Local, Explicit, and Charge-Conserving Electromagnetic Particle-In-Cell Algorithm on Unstructured Grids*

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Abstract—We present a charge-conserving electromagnetic particle-in-cell (EM-PIC) algorithm on unstructured grids based on a finite element time-domain (FETD) methodology with explicit field update, i.e., requiring no linear solver. The proposed explicit EM-PIC algorithm attains charge conservation from first principles by representing fields, currents, and charges by differential forms of various degrees, following the methodology put forth in [25]. The need for a linear solver is obviated by constructing a sparse approximate inverse (SPAI) for the FE system matrix, which also preserves the locality (sparsity) of the algorithm. We analyze in detail the residual error caused by SPAI on the motions of charged particles and beam trajectories and show that this error is several order of magnitude smaller than the inherent error caused by the spatial and temporal discretizations.

Index Terms—charge conservation, finite elements, particle-in-cell, plasma, sparse approximate inverse.

I. INTRODUCTION

In the past few decades, electromagnetic particle-in-cell (EM-PIC) algorithms coupled to time-dependent Maxwell’s equations [1]–[3] have been applied to a variety of problems involving charged particles and beam-wave interaction, including plasma-based accelerators [4]–[7], inertial confinement fusion [8], [9], and vacuum electronic devices [10]–[15]. Historically, EM-PIC algorithms have been mostly based upon regular grids and finite-difference approaches [16], [17] such as the celebrated Yee’s finite-difference time-domain (FDTD) algorithm. However, complex geometries involving curved (such as conformal cathodes and curved waveguide sections) or very fine geometrical features cannot be accurately modeled by regular grids because of ensuing ‘staircase’ (step-cell) effects. Although many studies have been done to ameliorate staircase errors in finite-differences, including the use of conformal finite-differences [18], [19], the most general solution to this problem is to employ irregular, unstructured grids (meshes). The finite-element (FE) method is a better option than FDTD in this case because it is naturally suited for such type of grids. In addition, FE enables a greater degree of space-adaptivity (using mesh refinement techniques) in a systematic fashion and can also be applied for transient problems using FE time-domain algorithms (FETD) [20], [21].

However, existing FE-based EM-PIC codes based on unstructured grids have three important drawbacks. First, FE-based EM-PIC algorithms tend to numerically violate charge conservation due to the fact that the continuity equation leaves residuals at the discrete level on unstructured grids. Past efforts to enforce charge conservation have included adding a posterior correction steps by Poisson’s solvers [16] or pseudo-currents [22]. However, the former approach requires a time-consuming linear solver at each time step and the latter introduces a diffusion parameter that may alter the physics. A recent charge-conserving PIC algorithm based on second-order vector wave equation for the electric field that does not require introduction of correction terms is described in [23], [24]. However, the solution space of the second-order vector wave equation in the time-domain includes spurious solutions with secular growth, of the form \( \nabla \phi \), which are not physical admissible solutions to Maxwell’s equations and can pollute the numerical results [25]–[27].

More recently, a gather-scatter algorithm with exact charge conservation on unstructured grids was described in [25], based on concepts borrowed from differential geometry [28], [29] and discrete differential forms [30], [31]. Charge-conserving PIC algorithms were also developed under similar tenets in [32], [33]. A second challenge for unstructured-grid EM-PIC algorithms is that the field solver is implicit, i.e., it requires the repeated solution of a linear system of equations sequentially at each time step [20]. Finally, a third challenge (shared by FDTD-based algorithms as well) is that their performance is hindered by the global Courant stability bounds on time steps used to advance fields and particles.

In order to overcome the second challenge noted above, a sparse approximate inverse (SPAI) strategy for unstructured meshes [34], [35] is incorporated here into an explicit FETD-based EM-PIC algorithm with exact charge-conserving properties developed in [25]. For a given mesh, the resulting SPAI explicit solver obtains an approximation for the inverse of the FE system matrix based on (powers of) the sparsity pattern of the original FE system matrix. This is done once-and-for all for any given mesh i.e., independently from any field excitation and particle distribution, and decoupled from the field update. The SPAI explicit solver is easily parallelizable and produces exponential convergence of the approximate inverse matrix.

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of the mesh, and \( \mathbf{B} \) in terms of Whitney 2 forms associated with faces of the mesh [25].

