An Envelope Tracking Approach for Particle in Cell Simulations

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Abstract—The state of the art in electromagnetic finite element particle-in-cell (EM-FEMPIC) has advanced significantly in the last few years; these have included understanding function spaces that must be used to represent sources and fields consistently, and how currents should be evolved in space and time. In concert, these achieve satisfaction of Gauss’ laws. All of these were restricted to conditionally stable explicit time stepping. More recently, there have been advances to the state of art: it is now possible to use an implicit EM-FEMPIC method while satisfying Gauss’ law to machine precision. This enables choosing time step sizes dictated by physics as opposed to geometry. In this article, we take this a step further. For devices characterized by a narrowband high-frequency response, choosing a timestep size based on the highest frequency of interest is considerably expensive. In this article, we use methods derived from envelope tracking to construct an EM-FEMPIC method that analytically provides for the high-frequency oscillations of the system, allowing for analysis at considerably coarser timestep sizes even in the presence of non-linear effects from active media such as plasmas. Consequently, we demonstrate how the point-wise metric used for measuring satisfaction of Gauss’ Laws breaks down when prescribing analytical fast fields and provide a thorough analysis of how charge conservation can be measured. Through a number of examples, we demonstrate that the proposed approach retains the accuracy of the regular scheme while requiring far fewer timesteps in systems where the stepsize is strongly decided by the bandwidth of the fields.

Index Terms—Coulomb gauge, envelope tracking, finite element method, Gauss’ laws, particle in cell (PIC), plasma detuning, quasi-Helmholtz decomposition.

I. INTRODUCTION

THE simulation of moving charges in an electromagnetic field distribution is of great interest in a number of engineering applications. These include particle accelerators, plasma processing applications such as sterilization of medical implements and etching of high-precision integrated chips [1], [2], [3], among many others. The foremost application in performing these simulations is the particle-in-cell (PIC) method that relies on self-consistently solving Maxwell’s equations for the fields and Newton equations for particles of the charged species. Traditional implementations of PIC have used finite difference time domain (FDTD) to evolve the fields [4], with many advances made to better handle complex geometries through conformal formulations [5]. Recent advances, however, have made it possible to use the finite element field solvers [6], [7], [8], [9] that similarly allow for better resolution of curvilinear grids, in addition to making the use of more complex function spaces accessible. In addition, work has been done on constructing symplectic structure preserving FEMPIC scheme [10], [11] based on Whitney forms defined by B-splines [12]. Furthermore, it is possible to sidestep the Courant–Friedrichs–Lewy (CFL) constraint on the timestep size by using unconditionally stable implicit time marching schemes while conserving charge to machine precision [13]. And finally, techniques have been very recently developed that allow for explicit satisfaction of the Coulomb Gauge, thus alleviating the problem of spurious null-space solutions that exist in most implicit implementations [14].

All-in-all, advances in electromagnetic finite element PIC (EM-FEMPIC) have made it possible to: 1) simulate plasma phenomena while capturing the underlying geometry to very good precision and 2) analyze the system in time at the frequency of interest for capturing the desired physics as opposed to the satisfaction of mesh-based stability criteria. Despite the massive progress that has been accomplished in recent years, there are still classes of devices for which the current state of the art is inefficient to capture large-scale problems. One such example is the analysis of devices that have a narrowband, high-frequency response. Similarly, devices with features smaller than the electromagnetic wavelength that are nonetheless important for the electrostatic physics are computationally untenable to solve contemporary techniques. Despite having a relatively small window of significant frequency content, to simulate such a device, one would need to...
discretize the simulation in time at a rate determined by the maximal frequency of interest.

Efficient ways to simulate these devices exist when one considers a purely electromagnetic analysis (i.e., without particles). Termed envelope tracking, these methods solve an altered form of Maxwell’s equations wherein the high-frequency component in the fields is analytically prescribed. Performing this operation effectively, a Hilbert transform of Faraday’s and Ampere’s laws yields a new set of equations that still vary in time, but can be discretized at the bandwidth of the signal, which is significantly lower than the maximal frequency in the unshifted system.

Extending these results to a system with moving macroparticles is challenging for two primary reasons.

1) While the fields themselves oscillate within a narrowband high-frequency window, the particle positions and velocities generally have significant dc components that force analysis of Newton’s equations at the highest frequency of interest.

2) While recent advances make it possible to conserve charge within an implicit time-marching scheme [13], these techniques break down when used with an analytically prescribed plane wave component (we discuss this in greater detail in Section III-B).

In the remainder of this article, we construct an EM-FEMPIC method wherein the fields are solved using an envelope tracking method, henceforth referred to as ET-FEMPIC. We address both of the challenges listed above 1) by constructing an integration scheme for the particle system that allows Newton’s laws to be solved at the highest frequency of interest while being mapped self-consistently with the Maxwell solver and 2) by constructing a quasi-Helmholtz framework to explicitly satisfy the Coulomb gauge. We show analytically and through numerical experiments that this framework conserves charge to machine precision while producing results that match a traditional EM-FEMPIC implementation.

II. PROBLEM STATEMENT

Consider a region $\Omega \in \mathbb{R}^3$ bounded by a surface $\partial \Omega$ containing a single-charged species. This region is subjected to an external field due to which the charged species accelerate, and in turn produce spatially and temporally varying electric and magnetic fields denoted by $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$, respectively, with $\mathbf{r} \in \Omega$ and $t \in [0, \infty)$. The dynamics of the particles in phase space can be represented by a distribution function (PSDF) $f(t, \mathbf{r}, \mathbf{v})$ that follows the Vlasov equation:

$$\partial_t f(t, \mathbf{r}, \mathbf{v}) + \mathbf{v} \cdot \nabla f(t, \mathbf{r}, \mathbf{v}) + \frac{q}{m} [\mathbf{E}(\mathbf{r}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{r}, t)] \cdot \nabla_v f(t, \mathbf{r}, \mathbf{v}) = 0. \quad (1)$$

In what follows, we assume that the background media in $\Omega$ is free space. As a result, we denote the permittivity and permeability of free space by $\varepsilon_0$ and $\mu_0$, respectively, and the speed of light by $c$. In what follows, we will assume that either the external fields impressed on $\Omega$ or the source exciting fields is narrowband in that the center frequency of the excitation $f_0 \gg f_{bw}$, where $f_{bw}$ is the bandwidth. Likewise, we will assume that the system is quiescent for $t \leq 0$.

III. FORMULATION

We follow the usual path of not solving (1) directly, instead representing the moments of the PSDF using a charge and current density as, $\rho(t, \mathbf{r}) = q \int \omega f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}$ and $\mathbf{J}(t, \mathbf{r}) = q \int \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}$. We then use a particle approximation of these moments, and evolve their location and velocity together with Maxwell’s equations. As a result, assuming a shape functions $S(\mathbf{r})$, one obtains

$$\rho(t, \mathbf{r}) = q \sum_{p=1}^{N_p} S(\mathbf{r} - \mathbf{r}_p(t)) \quad (2a)$$

$$\mathbf{J}(t, \mathbf{r}) = q \sum_{p=1}^{N_p} \mathbf{v}_p(t) S(\mathbf{r} - \mathbf{r}_p(t)) \quad (2b)$$

where $N_p$ denotes the number of macroparticles. Furthermore, $\mathbf{r}_p(t)$ and $\mathbf{v}_p(t)$ refer to the positions and velocities as a function of time of the $p$th macroparticle. With no loss of generality, we will assume that there exist a source $\mathbf{J}_i(\mathbf{r}_i, t) = \mathbf{J}_i(\mathbf{r}_i, t)e^{j \omega t}$ at points $\mathbf{r}_i$ that excites the system. Given this temporal dependence, we posit that the field and fluxes have a similar behavior, that is, $\mathbf{E}(\mathbf{r}, t) = \tilde{\mathbf{E}}(\mathbf{r}, t)e^{j \omega t}$ and $\mathbf{B}(\mathbf{r}, t) = \tilde{\mathbf{B}}(\mathbf{r}, t)e^{j \omega t}$. In these expressions, the quantities with a tilde are slowly varying with respect to time. Using these expressions in Maxwell’s equations, we can write

$$\nabla \times \tilde{\mathbf{E}}(\mathbf{r}, t) = -j \omega \varepsilon_0 \tilde{\mathbf{B}}(\mathbf{r}, t) - \partial_t \tilde{\mathbf{B}}(\mathbf{r}, t) \quad (3a)$$

$$\nabla \times \mu_0^{-1} \tilde{\mathbf{B}}(\mathbf{r}, t) = \tilde{\mathbf{J}}(\mathbf{r}, t) + \mathbf{J}(t, t)e^{-j \omega t} + j \omega \varepsilon_0 \tilde{\mathbf{E}}(\mathbf{r}, t) + \varepsilon_0 \partial_t \tilde{\mathbf{E}}(\mathbf{r}, t). \quad (3b)$$

