Unstructured-grid and conservative particle-in-cell algorithm: Application to micromachined beam-plasma slow-wave structures

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Abstract: We present an accurate and efficient electromagnetic particle-in-cell (EMPIC) algorithm on unstructured grids for the analysis and design of axisymmetric slow-wave structures. The use of unstructured grids allows for more fidelity in the modeling of micromachined geometries. The use of a reduced dimensionality algorithm decreases the computational costs significantly and enables its integration as a forward engine into a design loop. Special gather and scatter steps are employed to yield accurate beam plasma dynamics and exact charge conservation on unstructured grids. We provide numerical examples involving travelling-wave tube amplifiers designed to harness bunching effects arisen from Cherenkov radiation from plasma electron beams.

Keywords: Maxwell-Vlasov equations, particle-in-cell, plasma, vacuum electronics devices.

References:


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Introduction

Particle-In-Cell (PIC) algorithm for plasma simulations: Field solver, gather, relativistic particle pusher, and scatter

Modeling of beam-field interactions in vacuum electronics devices (VED)

Numerical Examples (TWT amplifier and BWO)

Concluding Remarks
Electromagnetic Particle-in-Cell (EM-PIC) Algorithms

- **Vlasov equation**
  - \( \frac{df_p(r(t), \dot{r}(t), t)}{dt} = 0 \) (collisionless)
  - \( \frac{\partial f_p}{\partial t} + \dot{v} \cdot \nabla r f_p + \frac{q_p}{m_p} [E + \dot{v} \times B] \cdot \nabla v f_p = 0 \)
  - Shape factor \( f_p \) represents spatial distribution for an ensemble of particles (number density of particles), described by a smaller set of “super-particles” (coarse graining of the phase-space).

- **Electromagnetic particle-in-cell (EM-PIC) algorithm**
  - Numerical approach to solve the MV system
  - Four major steps at each time-update

- **Applications based on EM-PIC simulations**
  - Plasma physics and astrophysics
  - Vacuum electron devices (VED)
Vacuum Electronics Devices (VED)
- VED are essential for high-power microwave (HPM) sources in variety of applications including pulsed radar systems, RF amplification, and others.
- Slow-wave structures (SWS) are often used to slow down the phase velocity of waves and excite Cerenkov radiation.
- Most VEDs are cylindrically axisymmetric (invariant along $\phi$).

Micromachined Slow-Wave Structures (SWS)
- Micromachining desirable for high performance operation at microwaves and, especially, terahertz frequencies.
- Either structured grids with conformal capabilities or unstructured grids (general solution) should be used to correctly capture the geometry of micromachined SWSs.

Main contribution of this work
- We introduce a EM-PIC algorithm for circularly symmetric VED which is (1) based on unstructured grids and (2) attains charge conservation from first principles.
3D cylindrical axisymmetry VED

- (1) Problem geometry, (2) EM fields, and (3) sources are cylindrically axisymmetric ($\frac{\partial}{\partial \phi} = 0$).

1. Reduction of the exterior derivative $d : d = \frac{\partial}{\partial \rho} d\rho + \frac{\partial}{\partial z} dz$

Two useful constraints to reduce the dimensionality of 3D cylindrically axisymmetric problems

1. Reduction of the exterior derivative $d : d = \frac{\partial}{\partial \rho} d\rho + \frac{\partial}{\partial z} dz$
2. Consideration of only TM eigenmodes with $m = 0$ ($m$ is an index for azimuthal modes)
Differential forms expressions for dynamic variables with a non orthonormal basis set of \((d\rho, d\phi, dz)\)

- \(\mathcal{E} = E_\rho \, d\rho + E_z \, dz\)
- \(\mathcal{B} = B_\phi \, dz \wedge d\rho\)
- \(\mathcal{H} = H_\phi \, d\phi\)
- \(\mathcal{D} = D_\rho \, d\phi \wedge dz + D_z \, d\rho \wedge d\phi\)
- \(J_* = J_{*\rho} \, d\rho + J_{*z} \, dz\)
- \(Q_* = \rho_{v*}\)
- \(\mathcal{J} = J_\rho \, d\phi \wedge dz + J_z \, d\rho \wedge d\phi\)
- \(\mathcal{Q} = \rho_v \, d\rho \wedge d\phi \wedge dz\)