Next, using the generalized Stoke’s theorem to obtain semi-discrete equations followed by a leap-frog discretization in time (second-order symplectic time integration), the following full-discrete FETD scheme is obtained [25], [34]:

\[
\begin{align*}
\mathbf{B}^{n+\frac{1}{2}} &= \mathbf{B}^{n-\frac{1}{2}} - \Delta t \left[ \mathbf{D}_{\text{curl}} \right] \cdot \mathbf{E}^n \quad (1) \\
\left[ \mathbf{s} \right] \cdot \mathbf{E}^{n+1} &= \left[ \mathbf{s} \right] \cdot \mathbf{E}^n + \\
&\quad \Delta t \left( \left[ \mathbf{D}_{\text{curl}} \right]^T \cdot \left[ \mathbf{s} \right]^{n-1} \left[ \mathbf{B}^{n+\frac{1}{2}} - \mathbf{J}^{n+\frac{1}{2}} \right] \right) \quad (2)
\end{align*}
\]

where \( \Delta t \) is the time step increment, the superscript \( n \) denotes the time step index, and \( \mathbf{B} \), \( \mathbf{E} \), and \( \mathbf{J} \) are column vectors representing \( \mathbf{B} \) on each face, and \( \mathbf{E} \) and \( \mathbf{s} \) on each edge, respectively. In addition, \( \left[ \mathbf{D}_{\text{curl}} \right] \) is the incidence matrix representing the discrete exterior derivative (or, equivalently, the discrete curl operator distilled from the metric, that is, with elements in the set \( \{-1, 0, 1\} \) on the mesh [28], [34], and \( \left[ \mathbf{s} \right] \) and \( \left[ \mathbf{s}^{n-1} \right] \) are discrete Hodge (mass) matrices whose elements are given by the volume integrals [31], [34]

\[
\begin{align*}
\left[ \mathbf{s} \right]_{i,j} &= \epsilon \int \hat{W}_{i}^{(1)} \cdot \hat{W}_{j}^{(1)} d\Omega \\
\left[ \mathbf{s}^{n-1} \right]_{i,j} &= \mu^{-1} \int \hat{W}_{i}^{(2)} \cdot \hat{W}_{j}^{(2)} d\Omega
\end{align*}
\]

where \( \hat{W}_{i}^{(1)}, i = 1 \ldots N_E \) and \( \hat{W}_{i}^{(2)}, i = 1 \ldots N_F \) are the vector proxies of Whitney 1- and 2-forms [28] that span the set of \( N_E \) edges and \( N_F \) faces of the mesh, respectively. It can be shown that \( \left[ \mathbf{D}_{\text{curl}} \right]^T = \left[ \mathbf{D}_{\text{curl}} \right] \), the incidence matrix on the dual mesh [25], [28], [29], [40], [41]. Eqs. (1) and (2) constitute an implicit field solver because \( \left[ \mathbf{s} \right] \) is nondiagonal: in order to update the electric field from eq. (2) it is necessary to solve a large linear system of equations at every time step. The explicit scheme proposed here is detailed in Section II.D below.

B. Gather-scatter and particle pusher steps

In the gather step, Whitney forms are used to determine the electric and magnetic field values at the position of each particle, as depicted schematically in Fig. 2a. Specifically, from the values of \( \mathbf{E}^n \) on edges and \( \mathbf{B}^{n+\frac{1}{2}} \) and \( \mathbf{B}^{n-\frac{1}{2}} \) on faces, vector proxies of Whitney forms are used to interpolate \( \hat{E}^n(\vec{r}) \) and \( \hat{B}^n(\vec{r}) \) at any ambient point \( \vec{r} \), and in particular at the charged particles’ locations, by

\[
\begin{align*}
\hat{E}^n(\vec{r}) &= \sum_{i=1}^{N_E} \left[ \mathbf{E} \right]_{i}^{n} \hat{W}_{i}^{(1)}(\vec{r}) \\
\hat{B}^n(\vec{r}) &= \sum_{i=1}^{N_F} \frac{1}{2} \left( \left[ \mathbf{B} \right]_{i}^{n+\frac{1}{2}} + \left[ \mathbf{B} \right]_{i}^{n-\frac{1}{2}} \right) \hat{W}_{i}^{(2)}(\vec{r})
\end{align*}
\]

where \( \left[ \mathbf{E} \right]_{i}^{n} \) denotes the \( i \)-th element of the column vector \( \mathbf{E} \) and likewise for \( \left[ \mathbf{B} \right]_{i}^{n+\frac{1}{2}} \) and \( \left[ \mathbf{B} \right]_{i}^{n-\frac{1}{2}} \). This is illustrated schematically in Fig. 2a. In the scatter step, we compute the particle current densities mapped to the edges of the mesh, i.e. to the mesh-based quantity \( \mathbf{J}^{n+\frac{1}{2}} \), for incorporation back into the field solver. We adopt here the charge-conserving scatter for unstructured grids recently proposed in [25]. By referring

Fig. 1: Basic steps in a full-wave EM-PIC algorithm. On unstructured meshes, conventional field solvers for the electric field update are implicit, requiring the solution of a (large) linear system at each time step.

