expensive and iterative solvers are used instead. We assume that a Krylov subspace based method like GMRES converges in N_{iter} steps for both leapfrog and Newmark-Beta. Assuming that the duration of analysis is T gives $N_{t,lf}$ and $N_{t,N\beta}$ as the number of time steps for leapfrog and Newmark-Beta, respectively. It follows that runtime scales as $\mathcal{O}(N_{t,lf} N_{iter} N_e)$ for leapfrog

and $\mathcal{O}(N_{t,N\beta}N_{iter}(N_e + N_f))$ for Newmark-Beta. It is apparent that the increased degrees of freedom required for a Newmark system could lead to higher costs; however, the time step sizes can be vastly different. Indeed, depending on the geometry (especially when discretization is driven by the need to capture feature sizes), the cost of the increased degrees of freedom can be counterbalanced by the number of time steps taken when there is flexibility in the time step size. Thus, as the ceiling of $\Delta_{t,LF}$ is fixed by the mesh, so is the number of time steps for a fixed duration of time. However, this is not the case for Newmark-Beta. The numerical experiment conducted next illustrates the cost tradeoff.

This experiment is shown in figure A.5 and is conducted using three $1\text{ m} \times 1\text{ m} \times 1\text{ m}$ cubes with Dirichlet boundary conditions. A normally-incident TEM plane wave is simulated propagating in free space. The electric field is defined in (A.25) with a center frequency of 110 MHz and a maximum frequency of 210 MHz. The Newmark-Beta time stepping scheme was run three times for the same amount of simulated time. Once at the maximum time step size for leapfrog, once at half that time step size, and once with a time step size of $1/20f_{max} \approx 238\text{ ps}$. GMRES was used with a diagonal preconditioner and a tolerance of 10^{-4} . When $\Delta_{t,N\beta} = 1/20f_{max}$, the runtime for Newmark-Beta was equal to

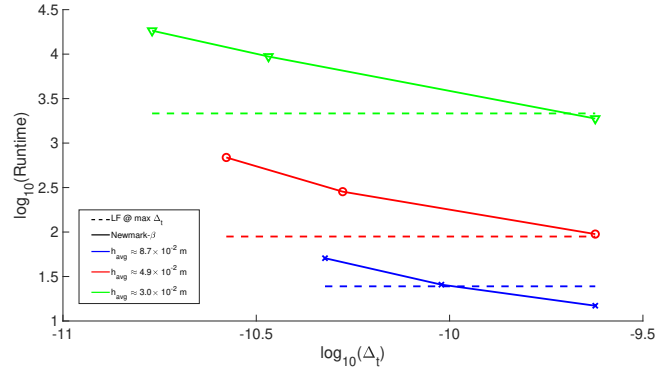


Figure A.5: Runtime Comparison

or faster than leapfrog. While this was a simple example, we expect to reap significant benefits as the model representation drives discretization.

A.4.3 Eigenvalues of Space-time matrix

In this test, we further verify the stability of the proposed Newmark-Beta time-marching scheme. To determine the stability of a time stepping schemes, we analyze the eigenvalues of a space-time matrix $\mathbf{A}$ that satisfies

$$\bar{\mathbf{u}}^{n+1} = \mathbf{A}\bar{\mathbf{u}}^n \quad (\text{A.27})$$

for some input vector $\bar{\mathbf{u}}_n$. The space-time matrix is an amplification matrix for some input and for it to have a bounded output, the absolute value of the eigenvalues must lie on or within the unit circle in the complex domain. For an energy-conserving system, all the eigenvalues lie on the unit circle, signifying that there is no numerical loss in the system. In this example, two different meshes discretize the same 1 m cube. The first mesh is nearly uniformly discretized, with a ratio of $h_{\max}/h_{\min} \approx 1.5$, where h is edge length. The second mesh is not uniformly discretized, in which the edges become smaller near one face. The ratio of the largest edge to smallest edge in the nonuniform mesh is ≈ 8 . Figures A.6, A.7, and A.8 compare the eigenvalues of the space-time matrices for both the leapfrog and Newmark-Beta time stepping schemes for varying time step size. The reference time step size $\Delta_t = 1/(30f_{\max})$.

