Charge-Conserving Relativistic PIC Algorithm on Unstructured Grids

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***Abstract*—We discuss the extension of an exact charge-conserving particle-in-cell (PIC) algorithm based on unstructured grids to the relativistic regime. The present PIC algorithm is based on the representation of grid-based variables such as fields, currents, and (nodal) charges as discrete differential forms of various degrees. In gather and scatter steps, Whitney functions are used as spatial interpolators from grid-based variables to kinetic variables. In the push step, Boris method is adopted to efficiently incorporate relativistic effects into the particle updates. Computational example of a plasma ball expansion and synchrotron charge acceleration are used to illustrate the proposed algorithm in the relativistic regime.**

I. Introduction

Accurate and reliable electromagnetic (EM) particle-in-cell (PIC) [1], [2], [3] algorithms based on time-dependent Maxwells equations are needed in a number of problems, including the analysis and design of beam-wave interaction structures. Historically, EM-PIC codes have been based on the finite-difference (FD) method and regular grids. However, complex geometries cannot be accurately modeled by regular grids because of ensuing staircase effects. For geometrical flexibility, unstructured (irregular) grids should be employed instead. The finite-element (FE) method is a preferred choice in this case because it naturally conforms to such geometries [4]. FE also enables a more seamless multi-physics integration with thermal solvers. However, conventional PIC algorithms on irregular grids violate charge conservation because the ensuing continuity equation leaves residuals at the discrete level. As such, there has been a longstanding need for a conservative full-wave EM-PIC algorithm on unstructured grids. Efforts along this direction have included correction potentials or pseudo-currents. The former approach requires a time-consuming Poisson solver (especially in complex geometries) at each time-step and the latter introduces a diffusion parameter that may alter the underlying physics. A recent charge-conserving full-wave PIC algorithm that does not require introduction of correction terms was proposed in [5]. However, this algorithm is based on the second-order vector wave equation for the electric field, with solution space including spurious modes of the form $\nabla\phi$, which are not physical admissible field solutions to Maxwells equations and can pollute the numerical results. More recently, a novel exact charge-conserving, non-relativistic PIC algorithm for unstructured grids was introduced in [6] based on the use of Whitney forms [7], [8] as self-consistent charge and current interpolants for the scatter step. Similar methodologies were discussed in [9], [10] as well. Here, we briefly describe the extension of the algorithm presented in [6] to the relativistic regime. The extension is based on the use of the Boris method [11] to introduce a modified velocity parameter incorporating the relativistic factor. We provide computational examples to show that exact charge-conservation on unstructured grids is retained in the relativistic regime.

II. Relativistic PIC Formulation

The overall time-update procedure for the PIC algorithm is carried out according to the following sequence [6]: (1) magnetic flux density $\mathbf{B}$ update; (2) gather step; (3) particles' positions and velocities update; (4) scatter step; and (5) electric field $\mathbf{E}$ update. By representing the fields in terms of differential forms [12], [13], the $\mathbf{E}$ and $\mathbf{B}$ fields are spatially discretized using Whitney 1-forms and 2-forms based on edges and faces of the grid, respectively. Likewise, the Hodge-dual of the current density $\mathbf{J}$ is represented as a 1-form defined on the edges of the grid. By applying a leap-frog time integration to the semi-discrete (spatially discretized) Maxwell's equation, we obtain full-discrete equations of the form [14]: $\mathbf{b}^{n+\frac{1}{2}} = \mathbf{b}^{n-\frac{1}{2}} + \Delta t\ \mathbf{C}\cdot\mathbf{e}^{n}$ and $[\star_\epsilon]\cdot\mathbf{e}^{n+1} = [\star_\epsilon]\cdot\mathbf{e}^{n} + \Delta t\left(\mathbf{C}^{T}\cdot\left[\star_{\mu^{-1}}\right]\cdot\mathbf{b}^{n+\frac{1}{2}} - \mathbf{i}^{n+\frac{1}{2}}\right)$, where $\mathbf{b}$ (face-based), $\mathbf{e}$ (edge-based), and $\mathbf{i}$ (edge-based) are the degrees-of-freedom (DoFs) for $\mathbf{B}$, $\mathbf{E}$, and $\mathbf{J}$, respectively, Δt is the time-step interval and, $\mathbf{C}$ is the incidence matrix of the grid [7], and $[\star_\epsilon]$ and $\left[\star_{\mu^{-1}}\right]$ are matrices representing the discrete Hodge star operator [7], [15]. The superscript denotes the time step index. As explained in [6], field values are interpolated at particles' positions in the gather step by also using Whitney functions. In the relativistic regime, we incorporate Boris algorithm into particle updates as follows. We introduce a modified velocity defined as $\mathbf{u}_p = \gamma_p\mathbf{v}_p$ where for the p-th particle the relativistic factor is given by $\gamma_p = (1+\left|\mathbf{v}_p/c^2\right|)^{-1/2}$, where $\mathbf{v}_p$ is the particle's velocity and c is the speed of light. We perform the particle push via ${\mathbf{r}_p}^{n+1} = {\mathbf{r}_p}^{n} + (\Delta t/\gamma_p^{n+\frac{1}{2}}){\mathbf{u}_p}^{n+\frac{1}{2}}$ and particle acceleration via ${\mathbf{u}_p}^{n+\frac{1}{2}} = {\mathbf{u}_p}^{n-\frac{1}{2}} + \frac{q\Delta t}{m_0}\left(\mathbf{E}^{n} + \frac{{\mathbf{u}_p}^{n}}{\gamma_p^{n}}\times\mathbf{B}^{n}\right)$ where $\mathbf{r}_p$ is the particle position. In the scatter step, we again use Whitney 0-form and 1-form as interpolatory functions, this time to assign