II. EXPLICIT FETD-PIC ALGORITHM

A typical EM-PIC algorithm consists of four basic steps [25]: (1) field solver (consisting of electric and/or magnetic field updates from Maxwell’s equations), (2) gather step (fields interpolation at each particle position), (3) scatter (assigning currents to grid edges and charges to grid nodes from the particle positions and velocities), and (4) particle acceleration and push (governed by Lorentz force and Newton’s law of motion). These four steps are sequentially performed at each time step, as illustrated in Fig. 1.

A. Field solver

In the language of differential forms for the electromagnetic field [39], the electric field \( \mathbf{E} \) and the (Hodge dual of the) current density \( *\mathbf{J} \) are represented as 1-forms, and the magnetic flux density \( \mathbf{B} \) is represented as a 2-form. On a mesh, 1-forms and 2-forms are associated to mesh edges and facets, respectively [28], [29]. Accordingly, in order to discretize Maxwell’s equations, the FETD algorithm expands \( \mathbf{E} \) and \( *\mathbf{J} \) in terms of Whitney 1-forms associated with edges
to the exact inverse matrix as the density (sparsity) of the former is increased (reduced) [34]. Importantly, since sparsity is retained, the algorithm remains local [35]. The explicit and sparse nature of the resulting EM-PIC algorithm enables integration with asynchronous time stepping techniques [36]–[38] designed to overcome the third challenge indicated above. We investigate in detail here the effect of the approximate inverse on the particle dynamics by comparing particle trajectories computed with the new proposed algorithm against analytical solutions (when available) and a conventional implicit EM-PIC algorithm employing a direct LU-solver. We show that the error caused by the SPAI approximation is several order of magnitude smaller than inherent space and time discretization errors.
to Fig. 2b, given the initial \( \vec{r}_p^n \) and final \( \vec{r}_p^{n+1} \) locations of a particle \( p \) with charge \( q_p \) during a time step \( \Delta t \), the associated current flowing along edge \( e \) is written as

\[
[j]^n_e = \frac{q_p}{\Delta t} \int_{\vec{r}_p^n}^{\vec{r}_p^{n+1}} \vec{W}^{(1)}(\vec{r}) \cdot d\vec{l} = \frac{q_p}{\Delta t} \left[ \lambda_1(\vec{r}_p^n) - \lambda_1(\vec{r}_p^{n+1}) \right]
\]

where \( \lambda_1(\vec{r}) \) are the barycentric coordinates of point \( \vec{r} \) w.r.t vertices 1 and 2 respectively (the boundary points of edge \( e \) in consideration). Analogous assignments follow for the other edges of the mesh.

C. Discrete continuity equation

As demonstrated in [25], the above scatter algorithm yields exact charge conservation at the discrete level because the variation of the charge at any node of the mesh exactly matches the total current flowing in or out of that particular node. In other words, the following discrete continuity equation (DCE) holds

\[
[D]^{\star}_{\text{div}} \cdot [j]^{n+\frac{1}{2}} + \frac{Q^{n+1} - Q^n}{\Delta t} = 0
\]

where \( [D]^{\star}_{\text{div}} \) is the incidence matrix associated to the discrete divergence operator in the dual mesh, which is also equal to \( [D]^{T}_{\text{grad}} \) [25], [28], [29], [40], [41], and \( Q^n \) denotes the column vector with the charge associated to each node of the mesh\(^1\). Note that the nodal charge at any node \( i \) is obtained from the sum of the nearby particle charges weighted by their corresponding barycentric coordinates w.r.t. particular node, that is

\[
[Q]^n_i = \sum_p q_p \lambda_i(\vec{r}_p^n).
\]

Barycentric coordinates can be identified as Whitney 0-forms associated to a particular node \( i \), i.e. \( W^{(0)}(\vec{r}_p^n) = \lambda_i(\vec{r}_p^n) \) [28], [29]. We provide a geometrical illustration of (8) in Fig. 2b. From eq. (9), the charge variation at node 1 due to a charged particle movement during \( \Delta t \) is proportional to

\[
\lambda_1(\vec{r}_p^{n+1}) - \lambda_1(\vec{r}_p^n).
\]

This quantity is represented by the blue-colored area in Fig. 2b. At the same time, from eq. (7), the current flowing along edge 1 is associated with the factor \( \lambda_1(\vec{r}_p^n)\lambda_2(\vec{r}_p^{n+1}) - \lambda_1(\vec{r}_p^{n+1})\lambda_2(\vec{r}_p^n) \), which is equal to the red-colored area in Fig. 2b. A similar factor is present for edge 2 which is indicated by the green-colored area. From the area equivalences, it is clear that the sum of the current flow out of node 1 along edges 1 and 2 is equal to the charge variation on node 1.