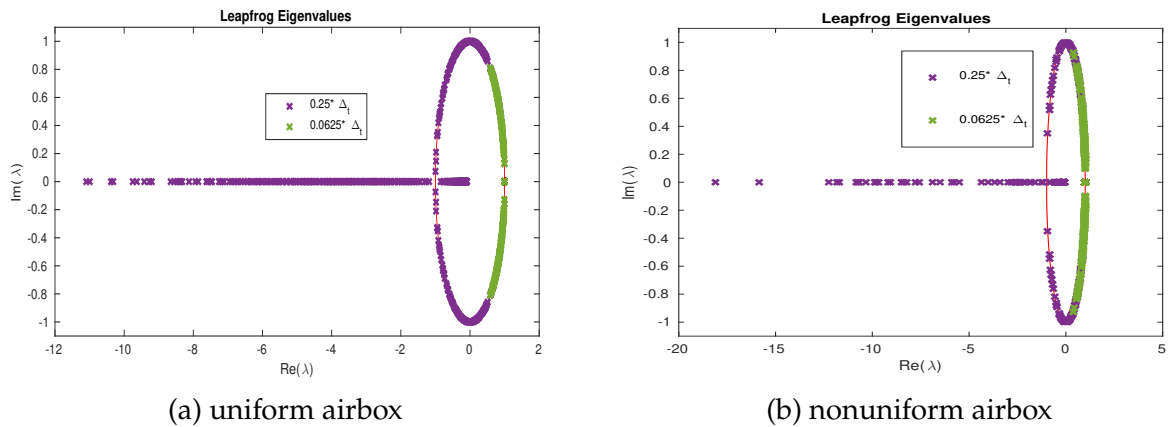


Figure A.6: Leapfrog Eigenvalues

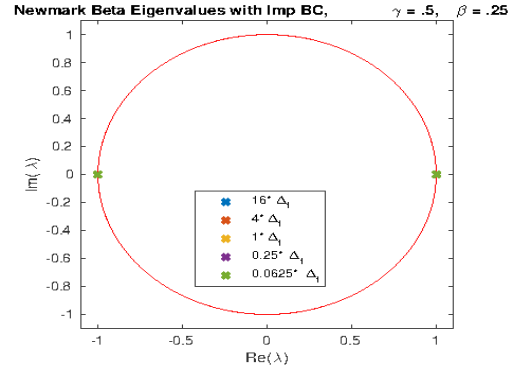
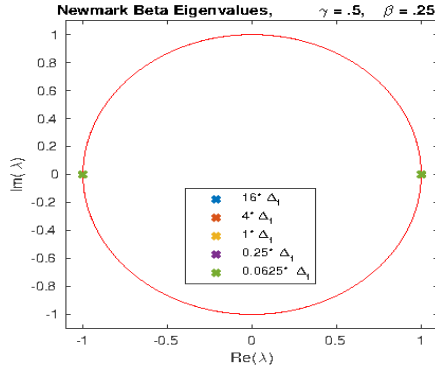


Figure A.7: Newmark-Beta Eigenvalues for Uniform Airbox

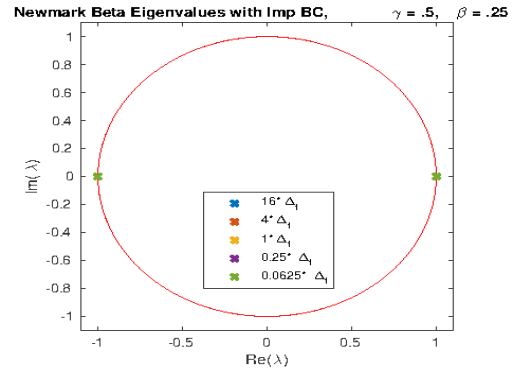
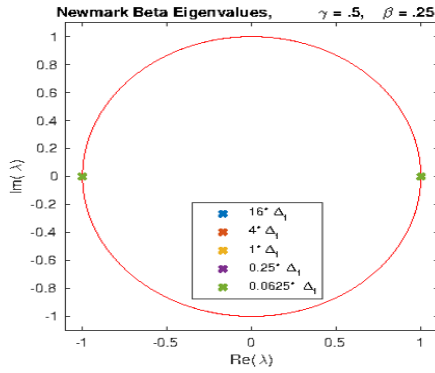
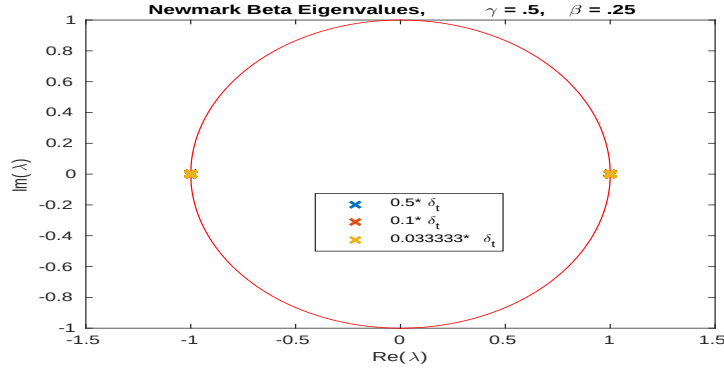