Following [13], we replace $\mathbf{J}(\mathbf{r}, t)$ with its time integral:

$$\mathbf{G}(\mathbf{r}, t) = \int_0^t \mathbf{J}(\mathbf{r}, \tau) d\tau = q \sum_{p=1}^{N_p} \int_0^t \mathbf{v}_p(\tau) \delta(\mathbf{r} - \mathbf{r}_p(\tau)) d\tau \quad (3c)$$

in (3b), to obtain

$$\nabla \times \mu_0^{-1} \tilde{\mathbf{B}}(\mathbf{r}, t) = \tilde{\mathbf{J}}(\mathbf{r}, t) + e^{j \omega t} \partial_t \mathbf{G}(\mathbf{r}, t) + j \omega \varepsilon_0 \tilde{\mathbf{E}}(\mathbf{r}, t) + \varepsilon_0 \partial_t \tilde{\mathbf{E}}(\mathbf{r}, t). \quad (3d)$$

and satisfy Gauss’ electric and magnetic laws

$$\nabla \cdot \varepsilon_0 \tilde{\mathbf{E}}(\mathbf{r}, t) = \rho_i(\mathbf{r}, t) + \rho(\mathbf{r}, t) \exp[-j \omega t] \quad (4a)$$

$$\nabla \cdot \tilde{\mathbf{B}}(\mathbf{r}, t) = 0. \quad (4b)$$

It is important to note at this point that $\mathbf{G}(\mathbf{r}, t)$ and $\rho(\mathbf{r}, t)$ are not necessarily narrowband. As a result, they cannot be decomposed into fast and slow varying components. As usual, boundary conditions need to be imposed on $\tilde{\mathbf{E}}(\mathbf{r}, t)$ and $\tilde{\mathbf{B}}(\mathbf{r}, t)$ on sections of the outer boundary $\partial \Omega$. These are assumed as either Dirichlet, Neumann, or impedance boundary conditions.
on non-overlapping surfaces \( \partial \Omega_D, \partial \Omega_N, \) and \( \partial \Omega_I \), and are defined as follows:

\[
\hat{n} \times \vec{E}(\mathbf{r}, \tau) = \Psi_D(\mathbf{r}, \tau) \text{ on } \Omega_D
\]

\[
(5a)
\]

\[
\hat{n} \times \mu^{-1}\vec{B}(\mathbf{r}, \tau) = \Psi_N(\mathbf{r}, \tau) \text{ on } \Omega_N
\]

\[
(5b)
\]

\[
\hat{n} \times \mu^{-1}\vec{B}(\mathbf{r}, \tau) - Y \hat{n} \times \vec{E}(\mathbf{r}, \tau) = \Psi_I(\mathbf{r}, \tau) \text{ on } \Omega_I.
\]

\[
(5c)
\]

Note, it is assumed that \( \partial \Omega_D + \partial \Omega_N + \partial \Omega_I = \partial \Omega \). The evolution of the macroparticles in space and time is determined by solving for the equations of motion with the acceleration determined by the Lorentz force. This yields the following coupled system of equations for ordinary differential equations (ODEs) \( \mathbf{v}_p(\tau) \) and \( \mathbf{r}_p(\tau) \):

\[
\frac{d\mathbf{v}_p(\tau)}{d\tau} = \frac{q}{m} [\vec{E}(\mathbf{r}_p(\tau), \tau) + \mathbf{v}_p(\tau) \times \vec{B}(\mathbf{r}_p(\tau), \tau)] \exp[j\omega_0\tau]
\]

\[
(6a)
\]

\[
\frac{d\mathbf{r}_p(\tau)}{d\tau} = \mathbf{v}_p(\tau)
\]

\[
(6b)
\]

In what follows, we present a method to self-consistently solve both Maxwell’s equations and equations of motion, especially under the narrowband approximation.

### A. Discretization in Space and Time

Solutions to (3) are obtained by spatially representing \( \vec{E}(\mathbf{r}, \tau) \) and \( \vec{B}(\mathbf{r}, \tau) \) in terms of Whitney edge and face basis functions, respectively (shown for a single tetrahedron in Fig. 1)

\[
\begin{align*}
\vec{E}(\mathbf{r}, \tau) & = \sum_{i=1}^{N_e} e_i(\tau) W^1_i(\mathbf{r}) \\
\vec{B}(\mathbf{r}, \tau) & = \sum_{i=1}^{N_f} b_i(\tau) W^2_i(\mathbf{r}).
\end{align*}
\]

\[
(7)
\]

Here, \( W^1_i(\mathbf{r}) \) and \( W^2_i(\mathbf{r}) \) represent the lowest order Whitney edge function defined on the \( i \)th edge and face function defined on the \( i \)th face, respectively. Further, \( N_e \) and \( N_f \) denote the number of edges and faces in the tetrahedral mesh used to discretize \( \Omega \); details on mixed finite elements can be found in [15], [16], [17], [18], [19] and references therein. Using Gherkin testing results in the following matrix ODE to solve for the vector of field coefficients \( \vec{B}(\tau) \) and \( \vec{E}(\tau) \) in time:

\[
\begin{bmatrix}
\vec{s} & \vec{\beta}(\tau) & \vec{\beta}(\tau) \\
\end{bmatrix} + \frac{1}{\epsilon_0} \begin{bmatrix}
\mu^{-1} & 0 \\
0 & \mu^{-1}
\end{bmatrix} \frac{\partial}{\partial \tau} \begin{bmatrix}
\vec{B}(\tau) \\
\vec{E}(\tau)
\end{bmatrix} = \vec{f}
\]

\[
(8)
\]

where the various matrix definitions are as follows:

\[
\begin{align*}
\vec{s} & = \begin{bmatrix}
0 & \nabla \times \mathbf{r} & 0 \\
-\nabla \times \mathbf{r} & 0 & 0 \\
\end{bmatrix}
\end{align*}
\]

\[
\begin{align*}
\vec{\beta}(\tau) & = \begin{bmatrix}
*_{\mu^{-1}} & 0 \\
0 & *_{\mu^{-1}}
\end{bmatrix}
\end{align*}
\]

\[
\vec{f} = \begin{bmatrix}
\frac{\partial G(t)}{\partial \tau}
\end{bmatrix}
\]

\[
(9)
\]

Furthermore, \( \vec{B}(\tau) = [b_1(\tau), b_2(\tau), \ldots, b_{N_f}(\tau)]^T \), \( \vec{E}(\tau) = [e_1(\tau), e_2(\tau), \ldots, e_{N_e}(\tau)]^T \), \( \vec{G}(\tau) = [g_1(\tau), g_2(\tau), \ldots, g_{N_e}(\tau)]^T \), where \( g_i(\tau) = \langle \mathbf{W}_i, \mathbf{G}(\mathbf{r}, \tau) \rangle \) and \( \vec{J}_i(\tau) = [j_1(\tau), j_2(\tau), \ldots, j_{N_f}(\tau)]^T \), where \( j_1(\tau) = \langle \mathbf{W}_i, \vec{J}(\mathbf{r}, \tau) \rangle \).