The particle push step computes the Lorentz force acting on each charged particle given the (interpolated) electric and magnetic fields at the particle location and its velocity, and applies Newton’s force law to accelerate the particle. This step is implemented here by extending the particle push described in [25] to the relativistic regime based on the methodology put forth in [42].

D. SPAI

As noted above, a linear solve (implicit time-update) is required in (2) due to the presence of \([\star_e]^{-1}\) multiplying the unknown \( \mathbb{E}^{n+1} \) on the l.h.s. Naively, this linear solve could be avoided by pre-multiplying both sides of (2) by \([\star_e]^{-1}\), leading to

\[
\mathbb{E}^{n+1} = \mathbb{E}^n + \Delta t \cdot [\star_e]^{-1} \cdot \left( [D]^{\star}_{\text{curl}} \cdot [\star_{\mu-1}] \cdot \mathbb{B}^{n+\frac{1}{2}} - [j]^{n+\frac{1}{2}} \right).
\]

This multiplication is, of course, wholly impractical for large problems because \([\star_e]^{-1}\) is dense and such a direct inversion is computationally very costly and scales poorly with size. Even for relatively small problems, the fact that \([\star_e]^{-1}\) is dense makes the algorithm non-local and unsuited for asynchronous time-update algorithms [36]. Instead, to obtain an explicit and local field update algorithm, we explore the fact that, in the continuum, not only \( \star_e \) but also \( \star_e^{-1} \) are strictly local operators [31], [35], [43]. This indicates that, although dense, \([\star_e]^{-1}\) should be well approximated by a sparse approximate inverse (SAPI), which we denote \([\star_e]_a^{-1}\). Each column of \([\star_e]_a^{-1}\) can be obtained independently (and in parallel fashion) once a suitable sparsity pattern for \([\star_e]_a^{-1}\) is chosen. Since the sparsity pattern of \([\star_e]\) encodes nearest-neighbor edge adjacency, good candidates for the sparsity pattern of \([\star_e]_a^{-1}\)

\[\text{Fig. 2: Charge-conserving gather and scatter steps [25]. (a) Interpolation of } \vec{E} \text{ and } \vec{B} \text{ at the position of the particle by edge-based (left) and face-based degrees of freedom contributions (right) (weighted by the Whitney functions) in the gather step. (b) Exact charge-conserving scatter scheme. The sum of the two colored areas in the left, representing the magnitude of the edge currents, is equal to the blue area in the left, representing the charge variation at node 1 during one time step.}\]
are $[\ast]^{k}_{\ast}$ for $k = 1, 2, \ldots$, which would encode $k$-nearest neighbor adjacency among edges (with larger $k$ providing better accuracy but denser matrices). A parallel algorithm for computing $[\ast]^{-1}_{\ast}$ along these lines is detailed in [34], where it is also shown that the Frobenius norm of the difference matrix $\| [\ast]^{-1}_{\ast} - [\ast]^{-1}_{\ast} \|_F$ has exponential convergence to zero for increasing $k$.

Once $[\ast]^{-1}_{\ast}$ is precomputed, the explicit and local SPAI-based field update simply writes

$$
E^{n+1} = E^n + \Delta t [\ast]^{-1}_{\ast} \cdot \left( [D^{\ast}_{\text{div}}] \cdot [\ast]^{-1}_{\ast} \cdot E^{n+\frac{1}{2}} - J^{n+\frac{1}{2}} \right) .
$$  \hspace{1cm} (11)

E. Discrete Gauss’ law

By premultiplying both sides of (11) by $[D^{\ast}_{\text{div}}] [\ast]_{\ast}$, where $[D^{\ast}_{\text{div}}]$ is the incidence matrix representing the discrete divergence operator on the dual grid, and using the identity $[D^{\ast}_{\text{div}}] [D^{\ast}_{\text{curl}}] = 0$ [28], [29], [40], we obtain

$$
[D^{\ast}_{\text{div}}] [\ast]_{\ast} E^{n+1} = [D^{\ast}_{\text{div}}] [\ast]_{\ast} E^n - \Delta t [D^{\ast}_{\text{div}}] J^{n+\frac{1}{2}} .
$$  \hspace{1cm} (12)