Figure A.8: Newmark-Beta Eigenvalues for Nonuniform Airbox

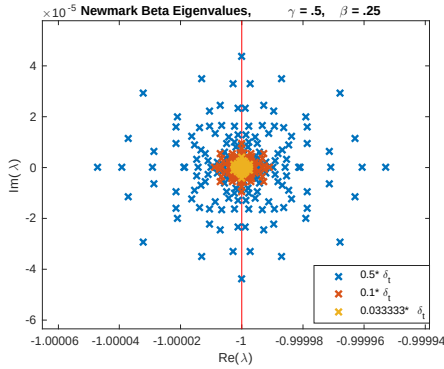
When the time step size of the leapfrog method satisfies the stability criterion, the eigenvalues all lie on the unit circle. However, when the time step size no longer satisfies the stability criterion, the eigenvalues close to -1 leave the unit circle and head toward 0 and $-\infty$.

Figure A.7 and A.8 show that the space-time eigenvalues of the Newmark-Beta time stepping scheme with $\gamma = .5$ and $\beta = .25$ always lie on the unit circle for a wide range of time step sizes, lending credence to it unconditionally stable nature. The eigenvalues of the system when these particular values are chosen are analytically ± 1 . Figure A.7 uses the uniformly discretized volume and figure A.8 uses the nonuniformly discretized volume, with both showing the behavior with Dirichlet boundary conditions and impedance boundary conditions. As the overall eigenvalue behavior holds as the basis function order

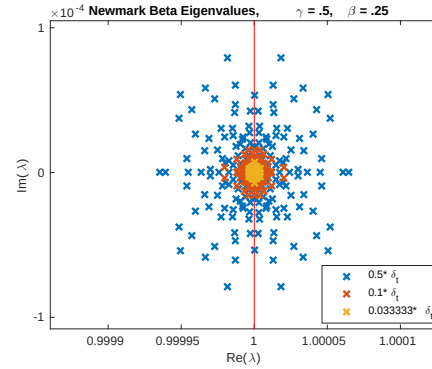
increases, similar results are seen in figures A.9 and A.10, which shows the space-time eigenvalues of the same uniform airbox with Dirichlet boundary conditions, but with first and second order basis functions. Closer inspection of the eigenvalues show that there is an error, as the eigenvalues lie outside the unit circle, but it is strictly numerical in nature and related to the condition number of the matrix $\mathbf{A}_1^{-1}\mathbf{A}_0$.



(a) First Order



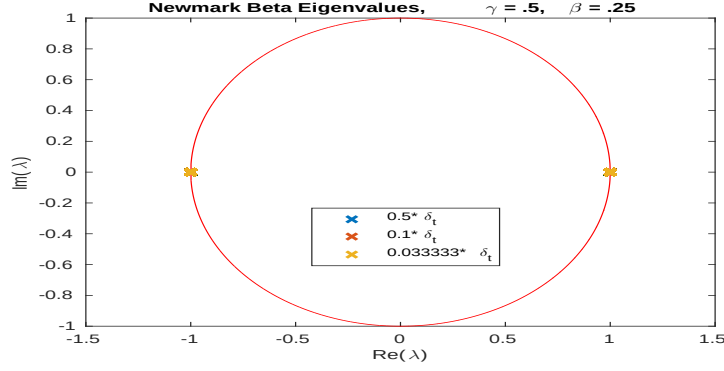
(b) p=1, Centered at $\text{Re}(\lambda) = -1$