We preface at this point that the method reduces to a traditional EM-FE PIC solve when \( \omega_0 = 0 \), so the proposed method represents a generalization of the EM-FE PIC formulation. To convert (8) into a discrete stencil at different intervals of time, we utilize a Newmark-\( \beta \) [20] scheme with \( \gamma = 0.5 \) and \( \beta = 0.25 \). Furthermore, we define \( \Delta t_{\omega_0} = (30\xi f_{\text{max}})^{-1} \) and \( \Delta t_{\text{cell}} = (30\xi f_{\text{cell}})^{-1} \) as the timestep size appropriate for the fast-varying and downshifted systems, respectively, with \( \xi \) being a real oversampling factor. This choice of parameters results in representing the field coefficients in terms of second-order Lagrange polynomials in time and testing with an average acceleration condition [represented by \( \mathbf{W}(\tau) \)] such that for \( t \in [t_{n-1}, t_{n+1}] \), where \( t_n = n\Delta t_{\text{cell}} \):

\[
\begin{align*}
\langle \vec{B}(\tau), \vec{E}(\tau) \rangle & = \sum_{k=0}^{2} N_{n, k}(\tau) \begin{bmatrix}
\vec{B}(t_{n+k-1}) \\
\vec{E}(t_{n+k-1})
\end{bmatrix} \\
L_{n, k}(\tau) & = \prod_{j=0}^{k-1} \frac{t - t_{n+1-j}}{t_{n+1-k} - t_{n+1-j}} \\
N_{n, k}(\tau) & = \left\{ \begin{array}{ll}
L_{n, k}(\tau), & t \in [t_{n-1}, t_{n+1}] \\
0, & \text{otherwise}
\end{array} \right.
\end{align*}
\]

\[
(10a)
\]

\[
(10b)
\]

\[
(10c)
\]
B. Discretization and Exact Charge Conservation

Next, we re-examine rubrics of a charge conserving PIC scheme from a slightly different perspective. The discrete divergence of the set of equations derived (8) should yield Gauss’ laws but a word of caution, the discrete equations are a result of measuring their continuous counterparts in time. More precisely, we note that the discrete divergence of Ampere’s laws yields

\[
\epsilon_0 \left[ \nabla \right]^T [\star_{\varepsilon}] \partial_t \bar{\mathbf{E}}(t) + j \omega_0 [\star_{\varepsilon}] \bar{\mathbf{E}}(t) = - \epsilon_0 \left[ \nabla \right]^T \left( \bar{\mathbf{J}}(t) + e^{-j\omega t} \partial_t \bar{\mathbf{G}}(t) \right).
\]  

(12)

Discretizing Gauss law, however, yields

\[
\epsilon_0 \left[ \nabla \right]^T [\star_{\varepsilon}] \bar{\mathbf{E}}(t) = \bar{\rho}_t(t) + \bar{\rho}(t)
\]  

(13)

where \(\bar{\rho}_t(t) = [\rho_1(t), \ldots, \rho_N(t)]^T\), \(\rho_i(t) = (W_{i0}(\mathbf{r}), \rho_0(\mathbf{r}, t))\), and \(\bar{\rho}(t) = [\rho(t), \ldots, \rho_N(t)]^T = \left[ \epsilon_0 \left[ \nabla \right]^T \bar{\mathbf{G}}(t) e^{-j\omega t} \right]^T\). Note, in the above equations, the \(\left[ \nabla \right]^T\) matrix effects a divergence of the flux density (which lies in the dual grid) in terms of quantities defined on the primal grid. In practice, as one only evolves the curl equations, the solution at every time step will automatically satisfy (12) provided care is taken in constructing the right-hand side \([13]\). But what is critical for satisfaction of Gauss’ law is that this discrete solution also satisfies (13). In the text that follows, we take some liberties in verbiage: 1) it will be understood that (12) and (13) are not explicitly discretized in time and evolved; 2) the system of equations resulting from taking the discrete divergence of the time-discretized Ampere’s laws and those from temporal discretization of (12) will be identical; 3) we use the word discretization and measurement interchangeably; they imply an inner product with a temporal basis function; and 4) our goal is to understand how one should measure or discretize (13) so as to be consistent with the measurement of (12). Indeed, if we choose different temporal basis to measure (12) and (13), it must be shown that the two measures are consistent. For instance, if the basis functions used to measure (12) are first order and those used to measure (13) are delta functions, they will yield different results; this is a point that we will return to later. Note, we have specifically assumed that \(\bar{\mathbf{G}}(t)\) is known. Indeed, as shown in \([13]\) and \([21]\), using \(\bar{\mathbf{G}}(t)\) is critical for exact satisfaction of Gauss’ electric law.

To understand these issues better, we analyze two cases: 1) \(\omega_0 = 0\) and 2) \(\omega_0 \neq 0\). To simplify our discussion, we assume both \(\bar{\mathbf{J}}(t) = 0 = \bar{\rho}_t(t)\).

1) Case 1 (\(\omega_0 = 0\)): When \(\omega_0 = 0\), (12) simplifies to

\[
\epsilon_0 \left[ \nabla \right]^T [\star_{\varepsilon}] \partial_t \bar{\mathbf{E}}(t) = - \left[ \nabla \right]^T \partial_t \bar{\mathbf{G}}(t).
\]  

(14)

Note, parenthetically, we note that \(\left[ \nabla \right]^T \bar{\mathbf{G}}(t) = - \bar{\rho}(t)\). In keeping with the Newmark-\(\beta\) scheme, to ensure late time stability, we have to use \(W_n(t)\) as testing functions in time.

If a scheme is charge conserving, then at any point \(t_n\), the system arising from the discrete divergence of Ampere’s law

\[
\left\{ W_n(t), \epsilon_0 \left[ \nabla \right]^T [\star_{\varepsilon}] \partial_t \bar{\mathbf{E}}(t) \right\} = \left\{ W_n(t), \partial_t \bar{\rho}(t) \right\}
\]  

(15)

should satisfy Gauss’ law, but under what measure. To make the ensuing text notationally less dense, we use \(\bar{\phi}(t) = \epsilon_0 \left[ \nabla \right]^T [\star_{\varepsilon}] \bar{\mathbf{E}}(t)\). Thus, (15) can be written as

\[
\left\{ W_n(t), \partial_t \bar{\phi}(t) \right\} = \left\{ W_n(t), \partial_t \bar{\rho}(t) \right\}.
\]  

(16)

Evaluation of this inner product results in

\[
\frac{\bar{\rho}^n+1 - \bar{\rho}^{n-1}}{2} - \frac{\bar{\rho}^n+1 - \bar{\rho}^{n-1}}{2} = 0
\]  

(17)

which is the relation that coefficients of the electric field will satisfy in keeping with the substitution defined earlier.

The questions are twofold: 1) since Gauss’ law in (13) is never solved, what is an equivalent discrete system and 2) will the update equation for this system be consistent with those obtained from (16). This may seem trivial as both sides of (14) have a time derivative and one can evaluate them analytically to obtain (13) together with null initial conditions.