This last equation can be rearranged as

$$
[D^{\ast}_{\text{div}}] [\ast]_{\ast} \left( \frac{E^{n+1} - E^n}{\Delta t} \right) = - [D^{\ast}_{\text{div}}] J^{n+\frac{1}{2}} ,
$$  \hspace{1cm} (13)

which, using (8), can be rewritten as

$$
[D^{\ast}_{\text{div}}] [\ast]_{\ast} \left( \frac{E^{n+1} - E^n}{\Delta t} \right) = Q^{n+1} - Q^n .
$$  \hspace{1cm} (14)

Eq. (14) implies that residuals of the discrete Gauss’ law (DGL) at any two successive time steps remain the same, in other words

$$
[D^{\ast}_{\text{div}}] [\ast]_{\ast} E^{n+1} - Q^{n+1} = [D^{\ast}_{\text{div}}] [\ast]_{\ast} E^n - Q^n ,
$$  \hspace{1cm} (15)

and by induction,

$$
[D^{\ast}_{\text{div}}] [\ast]_{\ast} E^n - Q^n = [D^{\ast}_{\text{div}}] [\ast]_{\ast} E^0 - Q^0 .
$$  \hspace{1cm} (16)

for all $n$, so that if initial conditions have $[D^{\ast}_{\text{div}}] [\ast]_{\ast} E^0 = Q^0$, then the DGL is verified for all time steps.

In the next Section, we analyze the error incurred by the above SPAI approximation to obtain an explicit field solver for EM-PIC simulations on unstructured grids.

III. Numerical Results and Discussion

In order to investigate the error caused by the SPAI-based explicit solver in EM-PIC simulations, we consider in this Section examples involving single charged-particle trajectories, a plasma ball expansion, and an accelerated electron beam.

A. Single-particle trajectories

Typical PIC simulations comprise an ensemble of superparticles effecting a coarse-graining of the phase-space. As such, instantaneous errors in individual particle trajectories may not always be relevant when computing grid-averaged physical quantities. Nevertheless, it is of interest to examine the secular trends on the particle trajectory discrepancies.

We investigate the motion of a single charged particle initially positioned at the origin in the presence of an external magnetic field $B^\text{ext}$ and electric field $E^\text{ext}$. In this case, the exact solution can be written as [44]

$$
x(t) = \frac{v_{x,0}}{\omega_c} \cos \omega_c t + \left( \frac{v_{x,0}}{\omega_c} + \frac{q_p E^\text{ext}}{m_p \omega_c^2} \right) \sin \omega_c t
$$

$$
- \frac{q_p E^\text{ext}}{m_p \omega_c^2} \frac{v_{y,0}}{\omega_c} t + \frac{v_{y,0}}{\omega_c} ,
$$

$$
y(t) = \frac{v_{y,0}}{\omega_c} \sin \omega_c t - \left( \frac{v_{x,0}}{\omega_c} + \frac{q_p E^\text{ext}}{m_p \omega_c^2} \right) \cos \omega_c t
$$

$$
+ \frac{q_p E^\text{ext}}{m_p \omega_c^2} + \frac{v_{y,0}}{\omega_c} ,
$$  \hspace{1cm} (17)

where $v_{x,0}$ and $v_{y,0}$ are the initial velocity components.

We examine two types of single-particle trajectories. The first corresponds a pure cyclotron motion ($B_z \neq 0$ and $E_y = 0$) and the second includes a drift motion as well ($B_z \neq 0$ and $E_y \neq 0$). We assume a superparticle with $q_p = -1.6 \times 10^{-15}$ [C] and mass $m_p = 9.1 \times 10^{-27}$ [kg]. In both cases, the initial velocity is set equal to $2 \times 10^8$ [m/s]. We consider three unstructured meshes labeled, from coarsest to finest, as 1, 2, and 3, all of which discretize the domain $\Omega = \{(x, y) \in [0, 1]^2 \}$. Table I provides information about the number of elements and other properties of the meshes considered. The parameter $\Delta l_{av}$ indicates the average edge length, which roughly halves for each mesh index increment.

<table>
<thead>
<tr>
<th>Table I: Number of elements in Meshes 1, 2, and 3</th>
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<tbody>
<tr>
<td>Mesh</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
</tbody>
</table>

The boundaries of the solution domain are truncated using a perfectly matched layer (PML) [26], [27], [45]. The time increment is chosen as $\Delta t = 10$, 5, and 2.5 [ps] for meshes 1, 2, and 3, respectively, and the simulation is terminated at $t = 150$ [ns].

