Numerical Instability Suppression in PSATD PIC Codes*

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Haber’s Pseudo-Spectral Analytical Time-Domain (PSATD) algorithm [1] offers numerous advantages for Particle-In-Cell beam simulations. It has dispersion-free electromagnetic wave propagation and no Courant limit in vacuum. It also possesses superior numerical stability properties [2], especially when combined with Esirkepov’s current deposition algorithm [3]. Vay’s recent research [4] suggests that it can be parallelized about as well as Finite-Difference Time Domain (FDTD) algorithms.

Despite its superior numerical stability, the PSATD algorithm exhibits both the numerical Cherenkov instability [5] in cold, relativistic beam simulations and the well-known quasi-electrostatic numerical instability [6] in cold, non-relativistic beam simulations. In this talk we extend the results of [2] by completely eliminating the primary mode of the numerical Cherenkov instability for all beam energies. Moreover, by using cubic interpolation and modest digitally filtering, we simultaneously minimize higher-order aliases of this instability. Finally, we demonstrate that a variant of PSATD eliminates the quasi-electrostatic numerical instability. These results, derived from the complete PSATD cold beam numerical dispersion relation, are confirmed by two-dimension WARP [7] simulations.


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Pseudo-Spectral “Analytical” Time Domain (PSATD) Algorithm*

- Numerical Cherenkov instability essentially eliminated for PSATD relativistic beam simulations
- Points way to suppressing Numerical Cherenkov instability in FDTD simulations
  - Contains this talk, some software; more to come
- Details from brendan.godfrey@ieee.org

Numerical Cherenkov Instability

• Serious issue in 2D, 3D EM PIC simulations of relativistic beams (accelerators, astrophysics, etc.)
  – Growth rates a large fraction of \((\omega_p^2 k_{\perp}^2 \Delta t / \gamma)^{1/3}\)
• Arises from differing approximations to \(\omega - k_z v\):
  – Lagrangian particle pusher \(-\sin \left( (\omega - k_z' v) \frac{\Delta t}{2} \right) / \frac{\Delta t}{2}\)
  – Eulerian field solver \(-\sin \left( \omega \frac{\Delta t}{2} \right) / \frac{\Delta t}{2} - v \sin \left( k_z \frac{\Delta z}{2} \right) / \frac{\Delta z}{2}\)
  – Difference leads to spurious beam-like normal modes, including aliases, which are unstable when interacting with light modes
• Typically addressed by substantial digital filtering
Generalized PSATD Algorithm

\[ E^{n+1} = E^n - 2iS_h k \times \frac{B^{n+1/2}}{k} - \frac{2S_h C_h \zeta:J^{n+1/2}}{k} \]

\[ + \frac{2S_h C_h}{k} k k \cdot \frac{\zeta:J^{n+1/2}}{k^2} - k k \cdot \frac{J^{n+1/2}\Delta t}{k^2} \]

\[ B^{n+1/2} = B^{n-1/2} + 2iS_h k \times \frac{E^n}{k} \]

Particle force: \[ F^n = \Psi_E : E^n + \Psi_B : \frac{(B^{n+1/2} + B^{n-1/2})}{2C_h} \]

with \( S_h = \sin \frac{k\Delta t}{2}, C_h = \cos \frac{k\Delta t}{2} \)

• \( \zeta, \Psi_E, \Psi_B \) — diagonal matrices, nine free parameters in 3D
• \( J \) assumed to conserve charge
  – e.g., Esirkepov algorithm or standard current correction
Extra Poles in Dispersion Relation

\[ C_0 + n \sum_m C_1 \csc \left( (\omega - k'_z \nu) \frac{\Delta t}{2} \right) \]
\[ + n \sum_m \left( C_{2x} + \frac{C_{2z}}{\gamma^2} \right) \csc \left[ (\omega - k'_z \nu) \frac{\Delta t}{2} \right]^2 \]
\[ + n \sum_m C_{3x} \frac{C_{3z}}{\gamma^2} \csc \left[ (\omega - k'_z \nu) \frac{\Delta t}{2} \right]^3 = 0 \]

with \( n \) the beam density divided by \( \gamma \)

and \( k'_z = k_z + m \frac{2\pi}{\Delta z} \) (aliases)

- Beam modes associated with \( C_1, C_{2x} \) are numerical artifacts, trigger numerical Cherenkov instability
Full Dispersion Relation Growth Rates

- Peak growth rates at resonances
  - \( m = 0 \) dominates for
    \[
    \frac{\Delta t}{\Delta x} > 2 \left( \frac{\Delta x}{\Delta t_c} - \frac{\Delta z}{\Delta x} \right)
    \]
  - \( m = -1 \) dominates otherwise