But it is important to remember that: 1) right-hand side of Ampere’s law is deliberately chosen to be different from the conventional one where one discretizes current \([9]\) and 2) we effect the solution of (8) by choosing temporal basis sets such that the solution is unconditionally stable, and do not treat it as a first order ODE. Under these circumstances, we can ask what should \(\bar{W}_n(t)\) to reduce (13) to a discrete system. To make our analysis as general as possible, let us denote \(\bar{W}_n(t)\) as a basis that is used to discretize (13)

\[
\left\{ \bar{W}_n(t), \epsilon_0 \left[ \nabla \right]^T [\star_{\varepsilon}] \bar{\mathbf{E}}(t) \right\} = \left\{ \bar{W}_n(t), \bar{\phi}(t) \right\}.
\]  

(18)

Using the abbreviated notation defined earlier, we get

\[
\left\{ \bar{W}_n(t), \bar{\phi}(t) \right\} = \left\{ \bar{W}_n(t), \bar{\rho}(t) \right\}.
\]  

(19)

Consider two potential choices: for \(\bar{W}_n(t) = \delta(t - t_{n+1})\), one gets

\[
\left\{ \delta(t - t_{n+1}), \bar{\phi}(t) \right\} = \left\{ \delta(t - t_{n+1}), \bar{\rho}(t) \right\} \rightarrow \bar{\rho}^{n+1} = \bar{\rho}^{n+1}
\]  

(20)

and for \(\bar{W}_n(t) = W_n(t)\), one gets

\[
\frac{\bar{\rho}^{n+1} + 2\bar{\rho}^n + \bar{\rho}^{n-1}}{4} - \frac{\bar{\rho}^{n+1} + 2\bar{\rho}^n + \bar{\rho}^{n-1}}{4} = 0.
\]  

(21)

In (21), if we were to assume a quiescent initial condition at \(t = 0\), it is trivial to show that one recovers solutions obtained in (17). However, for (21), one needs Gauss’ laws to be satisfied at both \(t = \{0, \Delta t\}\) for it to be consistent with solutions in (17). Indeed, one can use any test function as long as it is piecewise continuous, causal and one imposes additional initial conditions.

We digress a little to note that this is a consequence of using \(\bar{\mathbf{G}}(t, \mathbf{r})\) and not \(\mathbf{J}(t, \mathbf{r})\). To set the stage, consider \(\bar{\mathbf{J}}(t) = [\bar{j}_1(t), \bar{j}_2(t), \ldots, \bar{j}_N(t)]^T\) where \(\bar{j}_i(t) = (W_{i0}(t), \mathbf{J}(t, \mathbf{r}, t))\). The standard discretized Ampere’s law yields

\[
\epsilon_0 \left[ \nabla \right]^T [\star_{\varepsilon}] \partial_t \bar{\mathbf{E}}(t) = \left[ \epsilon_0 \left[ \nabla \right]^T \bar{\mathbf{J}}(t) \right]
\]  

(22)
Using $\tilde{\eta}(t) = [\nabla]^T \tilde{J}(t)$ and testing with $W_n(t)$ simplifies the notation to
\[ \{W_n(t), \, \tilde{\eta}(t)\} = \{W_n(t), \, \tilde{\eta}(t)\}. \tag{23} \]
Evaluating the integrals as listed above yields the following stencil:
\[ \phi^{n+1} - \phi^{n-1} = \Delta t,_{\text{coup}} \frac{\tilde{\eta}^{n+1} + \tilde{\eta}^{n-1}}{4}. \tag{24} \]
But Gauss’ law is slightly different; indeed, $\tilde{\rho}(t) = \int_0^t d\tau \tilde{\eta}(\tau)$. This implies that the discrete evolution of Gauss’ law yields
\[ \{W_n(t), \, \tilde{\rho}(t)\} = \{W_n(t), \, \tilde{\rho}(t)\}. \tag{25} \]
Then (25) simplifies to
\[ \phi^{n+1} + 2\phi^n + \phi^{n-1} = \tilde{\rho}^{n+1} + 2\tilde{\rho}^n + \tilde{\rho}^{n-1}. \tag{26} \]
But as only $\tilde{\eta}(t)$ is available, one would need to integrate this to obtain the charge density. Choosing a backward Euler scheme for illustration, we obtain
\[ \tilde{\rho}^n = \tilde{\rho}^{n-1} + \Delta t,_{\text{coup}} \tilde{\eta}^n. \tag{27} \]
Using (27) in (24) results in
\[ \phi^{n+1} - \phi^{n-1} = \frac{1}{4} \left( \phi^{n+1} + \phi^n - \phi^{n-1} - \phi^{n-2} \right). \tag{28} \]
It is apparent from above equations that, irrespective of the integration scheme, the coefficient obtained by solving Ampere’s law will not satisfy the discrete Gauss’ law.

The above discussion presents the nuances of the challenge in ensuring that the solution of the discrete curl equations satisfies Gauss’ law. When $\omega_0 = 0$, one can somewhat get around the challenge by defining $\tilde{G}(t)$. As we will see, this challenge cannot be overcome when $\omega_0 \neq 0$.

2) Case 2 ($\omega_0 \neq 0$): Next, we consider the effect of adding an analytically prescribed fast-varying function to our field solution. As before, we begin our analysis with the divergence of Ampere’s Law in (12) and obtain
\[ \epsilon_0 [\nabla]^T \left( [\epsilon_j] \frac{\partial}{\partial t} \tilde{E}(t) + j \omega_0 [\epsilon_j] \tilde{E}(t) \right) = -[\nabla]^T \left( e^{-j \omega_0 t} \frac{\partial}{\partial t} \tilde{G}(t) \right). \tag{29} \]
Using the notation defined earlier and testing with $W_n(t)$, we get
\[ \{W_n(t), \, \phi(t) + j \omega_0 \tilde{\rho}(t)\} = \{W_n(t), \, \exp(-j \omega_0 t) \bar{\delta}_t \tilde{\rho}(t)\}. \tag{30} \]
Evaluating the inner product integrals yields
\[ \left( j \omega_0 \frac{\Delta t,_{\text{coup}}}{2} + \frac{1}{2} \right) \phi^{n+1} = - j \omega_0 \frac{\Delta t,_{\text{coup}}}{2} \phi^n + j \omega_0 \frac{\Delta t,_{\text{coup}}}{4} \left( \phi^{n+1} + \phi^{n-1} (\omega_0) \phi^{n+1} \right) + \beta^n (\omega_0) \phi^n + \beta^{n-1} (\omega_0) \phi^{n-1} \tag{31} \]
where $\beta^{n+1}(\omega_0)$, $\beta^n(\omega_0)$, and $\beta^{n-1}(\omega_0)$ are defined in Section V. If charge conservation is achieved, then we should be able to find a testing function $\tilde{W}_n(t)$ that when used to measure Gauss’ Law will reduce it to a form that is satisfied by the solution to (31).

Let us first begin by setting $\tilde{W}_n(t) = \delta(t - t_n)$. Testing Gauss’ law with this function will lead to
\[ \{\delta(t - t_n), \, \tilde{\rho}(t)\} = \{\delta(t - t_n), \, \exp(-j \omega_0 t) \tilde{\rho}(t)\}. \tag{32} \]
which when evaluated leads to the following relation for $\phi^n$:
\[ \phi^n = \exp(-j \omega_0 t_n) \tilde{\rho}. \tag{33} \]
Comparing this relation to (31), we find that the point-wise relation for $\phi$ does not satisfy the stencil for the divergence of Ampere’s Law. Interestingly, the solutions do agree in the limit when $\omega_0 \to 0$, but otherwise, they are inconsistent. Likewise, if we were to perform a similar analysis with $\tilde{W}_n(t) = \tilde{W}(t)$, we end up with the following update expression for $\phi^{n+1}$:
\[ \frac{\Delta t,_{\text{coup}}}{4} \phi^{n+1} = - \frac{\Delta t,_{\text{coup}}}{2} \phi^n - \frac{\Delta t,_{\text{coup}}}{4} \phi^{n-1} + \alpha^{n+1} (\omega_0) \tilde{\rho}^{n+1} + \alpha^n (\omega_0) \tilde{\rho}^n + \alpha^{n-1} (\omega_0) \tilde{\rho}^{n-1}. \tag{34} \]
Once again, the coefficients $\alpha^{n+1}(\omega_0)$, $\alpha^n(\omega_0)$, and $\alpha^{n-1}(\omega_0)$ refer, respectively, to the inner products of $W_n(t)$ and $\exp(-j \omega_0 t)$ multiplying the basis functions used to represent the field quantities in time $N_{n,0}(t)$, $N_{n,1}(t)$, and $N_{n,2}(t)$, respectively, [defined in (10c)]. As before, (34) and (31) agree in the limit of $\omega_0 \to 0$, they are inconsistent for finite $\omega_0$.