An implicit solver based on LU decomposition is used as reference. Charged-particle trajectories calculated by using such LU solver are referred to as standard trajectories. On the other hand, particle trajectories obtained by the SPAI-based explicit field solver are designated as test trajectories. The effect of the inverse approximation error can be quantified by examining the discrepancy between standard and test trajectories. This discrepancy can be further compared to the discrepancy in particles’ trajectories between that result from
To quantify the error, we define the relative position difference (RPD), which is the ratio of the magnitude of the difference between the standard and test position vectors at certain time step \( n \) to the total travel length of the standard particle up to time step \( n \), i.e.,

\[
\text{RPD}_{\text{test}}^{n} = \frac{\frac{1}{n} \sum_{i=1}^{n} |\vec{r}_{p, \text{test}}^{i} - \vec{r}_{p, \text{std}}^{i}|}{|\vec{r}_{p, \text{std}}^{n}|} = \frac{|\vec{d}_{\text{test}}^{n}|}{|\vec{d}_{\text{std}}^{n}|} \tag{18}
\]

where \( \text{RPD}_{\text{test}}^{n} \) is the RPD for the \( j \)-th test particle at time instant \( n \), and \( \vec{r}_{p, \text{std}}^{n} \) and \( \vec{r}_{p, \text{test}}^{n} \) are the standard and test particle position, respectively, at time step \( i \).

For visualization purposes, we plot the RPD in a polar graph as shown in Fig. 3, with the radial coordinate represented in a logarithmic scale. The standard trajectory points computed by the implicit LU-based solver are indicated by \( \triangle \) and placed at the origin of the RPD for all times. The symbols \( \bigcirc, +, \times, \square \) represent, in turn, the relative position of test particles’ 1, 2, 3, and 4 w.r.t. to standard trajectory points, as given by the vector \( \vec{d}_{\text{test}}^{n}/|\vec{d}_{\text{std}}^{n}| \). As summarized in Table II, these four sets of points correspond, respectively, to the exact trajectory points obtained via an analytic solution and to the trajectory points obtained using the SPAI-based explicit field solver with \( k = 2, 4, \) and 6.

**Table II:** Conventional used for particle trajectory visualization.

<table>
<thead>
<tr>
<th>solver</th>
<th>test particle number</th>
<th>symbol used</th>
</tr>
</thead>
<tbody>
<tr>
<td>analytical sol.</td>
<td>1</td>
<td>\bigcirc</td>
</tr>
<tr>
<td>SPAI ( k = 2 )</td>
<td>2</td>
<td>+</td>
</tr>
<tr>
<td>SPAI ( k = 4 )</td>
<td>3</td>
<td>\times</td>
</tr>
<tr>
<td>SPAI ( k = 6 )</td>
<td>4</td>
<td>\square</td>
</tr>
</tbody>
</table>

1) Circular trajectory: In this case \( B_{x}^{\text{ext}} = 5.085 \times 10^{-3} \text{ [Wb/m}^{2}\text{]} \) and \( E_{y}^{\text{ext}} = 0 \text{ [V/m]} \) so that a pure cyclotron motion with angular frequency \( \omega_{c} = 6.05 \times 10^{2} \text{ [rad/s]} \) results. Fig. 4 illustrates the result of the SCP test for the circular trajectory. Figs. 4a, 4b, and 4c illustrate the trajectory of the SCP for Meshes 1, 2, and 3, respectively. Figs. 4d, 4e, and 4f show the RPDs for four test particles on each mesh. It is seen that RPDs for the analytic test particle is very large (several orders of magnitude) compared to the RPDs of the EM-PIC simulation with SPAI-based explicit field solver for \( k = 2, 4, \) and 6. We note again that the RPD for the analytic test particle arises from space and time discretization errors, whereas the other RPDs are due solely to the inverse approximation error. Therefore, these results indicate that inverse approximation error is negligible compared to the other inherent numerical errors. We also note, as expected, that the RPD due to the discretization error decreases as the mesh is progressively refined (curves with \( \bigcirc, +, \times, \) and \( \square \) in Figs. 4d, 4e, and 4f). Examining these figures, it is also observed that the error decreases as the parameter \( k \) increases.