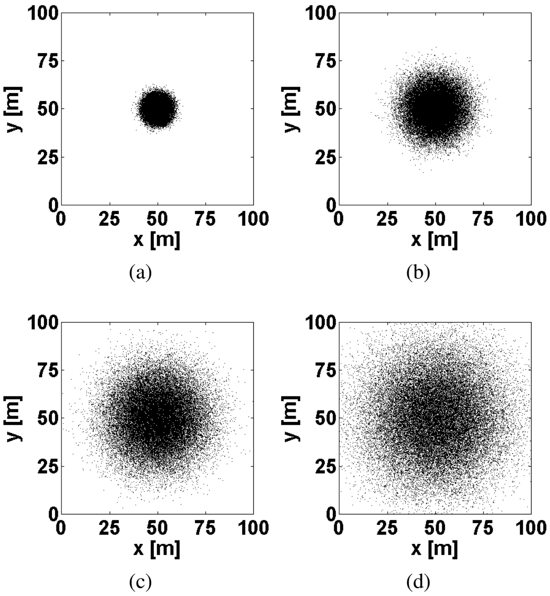

Fig. 1: Snapshots for plasma ball expansion. (a) $t = 40\Delta t$. (b) $t = 120\Delta t$. (c) $n = 200\Delta t$. (d) $n = 280\Delta t$.

particles' charges and currents onto nodes and edges of the grid, respectively [6].

III. Computational examples

We first consider the expansion of a plasma ball consisting of 40,000 electrons with Maxwellian distribution and thermal velocity $0.3 \times c$ at the initial state. Fig. 1. illustrates snapshots of plasma ball expansion for different time instants as indicated, with $\Delta t = 1$ ns. By computing the nodal charges a various grid nodes, charge conservation is verified at all time steps.

The second example presented deals with a relativistic synchrotron, where a particle is guided along a quasi-circular trajectory by external applied fields. Because the mass of the particle increases as the velocity of the particle approaches the speed of light, the frequency of external RF electric field should be modified according to the relativistic factor to match the varying period of motion. Fig. 2 shows the trajectory of the charged particle in the relativistic synchrotron case. It is seen that by applying the RF field in the proper synchronized fashion, the quasi-circular trajectory is obtained is retained the relativistic regime.

IV. Conclusion

We have extended a charge-conserving PIC algorithm on unstructured grids [6] to the relativistic regime. A modified particle update is implemented based on Boris algorithm to incorporate the relativistic factor in a consistent fashion. Examples including a plasma ball expansion and a relativistic synchrotron have been included to illustrate the proposed PIC algorithm.

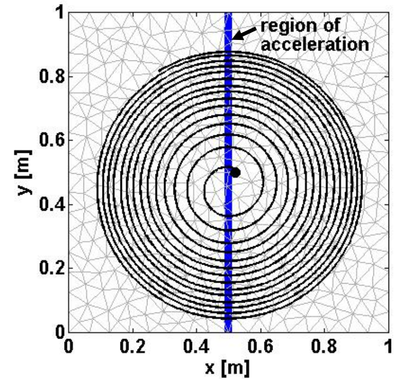

Fig. 2: Trajectory of an electron for relativistic synchrotron

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