While neither choice of $\tilde{W}_n(t)$ results in discrete systems that are consistent with (31), and there may never be, we take a different and more robust path. In addition to the above difficulties, we note the following: The standard Newmark time stepping scheme excites a null space that is time independent. While the null space can be small, it will not have a trivial divergence and will corrupt the satisfaction of Gauss’ law [16]. A way to overcome both problems is to use a Helmholtz decomposition or impose a Coulomb gauge in the discrete setting. The means to do so is elaborated next.

### C. Quasi-Helmholtz or Coulomb Gauge

Much of the development of what follows has been detailed in our earlier article [14]. The following discussion is purely for completeness of the article. In a nutshell, $\tilde{E}(r, t)$ and $\tilde{B}(r, t)$ can be decomposed into solenoidal (components that are divergence free) and non-solenoidal components (have a finite curl). We note that this decomposition is not a true Helmholtz decomposition since we do not separate the fields into divergence-free and curl-free components (as is possible in the continuous world). As a result, the resulting formulation is a quasi-Helmholtz decomposition. In this framework, Gauss’ laws are explicitly discretized and solved. Furthermore, while the solution for the solenoidal component has a null space, its divergence is exactly zero. As a result, Gauss’ laws are exactly satisfied.

In what follows, we use $\tilde{E}_n^a$ that refers to the non-solenoidal coefficients of the electric field at the nth timestep. Likewise, $\tilde{E}_n^a$ and $\tilde{B}_n^a$ refer to the divergence-free solenoidal coefficients of the electric field and magnetic flux density, respectively. A complete prescription of all submatrices involved is provided in Section V.
1) Requisite Projectors: To project the non-solenoidal components from the basis used for representing the electric field, we define projectors \( \hat{P}_{e}^{\Sigma} \) and \( \hat{P}_{b}^{\Lambda} \) that, when operated on the complete electric field, respectively, extract the non-solenoidal and solenoidal components (where \( \dagger \) represents a Moore–Penrose pseudoinverse).

\[
\begin{align*}
\hat{P}_{e}^{\Sigma} & = \Sigma \left( \Sigma^T \Sigma \right)^{\dagger} \Sigma^T \\
\hat{P}_{e}^{\Lambda} & = \mathcal{I} - \hat{P}_{e}^{\Sigma} \\
\hat{P}_{b}^{\Lambda} & = \mathcal{I} - \Sigma_m \left( \Sigma_m^T \Sigma_m \right)^{\dagger} \Sigma_m^T
\end{align*}
\]  

(35a)

(35b)

(35c)

where \( \Sigma = \epsilon_0 \hat{M}_e \) and \( \Sigma_m = [\nabla \cdot]^T \). Using these projectors, we can now define a decomposition for the electric flux density as

\[
\vec{D}(t) = \vec{\Sigma} \vec{E}_{\text{ns}}(t) + \left[ \hat{P}_{e}^{\Lambda} \right] \vec{D}(t)
\]

(36)

and the magnetic flux density as

\[
\vec{B}_e(t) = \left[ \hat{P}_{b}^{\Lambda} \right] \vec{B}(t).
\]

(37)

Using this projector, it is rather straightforward to show that the divergence of \( \vec{B}(t) \) is zero.

2) Discrete System: To use this decomposition, we use all of Maxwell’s equations. First given the divergence of the electric field system treated analytically. The specifics of the resulting integration rule can be written as

\[
\begin{align*}
\frac{d\vec{v}}{dt}(\vec{r}_p, t) &= \frac{q_p}{m_p} \text{Re} \left\{ \vec{E}(\vec{r}_p, t) \exp[j\omega_0 t] \right\} \\
&+ \frac{q_p}{m_p} \vec{v}(\vec{r}_p, t) \times \text{Re} \left\{ \vec{B}(\vec{r}_p, t) \exp[j\omega_0 t] \right\}
\end{align*}
\]

(40)

which can be numerically integrated with the fast-varying components treated analytically. The specifics of the resulting integration rule can be written as

\[
\begin{align*}
\vec{v}(\vec{r}_p^{n+1}, t_{n+1}) - \vec{v}(\vec{r}_p^n, t_n) &= \frac{q_p}{m_p} \sum_{k=0}^{2} \vec{E}(\vec{r}_p^{n-1-k}, t_{n-1-k}) \left( M_{n,k}^r + M_{n,k}^i \right) \\
&+ \frac{q_p}{m_p} \sum_{k=0}^{2} \vec{v}(\vec{r}_p^{n-1-k}, t_{n-1-k}) \times \vec{B}(\vec{r}_p^{n-1-k}, t_{n,1,k}) \\
&\quad \times (L_{n,k}^r + L_{n,k}^i)
\end{align*}
\]

(41)

where the operators used are defined as follows:

\[
\begin{align*}
L_{n,j,k}^r &= \int_{t_j}^{t_{j+1}} N_{n,j}(t) N_{n,k}(t) \cos(\omega_0 t) \, dt \\
L_{n,j,k}^i &= \int_{t_j}^{t_{j+1}} N_{n,j}(t) N_{n,k}(t) \sin(\omega_0 t) \, dt \\
M_{n,j}^r &= \int_{t_j}^{t_{j+1}} N_{n,j}(t) \cos(\omega_0 t) \, dt \\
M_{n,j}^i &= \int_{t_j}^{t_{j+1}} N_{n,j}(t) \sin(\omega_0 t) \, dt.
\end{align*}
\]

(42a)

(42b)

(42c)

(42d)

The particle positions can then be integrated consistently in time at \( \Delta t, \omega_0 \) through a fourth-order Adams–Bashforth stencil

\[
\vec{r}_p^{n+1} = \vec{r}_p^n + \Delta t, \omega_0 \left( \frac{55}{24} \vec{r}_p^n - \frac{59}{24} \vec{r}_p^{n-2} + \frac{37}{24} \vec{r}_p^{n-3} \right)
\]

(43)

Since the particle positions cannot be downshifted in the same way as the velocity update, some oversampling is still required to maintain accuracy, but as we show in Section IV-B, this factor is relatively small. The computed trajectories can then be used to obtain \( \vec{G}(t) \)

\[
\begin{align*}
\vec{G}_i^{\text{nt}} &= \left\{ \hat{W}_i^{(1)}(\vec{r}_p(n \Delta t, \omega_0)) \sum_{p=1}^{N_p} \int_{t_p^{(0)}}^{t_p^{(n \Delta t, \omega_0)}} \text{d} \vec{S} \left( \vec{r} - \vec{r}_p \right) \right\}
\end{align*}
\]

(44)

where \( n \) refers to the number of timesteps evolved by the EM system, and \( l \) refers to a specific edge in the EM system.

In systems where the number of particles is not very large, and therefore the cost of a particle update is negligible in relation to the cost of a field solve, we can follow a simpler integration setup and simply interpolate the electric field to time points that are spaced at \( \Delta t, \omega_0 \). To do this, one would have to use a predictor–corrector scheme, where an explicit particle push of sufficiently high polynomial order is used to compute.