Fig. 4g, 4h, and 4i show the RPD bands normalized by the analytic test particle’s RPD (i.e. setting the RPD of the analytical result to unity radius in the plot). In all cases, the normalized RPD bands rotate around the origin (LU-decomposition implicit solution) around nearly circular orbits. Such normalized RPD bands for test particles 2, 3, and 4 become larger as mesh is refined since the space and time discretization errors decrease, as noted above.

2) Trajectory with drift: In this case, we set \( B_{z}^{\text{ext}} = 5.085 \times 10^{-3} \text{ [Wb/m}^{2}\text{]} \) and \( E_{y}^{\text{ext}} = -5 \times 10^{3} \text{ [V/m]} \). This add a drift motion to the trajectory of the particle, as seen in Fig. 5a. We consider mesh 3 result only, for brevity. The RPD data is shown in Fig. 5b and Fig. 5c. Similar to the pure circular trajectory case, the RPDs for different \( k \) are very small compared to analytic RPD. It is again seen that the bands converge to the center of the circle, which stands for the position of the standard particle, as \( k \) increases.

**B. Plasma ball expansion**

In the next example, we consider the simulation of an expanding plasma ball. We consider \( 5 \times 10^{4} \) superparticles, each representing 200 electrons, initially placed uniformly within a circle of 0.5 \text{ [m]} radius centered at the origin. At \( t = 0 \) positive and negative charged particles overlap, with net zero charge everywhere. Negative particles are initialized with Maxwellian distribution with thermal velocity \( v_{th} = 0.1 \times c \text{ [m/s]} \). Positive charged are assumed with zero velocity at all times. The initial density of particles is \( n \approx 6.37 \times 10^{4} \text{ [m}^{-3}\text{]} \) and the Debye length is \( \lambda_{D} \approx 0.663 \text{ [m]} \), resulting on a plasma parameter \( \Lambda = 4\pi n_{e} \lambda_{D} \approx 2.34 \times 10^{5} \). The unstructured mesh used in this simulation has 1880 faces, 2884 edges, and 1005 nodes. A PML is used to truncate the solution domain. A time step increment \( \Delta t = 5 \text{ [ps]} \) is used, and the simulation is terminated at 10 \text{ [ns]}.

Fig. 6 shows the radial current density from the plasma expansion at \( t = 9 \times 10^{5} \Delta t \) as a function of the radial
coordinate computed by implicit LU-based and explicit SPAI-based field solvers with $k = 2, 4,$ and $6$. The picture in the inset of Fig. 6 shows a snapshot of the particle distribution at $t = 9 \times 10^3 \Delta t$. There is no discernible difference in the current density profile among the results shown in Fig. 6.

In order to check charge conservation, we plot in Fig. 7a the normalized residual (NR) for DCE (8) and DGL (14). These residuals are evaluated for each time step $n + 1$ or $n$ and node $i$, and defined as

$$\text{NR}_{\text{DCE}}^{n+1/2} = 1 + \frac{[Q]^{n+1} - [Q]^n}{\Delta t} \sum_{j=1}^{N_e} [D^*_\text{div}]_{i,j} [\beta]^{n+1/2}$$

$$\text{NR}_{\text{DGL}}^n = 1 - \frac{[Q]^n}{\sum_{j=1}^{N_e} [D^*_\text{div}]_{i,j} \left( \sum_{k=1}^{N_v} [\star]_{i,j,k} [E]^n_k \right)}$$

(19) (20)

where $N_v$ denotes the total number of nodes in the mesh. Fig. 7a shows $|\text{NR}_{\text{DCE}}^{n+1/2}|$ at $n = 20,000$ versus the nodal index for different solvers. As seen, $|\text{NR}_{\text{DCE}}^{n+1/2}|$ is fairly low, about $10^{-13}$, in all cases. The small noise above the double-precision floor $10^{-15}$ can be attributed from arithmetic round-off errors in the scatter process. Fig. 7b shows a similar plot now for $|\text{NR}_{\text{DGL}}^n|$, which is very close to the double-
Fig. 5: Results for a trajectory with drift. (a) Particle trajectory history. (b) RPDs versus time for the four test particles. (c) Normalized RPD bands for the four test particles.

Fig. 6: Radial current versus radius coordinate for the expanding plasma at time step \( n = 9 \times 10^4 \) using the LU-based implicit fields solver and the SPAI-based explicit field solver with \( k = 2, 4, \) and 6.