Hodge star operator for fields and sources

\[
\mathcal{H} = \star \mu^{-1} \mathcal{B} \\
LHS = H_\phi \, d\phi \\
RHS = \star \mu^{-1} \left( B_\phi \, dz \wedge d\rho \right) \\
= \mu_0^{-1} B_\phi \star (dz \wedge d\rho) = \mu^{-1}(\rho) B_\phi \, d\phi
\]

\[
\mathcal{D} = \star \mathcal{E} \\
LHS = D_\rho \, d\phi \wedge dz + D_z \, d\rho \wedge d\phi \\
RHS = \star \epsilon \left( E_\rho \, d\rho + E_z \, dz \right) = \\
= \epsilon \left[ E_\rho (\rho d\phi \wedge dz) + E_z (d\rho \wedge \rho d\phi) \right] \\
= \epsilon(\rho) \left( E_\rho \, d\phi \wedge dz + E_z \, d\rho \wedge d\phi \right)
\]

- We introduce an (1) artificial inhomogeneous medium with dependency on \(\rho\) and (2) rescaled sources.

3D axisymmetric problems w.r.t. geometry, fields, and sources can be modeled by 2D equivalent problems by $\text{TE}^\phi$-polarized fields, artificial inhomogeneous medium, and scaled sources.

- The continuous ring of particles along $\phi$-axis matches a particle at the meridian plane.
Mixed $\mathcal{E} - \mathcal{B}$ FETD Scheme for (2+1) Theory

\[
d\mathcal{E} = -\frac{\partial \mathcal{B}}{\partial t}, \quad d\mathcal{H} = \frac{\partial \mathcal{D}}{\partial t} + J, \quad d\mathcal{D} = Q, \quad d\mathcal{B} = 0
\]

Spatial discretization by expanding variables as

**In primal mesh**
- $\mathcal{E} = \sum_{i=1}^{N_1} \mathbb{E}_i^n \Psi_i^n$ (1-form)
- $\mathcal{B} = \sum_{i=1}^{N_2} \mathbb{B}_i^{n \frac{1}{2}} \Psi_i^n$ (2-form)
- $J_* = \sum_{i=1}^{N_1} \mathcal{J}_i^n \Psi_i^n$ (1-form)
- $Q_* = \sum_{i=1}^{N_0} \mathcal{Q}_i^n \Psi_i^n$ (0-form)

**In dual mesh**
- $\mathcal{H} = \sum_{i=1}^{N_0} \mathbb{H}_i^{n \frac{1}{2}} \tilde{\Psi}_i^0$ (0-form)
- $\mathcal{D} = \sum_{i=1}^{N_1} \mathcal{D}_i^n \tilde{\Psi}_i^1$ (1-form)
- $J = \sum_{i=1}^{N_1} \mathcal{J}_i^n \tilde{\Psi}_i^1$ (1-form)
- $Q = \sum_{i=1}^{N_2} \mathcal{Q}_i^n \tilde{\Psi}_i^0$ (0-form)

Paring, generalized Stokes Theorem, and leapfrog time scheme

Mixed $\mathcal{E} - \mathcal{B}$ FETD Scheme: Kim and Teixeira, IEEE T-AP, vol. 59, p. 2350 (2011)

\[
[\mathcal{B}]^{n + \frac{1}{2}} = [\mathcal{B}]^{n - \frac{1}{2}} + \Delta t [\mathcal{D}_{\text{curl}}] \cdot [\mathcal{E}]^n
\]

\[
[\mathcal{B}] \cdot [\mathcal{E}]^{n + 1} = [\mathcal{B}] \cdot [\mathcal{E}]^n + \Delta t \left( [\mathcal{D}_{\text{curl}}] \cdot [\mathcal{B}]^{n + \frac{1}{2}} - [I] \cdot [J_*]^{n + \frac{1}{2}} \right)
\]