---

D. Particle Push and Integration Scheme for \( \vec{G} \)

Next, we describe the framework used to evolve particle trajectories following (6). We recall from Section III-C that the error in the non-solenoidal component of the electric field is tied intimately to the accuracy in the evaluation of \( \vec{G}(t) \), making it important to evaluate the particle positions and velocities to high accuracy. But it is also known that the Fourier transform of the velocity or the position of any particle is not necessarily narrowband. As a result, the equations of motion and the path integral need to be evaluated at a step size \( \Delta t, \omega_0 \), while samples of the field are only known at \( \Delta t, \omega_0 \) times. There are two ways to get around this mismatch. First, one can incorporate the analytically known fast varying field components into the Lorentz update

\[
\begin{align*}
\frac{d\vec{v}}{dt}(\vec{r}_p, t) &= \frac{q_p}{m_p} \text{Re} \left\{ \vec{E}(\vec{r}_p, t) \exp[j\omega_0 t] \right\} \\
&+ \frac{q_p}{m_p} \vec{v}(\vec{r}_p, t) \times \text{Re} \left\{ \vec{B}(\vec{r}_p, t) \exp[j\omega_0 t] \right\}
\end{align*}
\]

(40)
the fields at the next timestep. After this, the magnitudes of the electric fields and magnetic flux density at the location of a given particle $p$ can be reconstructed from the downshifted quantities at a given time $t \in [t_{n-1}, t_{n+1}]$ as

$$ E(r, t) = \sum_{j=1}^{N_p} \sum_{k=0}^{2} N_{n,k}(t) \hat{E}_j^k \exp\{ j \omega_0 t_{n-1+k} \} W_j^1 (r_p) \quad (45a) $$

$$ B(r, t) = \sum_{j=1}^{N_p} \sum_{k=0}^{2} N_{n,k}(t) \hat{B}_j^k \exp\{ j \omega_0 t_{n-1+k} \} W_j^2 (r_p) \quad (45b) $$

These fields can then be used in an implicit Lorentz update at the smaller stepsize. Since the particle paths are now known at the finer timestep size $\Delta_{t,0}$, the path integral in (44) can be evaluated as

$$ \int_{r(0)}^{r(n \Delta_{t,0})} d\tilde{r}S(r-\tilde{r}) = \sum_{j=0}^{M-1} \int_{r(p(j \Delta_{t,0})}^{r(p((j+1) \Delta_{t,0}))} d\tilde{r}S(r-\tilde{r}) \quad (46) $$

where $M$ refers to the number of timesteps needed at $\Delta_{t,0}$ to advance to a time of $n \Delta_{t,0}$. We show, once again, in Section IV-B that this approach can be used to get precision similar to the actively downshifted integration scheme described earlier in the section, but the rate of oversampling required is larger. Note, in both these methods, we have assumed non-relativistic motion. Studies are underway on efficient methods in relativistic regimes.

**IV. Numerical Experiments**

In this section, we detail results obtained from an implementation of the ET-FEMPIC scheme described above. The results will be structured as follows: 1) first, we demonstrate the viability and computational gains of using envelope tracking in a linear EM system without particles by analyzing the radiated power due to a monopole antenna and 2) next, we demonstrate the accuracy of the integration scheme developed in Section III-D. Then, we proceed to analyze two systems with particles, thereby including non-linear effects from the active media. As a prelude, we note that the modulated Gaussian functions used in some of the numerical examples are defined as follows:

$$ v(t) = \cos(\omega_0 t) \exp\left(-\frac{(t-\sigma)^2}{2\sigma^2}\right) $$

$$ \sigma = \frac{2}{\omega_{bw}} \quad (47) $$

**A. Radiated Power From a Monopole Antenna**

We consider a conducting strip suspended over a finite ground plane, as specified in Fig. 2(a). The coupling between the EM system and the driving circuit is achieved across a vertical 1 cm edge going from the conducting plane to the strip. The current driving the antenna is generated by a Thevenin source characterized by $f_0 = 300$ MHz and $f_{bw} = 200$ MHz connected in series to a 100 $\Omega$ resistor. The circuit subsystem itself was modeled through a modified nodal analysis network [22], with the constituent equations appropriately modified to account for the analytically known fast field components. The voltage and current across the port feed were then used to compute the complex impedance of the feed as a function frequency. The radiated power curves for the antenna were computed from the impedance obtained from a regular MFEM solve and through the envelope tracking technique described in this work. As can be seen in Fig. 2(b), there is good agreement in the radiated power as a function of frequency between a regular MFEM and the envelope tracking method, despite the timestep size in the latter being 2.5 times larger.

**B. Fidelity of the Particle Push Routine**

Since the particle positions and velocities are not known to conform to the same frequency spread as the fields, we proposed two different time-stepping schemes in Section III-D to accurately evolve Newton’s equations. The numerical results presented in this section demonstrate the viability of both
TABLE I

| $f_{\text{op}}$ (MHz) | $N_{\text{Regular}}$ | $e^{\text{err}}$ ($N_{\text{Regular}}$) | $N_{\text{Downshift}}$ | $e^{\text{err}}$ ($N_{\text{Downshift}}$) |
|----------------------|-----------------------|--------------------------------------|------------------------|--------------------------------------|
| 20                   | 100                   | $4.135 \times 10^{-9}$              | 21                     | $3.916 \times 10^{-9}$              |
| 10                   | 200                   | $3.308 \times 10^{-9}$              | 54                     | $6.392 \times 10^{-9}$              |
| 5                    | 400                   | $2.591 \times 10^{-9}$              | 117                    | $7.997 \times 10^{-9}$              |
| 1                    | 2000                  | $1.195 \times 10^{-9}$              | 501                    | $2.410 \times 10^{-8}$              |

The comparison was done against numerically obtained data at $\Delta t_{\text{bench}} = \Delta t_{\text{bench}}/10$. $N_{\text{Regular}}$ and $N_{\text{Downshift}}$ refer to the oversampling factor for the naively oversampled and downshifted methods respectively, and $e^{\text{err}}$ refers to the $L^2$ error of a given method compared against the benchmark data. We note that the oversampling factor required for the downshifted method is significantly lower than with naive oversampling. In each case, $f_0 = 2$ GHz.

methods. To set the stage, we consider a system consisting of one particle moving under the influence of $E(r, t) = \hat{x}v(t)$ and $B(r, t) = \hat{z}v(t)$ with $v(t)$ as defined in (47). The positions of the fields and velocities are then solved using two different methods. First, we use a particle solver that operates at a smaller timestep size $\Delta t_{\text{max}}$ than the field solve. The values of the field are then interpolated to the finer timesteps and used to evolve Newton’s equations. Since the fields conform to the bandwidth amenable for an envelope tracking analysis, the interpolation should be as accurate as a time-marching routine that evolves at steps of $\Delta t_{\text{max}}$. Second, we evolve the particle using the downshifted integration scheme described in Section III-D. The final position curves obtained from both methods were compared against a solution obtained using a fourth-order Adams–Bashforth method evolved at $\Delta t_{\text{bench}} = \Delta t_{\text{max}}/10$. The relative error of the two methods in relation to this benchmark is reported in Table I. As is evident, both methods yield the same order of error over a range of center frequency/bandwidth combinations.

C. Klystron Excited by a Gap Voltage

Next, we analyze the EM response for a device with strong particle effects. Specifically, we examine the reduction in the quality factor of a Klystron under beam loading, with the setup as shown in Fig. 3. A sinusoidal RF source placed at the connecting neck, a 40-kV, 3 A beam was introduced on one end of the feed-tube. The gap voltage as a function of frequency was then computed from the Fourier transform of the measured electric field across an edge spanning the walls of the neck. The quality factor of the cavity was estimated by locating the half power points beneath the resonance peak, and computing $Q$ as

$$Q = \frac{f_{\text{peak}}}{\Delta f}.$$  (48)

We note from Fig. 4 and Table II that the quality factor when the klystron is loaded drops slightly in comparison to an unloaded run, with some of the energy of the cavity used to accelerate the particles. This acceleration can be seen by observing a histogram of particle velocities as a function of position along the length of the tube, as shown in Fig. 5. Likewise, we note in Fig. 6 that Gauss’ Laws are satisfied to machine precision. Furthermore, the quality factor derived using ET-FEMPIC is close to those derived from a traditional EM-FEMPIC solve but computed at approximately the tenth the number of timesteps. Furthermore, the drop observed is similar to that observed in [23] simulated using an axi-symmetric FDTD code. For a one-on-one comparison, we note from Fig. 7 that the results from the downshifted simulation agree closely with equivalent results run in a normal EM-FEMPIC solver. Finally, we note from Fig. 6 that Gauss’ Law is satisfied to machine tolerance.