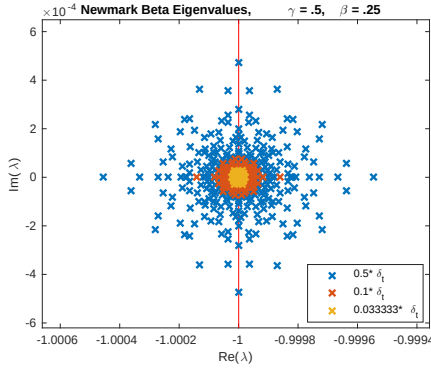
(c) p=1, Centered at $\text{Re}(\lambda) = 1$

Figure A.9: Newmark-Beta Eigenvalues for Uniform Airbox with First Order Basis functions

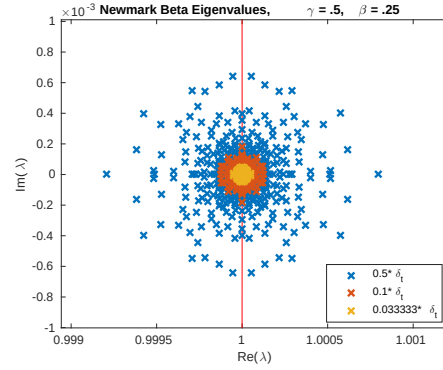
Finally, to numerically confirm late-time stability, figure A.11 shows the electric field and magnetic flux density run for 100,000 time steps at a time step size of $\Delta t_{N\beta} = 1/10 f_{max}$ or 4.762 ns. There is a noise floor that corresponds to a DC null space. However, the noise does not grow over time, indicating the nullspace does not contain $t\nabla\phi(\vec{r})$ present in TD-FEM.



(a) Second order



(b) $p=2$, centered at $\text{Re}(\lambda) = -1$



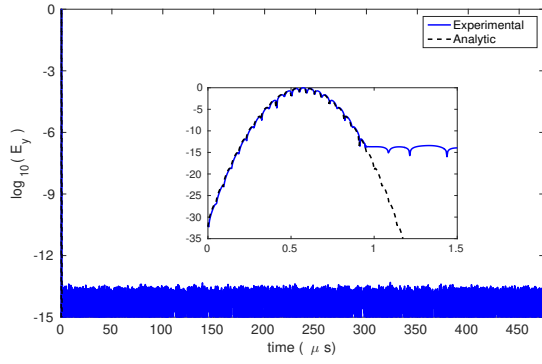
(c) $p=2$, centered at $\text{Re}(\lambda) = 1$

Figure A.10: Newmark-Beta Eigenvalues for Uniform Airbox with Second Order Basis Functions

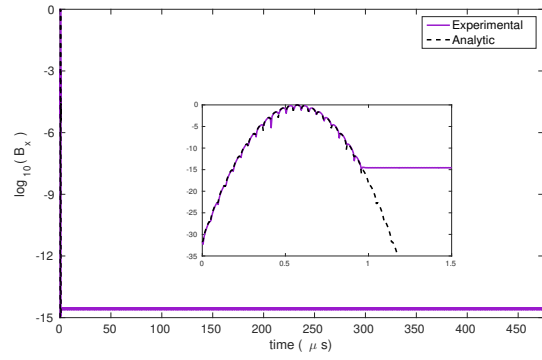
A.5 Summary

In this work, it was proven that the Newmark-Beta algorithm can be used to create an unconditionally stable time stepping framework for solving TD-MFEM. We proved stability for systems arising from different boundary conditions, as well as showed convergence and energy conservation. The benefit of being able to use different time step sizes is apparent. In future work, this method will be applied to simulating plasmas. Utilizing higher order basis sets with optimal particle pushing strategies will be investigated. Preconditioning strategies will also be developed to improve the use of iterative solvers for TD-MFEMs.

This work was supported by the Department of Energy Computational Science Graduate fellowship under grant DE-FG02-97ER25308. The authors would also supported in part by the HPCC Facility at Michigan State University under Grant NSF ECCS-1408115, and



(a) Electric Field



(b) Magnetic Flux Density

Figure A.11: Plane Wave Simulation for 100,000 Time Steps

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