Mixed Hodge matrices

\[
[\star_{\epsilon}]_{ij} = \int_K \epsilon(\rho) \omega_i^1 \wedge \star \omega_j^1
\]

\[
[\star_{\mu^{-1}}]_{ij} = \int_{\tilde{K}} \mu^{-1}(\rho) \omega_i^2 \wedge \star \omega_j^2
\]
Gather

- EM field values are interpolated at the instant positions of particles by using interpolants of Whitney forms
  \[
  \vec{E}_p^n = \sum_{i=1}^{N_1} \vec{E}_i^n \overrightarrow{W}_i^1 (\vec{r}_p^n)
  \]
  \[
  \vec{B}_p^n = \frac{\vec{B}_p^{n+\frac{1}{2}} + \vec{B}_p^{n-\frac{1}{2}}}{2} = \sum_{i=1}^{N_2} \left( \frac{\vec{E}_i^{n+\frac{1}{2}} + \vec{E}_i^{n-\frac{1}{2}}}{2} \right) \overrightarrow{W}_i^2 (\vec{r}_p^n)
  \]

- Relativistic particle pusher
  - Lorentz force and Newton’s law of motion
  - Updates of particles’ position and velocity
  - Relativistic factor, \( \gamma = \frac{1}{\sqrt{1 - (\frac{v_p}{c})^2}} \)
  - Boris or Vay algorithms
  - Beam focusing system (BFS)
BFS prevents particles to radially deviate from electron beams due to the repulsive forces

- It computes effects by self-fields and BFS and neglects $\phi$ motions due to continuous rings of particles.
Exact Charge-Conserving Scatter

Discrete continuity equation

\[
\frac{[I] \cdot [Q_*]^{n+1} - [I] \cdot [Q_*]^{n}}{\Delta t} = -[\mathcal{D}_{\text{div}}] \cdot [I] \cdot [J_*]^{n+\frac{1}{2}}
\]

Rate of charge variation at \( n_1 \)

\[
\frac{Q_{*,n_1}^{n+1} - Q_{*,n_1}^n}{\Delta t} = \frac{q}{\Delta t} \left( \frac{\rho_f + \rho_2 + \rho_3 \lambda_1^f}{3} - \rho_s + \frac{\rho_2 + \rho_3 \lambda_1^s}{3} \right) = -\frac{q}{\Delta t} \left[ \rho_f \lambda_1^f - \rho_s \lambda_1^s + (\rho_2 + \rho_3)(\lambda_1^f - \lambda_1^s) \right]
\]

Net currents flowing outward from \( n_1 \)

\[
\mathbb{J}_{*,e_i}^{n+\frac{1}{2}} = \frac{q}{\Delta t} \left( \rho_f \lambda_1^f - \rho_s \lambda_1^s + (\rho_2 + \rho_3)(\lambda_1^f - \lambda_1^s) \right)
\]

discrete charge

\[Q_{*,n_i} \equiv q(x, \rho w_{n_i}^0)\]

discrete current

\[\mathbb{J}_{*,e_i} \equiv \frac{q}{\Delta t} (l, \rho w_{e_i}^1)\]
Example 1: Vacuum Diode

- Proposed charge-conserving (CC) scheme vs. conventional non charge-conserving (NCC) scheme

Cathode  Anode

CC & SPAI $k = 2$

CC & LU dcmp.

NCC & LU dcmp.

Particle dist.

Self-fields

electron beam

non-physical bunching

spurious fields

Example 1: Vacuum Diode
- Electron beam, input RF signal, SWS
- Sinusoidal Corrugated Circular Waveguide (SCCW)
  \[ R_0 = 0.04, \epsilon_R = 0.025, p_c = 0.02 \]
- Electron bunching due to forward Cerenkov radiation
- Confinement of the electron beam by BFS

Example 2: Traveling Wave Tube (TWT) Amp.