D. Cascaded Klystron

Finally, in order to demonstrate the efficacy of ET-FEMPIC on a complex, larger scale problem, we consider an extension of the Klystron experiment from Section IV-C by analyzing a cascaded system. Specifically, we look at a two-cavity klystron. We first find an optimal spacing between the two-cavity openings such that the mutual coupling is maximized. This separation distance was estimated by analyzing the Fourier-domain response of the system (as shown in Table III). Here, this occurs when they are placed 15 cm apart along the feed-tube. As in the previous run, a background axial magnetic
TABLE II
TABULATED QUALITY FACTOR DATA IN THE KLYSTRON SOLVE

| \( t_{\text{max}}(\text{ns}) \) | \( N_t_{\text{ET-FEMPIC}} \) | \( Q_{\text{ET-FEMPIC}} \) | \( N_t_{\text{MPEM}} \) | \( Q_{\text{MPEM}} \) | \( Q_{\text{EM-FEMPIC}} \) | \( Q_{\text{ET-FEMPIC}} \) |
|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 135.6          | 1500           | 1079.1         | 13500          | 1084           | 903.7          | 899.4          |
| 90.4           | 1000           | 556.4          | 9000           | 561.4          | 484.9          | 488.4          |
| 67.8           | 750            | 231.4          | 6750           | 246.7          | 211.5          | 207.8          |

Here, \( N_t \) and \( Q \) refer respectively to the number of timesteps used in the analysis and the respective quality factor obtained. As can be seen in the table, the Envelope tracking approach closely tracks the results predicted by the MPEM solve.

Fig. 5. Velocity histogram at \( t = 100 \text{ ns} \) along the length of the Klystron showing particle acceleration when exposed to the RF source.

Fig. 6. Plot of relative error per particle in satisfaction of discrete Gauss’ Law for the Klystron setup simulated through ET-FEMPIC.

Fig. 7. Comparison between the loaded cavity responses obtained through the regular and downshifted frames.

Fig. 8. Plot of relative error per particle in satisfaction of discrete Gauss’ Law for the cascaded Klystron system simulated through ET-FEMPIC.

Once again, the RF-excitation at each port was set to be a modulated Gaussian pulse. The quality factor \( Q \) was measured at each peak by locating the resonance peak and finding the half power points. The specific values of the quality factor are reported in Table IV. We note that, as in the previous experiment, ET-FEMPIC yields very similar results as a traditional PIC solve, but at a significantly smaller timestep count.

Finally, we see in Fig. 8 that Gauss’ Laws are satisfied to machine precision.

E. Relativistic MILO

To stress the viability of the algorithm for a complex real-world device, we considered a setup with a relativistic MILO, as discussed in [24]. The layout of an axial cross section of

field of strength 1.5 \( T \) was applied and a 40-kV, 1.5 A beam was injected into the feed-tube. Since the cavities have the same dimensions, their resonance peaks coincided, allowing us to downshift the EM system from 4.1 GHz to baseband.
TABLE IV

| $\ell_{\text{max}}$ (ns) | $N_t$ | $Q_{\text{FEMPIC}}$ | $Q_{\text{FEMPIC}}$ | $Q_{\text{FEMPIC}}$ | $Q_{\text{FEMPIC}}$ | $Q_{\text{FEMPIC}}$ | $Q_{\text{FEMPIC}}$ |
|------------------------|-------|------------------|------------------|------------------|------------------|------------------|------------------|
| 135.6                  | 13500 | 1081.9           | 1086.1           | 1500             | 1075.1           | 1060.1           |                  |
| 90.4                   | 9000  | 503.4            | 499.4            | 1000             | 500.1            | 491.1            |                  |
| 67.8                   | 6750  | 247.3            | 248.1            | 750              | 246.1            | 235.1            |                  |

All reported values are for the beam-loaded setup. $N_t$ and $Q$ refer respectively to the number of timesteps used in the analysis and the respective quality factor obtained. Likewise, quantities with subscripts $P_1$ and $P_2$ respectively refer to measurements made at ports 1 and 2 respectively. As can be seen in the results, the Envelope tracking approach closely tracks the results predicted by the MFEMPIC solve.

the device is shown in Fig. 9, with red sections denoting PEC surfaces, green sections representing surfaces with an applied potential difference $V_{in}(t)$, dark green sections representing locations of particle emitters, and finally dashed blue sections representing surfaces where the output power $P_{out}(t)$ in the form of the Poynting flux across the surface is measured. $V_{in}(t) = \sin(2\pi f_0 t)$ was defined as a sinusoidal impulse with magnitude 1.8 MV at a center frequency of $f_0 = 1.2$ GHz. Likewise, the particles were emitted from inner conductor with a purely radial velocity of $2.12 \times 10^8$ ms$^{-1}$. Due to the high particle velocities in this example, the particle push algorithm described earlier was modified to solve the relativistic momentum. The particle current was set to 50 kA. This setup was simulated using the proposed method with a timestep size $\Delta t = 33.3$ ps. To provide a direct comparison, we also simulated this setup on XOOPIC [25] for the same parameters with $\Delta t = 1$ ps. A $z-r$ phase plot of the particles is shown in Fig. 9. Likewise, the spectrum of the output power is reported in Fig. 10. We note from both figures that the proposed method predicts particle distributions that agree closely with XOOPIC and further predicts an output spike at 1.2 GHz, as expected from other similar results in the literature [24].

F. Computational Complexity

Finally, we discuss the computational complexity of the method, and the range devices with the technique maximize savings in compute time. We wish to emphasize at this point that any time domain simulation method approach requires some means of fixing $\Delta t$. For explicit schemes with a mesh-dependant stability constraint, this is done quite trivially by looking at the smallest mesh features. For implicit methods that are similarly constrained by the mesh, the user needs to estimate a good $\Delta t$ based on a presumptive highest frequency of interest. Typically, this timestep size is inversely related to a factor multiplied by the highest frequency, that is,

$$\Delta t = \frac{1}{\xi (f_0 + f_{bw})}.$$  \hspace{1cm} (49)

As noted previously, when $\omega_0 = 0$, the method reduces back to a traditional EM-FEMPIC solve, so for highly broadband devices, the method is no more expensive than a traditional implicit EM-FEMPIC solve. For narrowband devices whose step size is heavily determined by the frequency offset in the fields, as opposed to the feature scales of the geometry, the savings in the number of timesteps can be estimated as follows. Under the proposed method, the frequency offset is analytically provided for, leading to a new timestep size given by

$$\Delta t = \frac{1}{\xi (f_{bw})}.$$  \hspace{1cm} (50)

Therefore, the number of timesteps required to go to a certain simulation time is reduced by a factor of $f_{bw}/(f_0 + f_{bw})$. This figure represents the reduction in number of steps for a device whose stepsize is determined entirely by the bandwidth of the fields. If the geometry of the simulation setup demands a smaller stepsize (as in the case of the relativistic MILO),

![Fig. 9. Layout and z-r phase distribution of particle positions along the MILO at 50 ns. Red sections denote conducting surfaces, green sections denote places with imposed potential differences, and dashed blue segments represent surfaces where the output power spectrum is measured.](image1)

![Fig. 10. Plot of the spectrum of output power obtained from the MILO using the method proposed in this work. We recover a peak at 1.2 GHz, as predicted by similar experiments in the literature [24].](image2)
one may have to choose a smaller stepsize than what would be demanded by the physics.