- Parameters
  - \( \frac{\nu \Delta t}{\Delta z} = 1.2, \nu \approx 1 \)
  - Linear interpolation

Use digital filtering to eliminate \( m=0,-1 \) resonant instabilities
Select free parameters to suppress nonresonant instabilities
Appropriate \( \zeta \), Cubic Interpolation, Filtering: Good Stability for \( \nu \Delta t/\Delta z \geq 1 \)

- Choose \( \zeta \) to set \( C_2 = 0 \), multiply by \( \sin^{1/6}(k_z \Delta z/2) \)
- Residual instability at \( \nu \Delta t/\Delta z > 1 \) from \( m = \pm 2 \) aliases
• Collect currents with twice usual resolution, discard upper half of $k_z$, use rest to push fields
• Interpolation scale-length modestly impacts stability
Using $\psi$ Instead of $\zeta$ Also Gives Excellent Results

- Choose $\zeta$ to set $C_{3x} = 0$ (finite-$\gamma$ third-order pole)
- No need to eliminate odd aliases (lower cost)
\( \zeta \)-based Option with \( E_Z \) Shifted by \( \Delta z/2 \) Suppresses Low-\( \gamma \) Instability

- Superior at high \( \gamma \), equally effective at low \( \gamma \) as “energy-conserving” algorithms (which also shift \( E_Z \))
- \( \psi \)-based options presumably also work well
Instability Predicted by Birdsall-Langdon is Price of no Courant Limit

- Occurs in narrow bands at $k \approx l\pi/\Delta t$ ($l$ odd)
- Insignificant at relativistic energies
- Plot parameters: $\zeta$-based option, no odd aliases
\[ \Psi \text{-based Option Can be Extended to FDTD with Very Good Results} \]

- Choose \( \frac{\psi_E}{\psi_B} \) to set \( C_{2x} = 0 \) (in \( k \)-space)

- Approximate by ratio of polynomials in \( \sin^2 \left[ \frac{k_z \Delta z}{2} \right] \)
  - *Mathematica* `RationalInterpolation` works well
  - High accuracy essential – of order \( 10^{-6} \)

- Set \( \psi_E \) to numerator, \( \psi_B \) to denominator
  - Corresponds to \( 2n + 1 \) stencil in \( z \), with \( n \) the degree of the polynomial

- Use with cubic interpolation, modest digital filtering

- Setting \( \psi_E \) to ratio, \( \psi_B \) to 1 also possible but requires matrix inversion, more filtering at larger \( \nu \Delta t/\Delta z \)
Sample $\Psi$-Based Multipliers

\[ \psi = 1 + \alpha_1 \sin^2 \left( \frac{k_z \Delta z}{2} \right) + \alpha_2 \sin^4 \left( \frac{k_z \Delta z}{2} \right) + \alpha_3 \sin^6 \left( \frac{k_z \Delta z}{2} \right) + \alpha_4 \sin^8 \left( \frac{k_z \Delta z}{2} \right) \]

\[ \alpha_E = \{-2.92128, 3.04729, -1.31363, 0.187765\} \]

\[ \alpha_B = \{-2.54796, 2.20374, -0.709955, 0.054882\} \]

"Uniform" Yee C-K with $\nu \Delta t / \Delta z = 0.9$
"Uniform" Yee C-K Interpolation

- ψ-based: 4\textsuperscript{th} order polynomials, 2-pass filter
- $\Psi_{Ex}$: ratio of 4\textsuperscript{th} order polynomials ($E_x$ only), 2-pass filter
- Baseline: cubic interpolation, 8-pass filter
“Galerkin” Yee C-K Interpolation

- \( \Psi \)-based: 4\(^{th}\) order polynomials, 2-pass filter
- \( \Psi_{Ex} \): ratio of 4\(^{th}\) order polynomials (\( E_x \) only), 2-pass filter
- Baseline: cubic interpolation, 8-pass filter
Next Steps

• Seek PSATD and FDTD options that increase usable $k$-space while preserving instability suppression
• Explore EM potentials version of PSATD
• Add related material to http://hifweb.lbl.gov/public/BLAST/Godfrey/
Backup
PSATD Normal Modes

EM modes
• \( \omega = \pm \text{Mod} \left[ k, \frac{2\pi}{\Delta t} \right] \)

Spurious beam modes
• \( \omega = \text{Mod} \left[ k_z', \frac{2\pi}{\Delta t} \right] \)

Intersections trigger numerical Cherenkov instability

EM modes fold over when \( \Delta t > \Delta t_c = (\Delta z^{-2} + \Delta x^{-2})^{-\frac{1}{2}} \)