Dispersion relations for SCCW

Distribution of the electron beam
Residual analysis for discrete Gauss law (DGL)

\[
\text{DGL} : [\mathcal{D}_\text{div}] \cdot [\star \epsilon] \cdot [\mathcal{E}]^n = [Q_\star]^n
\]

The residuals for DGL at any two successive time-steps remain the same, in other words, if initial conditions have

\[ [\mathcal{D}_\text{div}] \cdot [\star \epsilon] \cdot [\mathcal{E}]^0 = [Q_\star]^0, \]

DGL for all time-steps is verified.

Premultiplying \([\mathcal{D}_\text{div}] \cdot [\star \epsilon]\) into DAL, using \([\mathcal{D}_\text{div}] \cdot [\mathcal{D}_\text{curl}] = 0\), and rearranging the equation yield

\[
[\mathcal{D}_\text{div}] \cdot [\star \epsilon] \cdot \left( \frac{[\mathcal{E}]^{n+1} - [\mathcal{E}]^n}{\Delta t} \right) = -[\mathcal{D}_\text{div}] \cdot \left( \mathcal{J}_\star \right)^{n+\frac{1}{2}}.
\]

Substituting DCE into above equation and rearranging it give

\[
[\mathcal{D}_\text{div}] \cdot [\star \epsilon] \cdot [\mathcal{E}]^{n+1} - [Q_\star]^{n+1} = [\mathcal{D}_\text{div}] \cdot [\star \epsilon] \cdot [\mathcal{E}]^n - [Q_\star]^n.
\]

By induction,

\[
[\mathcal{D}_\text{div}] \cdot [\star \epsilon] \cdot [\mathcal{E}]^n - [Q_\star]^n = [\mathcal{D}_\text{div}] \cdot [\star \epsilon] \cdot [\mathcal{E}]^0 - [Q_\star]^0
\]

\[ |NR_{\text{DGL}}^n| = 1 - \frac{[Q_\star]^n + 1}{\sum_{j=1}^{N_0} [\mathcal{D}_\text{div}]_{i,j} \left( \sum_{k=1}^{N_1} [\star \epsilon]_{j,k} [\mathcal{E}]_{k}^{n} \right)} \]

Normalized residuals for DGL

\[ |NR_{\text{DGL}}^i| = 1 - \frac{[Q_\star]_{i}^{n+1}}{\sum_{j=1}^{N_0} [\mathcal{D}_\text{div}]_{i,j} \left( \sum_{k=1}^{N_1} [\star \epsilon]_{j,k} [\mathcal{E}]_{k}^{n} \right)} \]

Example 2: Traveling Wave Tube (TWT) Amp. (cont')
Example 3: Backward Wave Oscillator (BWO)

- Small perturbation by the electron beam generates RF signals in the positive feedback system (BWO).
- Rectangular corrugated cylindrical waveguide: \( R_{in} = 0.04 \text{ [m]}, R_{out} = 0.045 \text{ [m]}, p_c = 0.045 \text{ [m]} \)

- \( V_a = 500 \text{ [kV]} \) yields relativistic electron beams with \( v_p = 0.83c \).
- Electron bunching due to backward Cerenkov radiation
New electromagnetic particle-in-cell (EM-PIC) algorithm developed to solve Maxwell-Vlasov system on unstructured grids.

Exterior calculus of differential forms\textsuperscript{1} was used to derive an exact charge-conserving gather and scatter schemes on unstructured grids\textsuperscript{2}.

SPAI algorithm was used to accelerate the field update\textsuperscript{3}.

Relativistic particle pusher has been implemented by using Boris algorithm.

Successfully applied to simulate plasma-beam dynamics in axisymmetric VED devices, including travelling wave tube (TWT) amplifiers and backward wave oscillators (BWO).

\textsuperscript{1}F. L. Teixeira, \textit{PIER} 148, 113-128 (2014).


Thank You!

Q&A

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