V. CONCLUSION

In this article, we have proposed a technique to greatly improve the computational performance of EM-FEMPIC codes for a class of narrowband high-frequency devices. Using a quasi-Helmholtz setup, we show that our method exactly satisfies charge conservation and achieves similar fidelity to a traditional FEMPIC solve. As an aside, we have spent considerable fraction of the article examining nuances of charge conservation from a different perspective. The upshot of this discussion is that the underlying rubric of quasi-Helmholtz decomposition is always robust and immune to null spaces that would otherwise corrupt the system. Additionally, our results demonstrate real-world speedups equal to the ratio between the frequency shift and the bandwidth. In particular, the Klystron example is used close to a tenth the number of timesteps compared to a traditional EM-FEMPIC solve. This is before any kind of additional speedup up for parallel processing is applied.

APPENDIX A
MATRICES INVOLVED IN THE QUASI-HELMHOLTZ DECOMPOSITION

As a prelude, we define the sets $N$, $E$, $F$, and $T$ as the set of nodes, edges, faces, and tetrahedrons, respectively, having $N_n$, $N_f$, $N_e$, and $N_t$ elements. The various submatrices used in describing the quasi-Helmholtz framework in Section III-C are as follows:

\begin{align}
[\bullet_i]_{i,j} &= \left[ W_1^{(1)}(r), \varepsilon \cdot W_j^{(1)}(r) \right] ; \quad i, j \in E \\
[\bullet_{\mu-1}]_{i,j} &= \left[ W_2^{(2)}(r), \mu^{-1} \cdot W_j^{(2)}(r) \right] ; \quad i, j \in F \\
[\bullet_{\rho}]_{i,j} &= \left[ W_3^{(3)}(r), W_j^{(3)}(r) \right] ; \quad i, j \in T
\end{align}

where $W_1^{(1)}$, $W_2^{(2)}$, and $W_3^{(3)}$ are the Whitney edge, face, and volume basis functions, respectively. Further, we define the following matrices:

\begin{align}
[M_g]_{i,j} &= \left[ W_1^{(1)}(r), \nabla W_j^{(0)}(r) \right] ; \quad i \in E, \quad j \in N \\
[M_e]_{i,j} &= \left[ W_2^{(2)}(r), \nabla \cdot W_j^{(2)}(r) \right] ; \quad i \in F, \quad j \in E \\
[M_d]_{i,j} &= \left[ W_3^{(3)}(r), \nabla \times W_j^{(3)}(r) \right] ; \quad i \in T, \quad j \in F \\
[\nabla] &= \varepsilon [\bullet_e]^{-1} [M_g] \\
[\nabla \times] &= \mu^{-1} [\bullet_{\mu-1}]^{-1} [M_e] \\
[\nabla \cdot] &= [\bullet_{\rho}]^{-1} [M_d]
\end{align}

Likewise the submatrices involved in (39) are as follows: where the various submatrices involved in (39) are defined as:

\begin{align}
[Z]_{11} &= \left[ C^b_c \right]^T \left[ P \right]_b^{\Lambda} \left[ C^b_c \right] \\
[Z]_{12} &= \left[ C^b_c \right]^T \left[ \nabla \times \right] [\bullet_e]^{-1} [P \left[ \bullet_{\mu-1} \right]^{\Lambda} [C^b_c]
\end{align}

where the $[C^b_c]$ matrices are mappings that identify unknowns that reside on the core. Constructing this mapping is trivial for simply connected structures, but is trickier for multiply connected geometries.

APPENDIX B
INCOMPATIBILITY OF $W$ AND $\delta$-TESTING

Suppose $\phi(t) = \tilde{\phi}(t)e^{j\omega t}$. We can represent this as

$$
\phi(t) = \sum_{i=-1}^{n+1} \tilde{\phi}^i N_i(t)e^{j\omega t}
$$

where $N_i(t)$ represents the regular second-order Newmark basis functions. $\rho$ is defined as is normally done in Newmark

$$
\rho(t) = \sum_{i=-1}^{n+1} \rho^i N_i(t).
$$

Now, $\partial_t \phi - \partial_t \rho$ becomes

$$
\sum_{i=-1}^{n+1} \left[ \tilde{\phi}^i \partial_t N_i(t)e^{j\omega t} + \rho^i \partial_t N_i(t) \right] = 0
$$

W-testing gives us

$$
\left\langle W(t), \sum_{i=-1}^{n+1} \left[ \tilde{\phi}^i \partial_t N_i(t)e^{j\omega t} + \rho^i \partial_t N_i(t) \right] \rightangle = \left\langle W(t), \sum_{i=-1}^{n+1} \tilde{\phi}^i \left( N_i(t)e^{j\omega t} \right) + e^{j\omega t} \partial_t N_i(t) \right\rangle
$$

$$
+ \left\langle W(t), \sum_{i=-1}^{n+1} \rho^i \partial_t N_i(t) \right\rangle = 0.
$$

Thus, there are six relevant terms in the expansion of $\langle W, \phi(t) \rangle$. They are as follows:

$$
\langle W(t), \partial_t \left( N_k e^{j\omega t} \right) \rangle = e^{j\omega t} \sum_{k=-n-1}^{n+1} \left[ \alpha_{k,0} + \alpha_{k,\Delta_t} e^{j\omega \Delta_t} + \alpha_{k,-\Delta_t} e^{-j\omega \Delta_t} \right]
$$

where

\begin{align}
\alpha_{n+1,0} &= \frac{4j + 2\omega \Delta_t}{2\omega^2 \Delta_t^3} \\
\alpha_{n+1,-\Delta_t} &= -\frac{2j + \omega \Delta_t}{2\omega^2 \Delta_t^3} \\
\alpha_{n+1,\Delta_t} &= \frac{-2j - 3\omega \Delta_t + 2(j \omega \Delta_t)^2 + 2(\omega \Delta_t)^3}{2\omega^2 \Delta_t^3} \\
\alpha_{n,0} &= \frac{-4j - 2(j \omega \Delta_t)^2}{\omega^2 \Delta_t^3}
\end{align}
\[ \alpha_{n,-\Delta t} = \frac{2j - 2\alpha \Delta t}{\omega^2 \Delta t^3} \]  
\[ \alpha_n,\Delta t = \frac{2j + 2\alpha \Delta t}{\omega^2 \Delta t^3} \]  
\[ \alpha_{n-1,0} = \frac{4j - 2\alpha \Delta t}{2(\omega \Delta t)^3} \]  
\[ \alpha_{n-1,-\Delta t} = \frac{-2j + 3\alpha \Delta t + j(\omega \Delta t)^2 - 2(\omega \Delta t)^3}{2(\omega \Delta t)^3} \]  
\[ \alpha_{n-1,\Delta t} = \frac{-2j - \omega \Delta t}{2(\omega \Delta t)^3}. \]  

We can conclude by inspection from the coefficients defined in (61a) that for general \( \omega \), all nine coefficients can be non-zero. As a result, the quantities \( \beta_k = \left[ a_k,0 + a_k,\Delta t e^{i\omega \Delta t} + a_k,-\Delta t e^{-i\omega \Delta t} \right] \) defined for \( k = \{n-1, n, n+1\} \) must also generally be non-zero. Then

\[ \langle W(t), \tilde{\phi}_n \phi_j \tilde{\rho} \rangle = \beta_{n+1} \phi^{n+1} + \beta_n \phi^n + \beta_{n-1} \phi^{n-1} e^{i\omega \Delta t} - \frac{\left( \phi^{n+1} - \phi^{n-1} \right)}{2} = 0 \]  

(62)
cannot be captured in a point-wise manner, since all three coefficients multiplying \( \phi^k \) can generally be non-zero, while the coefficients multiplying \( \phi^k \) only exist when \( k = \{n-1, n+1\} \).

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