Fig. 7: (a) Normalized residuals of the discrete continuity equation for the plasma ball expansion example using different field solvers, at \( t = 2 \times 10^4 \Delta t \). (b) Similar results for the discrete Gauss’ law. (c) Averaged normalized residuals for the discrete Gauss’ law versus time step index.
indicating the robustness of the SPAI-based explicit solver. In order to verify that residual levels of the DGL are maintained by (16) during the time-update, we also plot \(|NR_{DGL}^n_i|\) averaged across all nodes of the mesh, i.e. \(NR_{DGL,ave}^n = \sum_{i=1}^{N_R} NR_{DGL,i}^n / N_R\) as a function of the time step \(n\) in Fig. 7c. As seen, \(NR_{DGL,ave}^n\) has nearly constant values close to the double-precision floor, with only a very small increase due to cumulative round-off error.

C. Electron beam

In order to further verify charge conservation and stability for long-time simulations, we simulate next an electron beam accelerated by a vacuum diode. The domain \(\Omega = \{x, y\} \in [0, 1]^2\) has lateral walls representing anode and cathode surfaces with potential difference set as \(1.5 \times 10^5\) V. The top and bottom boundaries of the domain are truncated by a PML. The unstructured mesh has 2301 faces, 3524 edges, and 1224 nodes. The time step interval is set to \(\Delta t = 270\) [ps], and the simulation is run up to 16,2 [ns]. Each superparticle used in the simulation represents 50 \(\times\) \(10^6\) electrons. For the thermionic emission of electrons from the cathode at the left boundary, a slow initial mean velocity of \(10^4\) [m/s] is assumed for the electrons. Fig. 8 presents snapshots of the particle distribution and the self-field (electric) profile. Fig. 8a and Fig. 8d show the field and particle distribution for the charge-conserving EM-PIC algorithm with LU-based implicit field solver. Fig. 8b and Fig. 8e show the field and particle distribution for the charge-conserving EM-PIC algorithm with SPAI-based \((k = 2)\) explicit field solver. Finally, Fig. 8c and Fig. 8f show the field and particle distribution for an EM-PIC with LU-based implicit field solver and conventional gather step (non-charge-conserving on an unstructured grid) where edge currents are obtained from the straightforward projection of the instantaneous product \(q_\mathbf{v}\), summed over all particles, onto the edge element \(\mathbf{W}^{(1)}_i\), i.e.

\[
[j]_{i-1/2}^{n+1/2} = \sum_p q_p \mathbf{r}_p^{n+1/2} \cdot \mathbf{W}^{(1)}_{i} \left( \mathbf{r}_p^{n+1/2} \right)
\]

(21)

where \(\mathbf{r}_p^{n+1/2} = (\mathbf{r}_p^{n+1} + \mathbf{r}_p^{n})/2\). In the latter case, violation of the continuity equation produced spurious bunching of the charges into strips of higher density. In addition, the self field is highly asymmetric and randomly oriented near the beam center. These spurious effects are not present in either the implicit or the explicit charge-conserving simulations.

Fig. 9 shows the average particle density and the average velocity of particles across a transverse section of the beam versus the longitudinal direction \(x\) along the beam at time step \(n = 3000\), for the charge-conserving algorithm with LU-based implicit solver and with SPAI-based explicit solver using \(k = 2, 4, 6\). As expected, the number density of particles monotonically decreases as the average velocity of particles increases, keeping a uniform current flow in steady-state across \(x\). There is an excellent agreement among all these cases, indicating the robustness of the SPAI-based explicit solver.

IV. CONCLUSION

We have developed a EM-PIC algorithm suited for unstructured grids that combines a local explicit field solver with a charge-conserving scatter-gather scheme. A sparse approximate inverse is pre-computed to obviate the need for a linear solver at each time step and to retain the local nature of the algorithm. Excellent agreement was verified between EM-PIC simulations utilizing the proposed field solver and a conventional (implicit) field solver based on a LU-solver. The explicit and local nature of the proposed EM-PIC algorithm makes it suitable for integration with asynchronous time stepping techniques as well.

REFERENCES

[15] E. Schamiloglu, “High power microwave sources and applica-
Fig. 8: Results for the accelerated electron beam at $t = 6 \times 10^4 \Delta t$. (a) (b) Particle distribution snapshot from charge-conserving EM-PIC algorithms using an LU-based implicit solver and a SPAI-based ($k = 2$) explicit solver, respectively. (c) Particle distribution snapshot from a conventional (non-charge conserving on the unstructured grid) EM-PIC algorithm with an LU-based implicit solver. (d) (e) (f) Corresponding electric-field profile distributions.

Fig. 9: Number density and average velocity of particles across a transversal section of the electron beam at $t = 3 \times 10^3 \Delta t$, after steady-state has been reached.
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