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.

[1] I. Haber, R. Lee, H. Klein, and J. Boris, *Proc. Sixth Conf. Numerical Simulation of Plasmas*, Berkeley, CA USA, Jul 16-18, 1973, pp. 46-48.
[2] B. B. Godfrey, J.-L. Vay, and I. Haber, submitted to *J. Comp. Phys.*
[3] T. Z. Esirkepov, *Comp. Phys. Comm.* **135**, 144-153 (2001)
[4] J.-L. Vay, I. Haber, and B. B. Godfrey, *J. Comp. Phys.* **243**, 260-268 (2013).
[5] B. B. Godfrey, *J. Comp. Phys.* **15**, 504-521 (1974).
[6] A. B. Langdon, *Proc. Fourth Conf. Numerical Simulation of Plasmas*, Washington DC USA, Nov 2-3, 1970, pp. 467-495.
[7] D.P. Grote et al., *AIP Conference Proceedings*, **749**, 55-58 (2005).

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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
- Numerical stability software collection at http://hifweb.lbl.gov/public/BLAST/Godfrey/
  - Contains this talk, some software; more to come
- Details from brendan.godfrey@ieee.org

*Introduced by I. Haber, *et. al.*, Sixth Conf. Num. Sim. Plas. (1970)
Expanded upon by J.-L. Vay, *et. al.*, J. Comp. Phys. **243**, 260-268 (2013).

Numerical Cherenkov Instability

- Serious issue in 2D, 3D EM PIC simulations of relativistic beams (accelerators, astrophysics, *etc*.)
  - Growth rates a large fraction of $\left(\omega_p{}^2 k_\perp{}^2 \Delta t/\gamma\right)^{1/3}$
- 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

$$\boldsymbol{E}^{n+1} = \boldsymbol{E}^{n} - 2iS_h\boldsymbol{k} \times \frac{\boldsymbol{B}^{n+½}}{k} - \frac{2S_hC_h\boldsymbol{\zeta}:\boldsymbol{J}^{n+½}}{k}$$

$$+\frac{2S_hC_h}{k}\boldsymbol{kk}\cdot\frac{\boldsymbol{\zeta}:\boldsymbol{J}^{n+½}}{k^2} - \boldsymbol{kk}\cdot\frac{\boldsymbol{J}^{n+½}\Delta t}{k^2}$$

$$\boldsymbol{B}^{n+½} = \boldsymbol{B}^{n-½} + 2iS_h\boldsymbol{k} \times \frac{\boldsymbol{E}^{n}}{k}$$

Particle force: $\boldsymbol{F}^n = \boldsymbol{\psi}_E:\boldsymbol{E}^n + \boldsymbol{\psi}_B:\frac{(\boldsymbol{B}^{n+½}+\boldsymbol{B}^{n-½})}{2C_h}$

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

- $\boldsymbol{\zeta}, \boldsymbol{\psi}_E, \boldsymbol{\psi}_B$ – diagonal matrices, nine free parameters in 3D
- $\boldsymbol{J}$ assumed to conserve charge
  - *e.g.*, Esirkepov algorithm or standard current correction

Extra Poles in Dispersion Relation

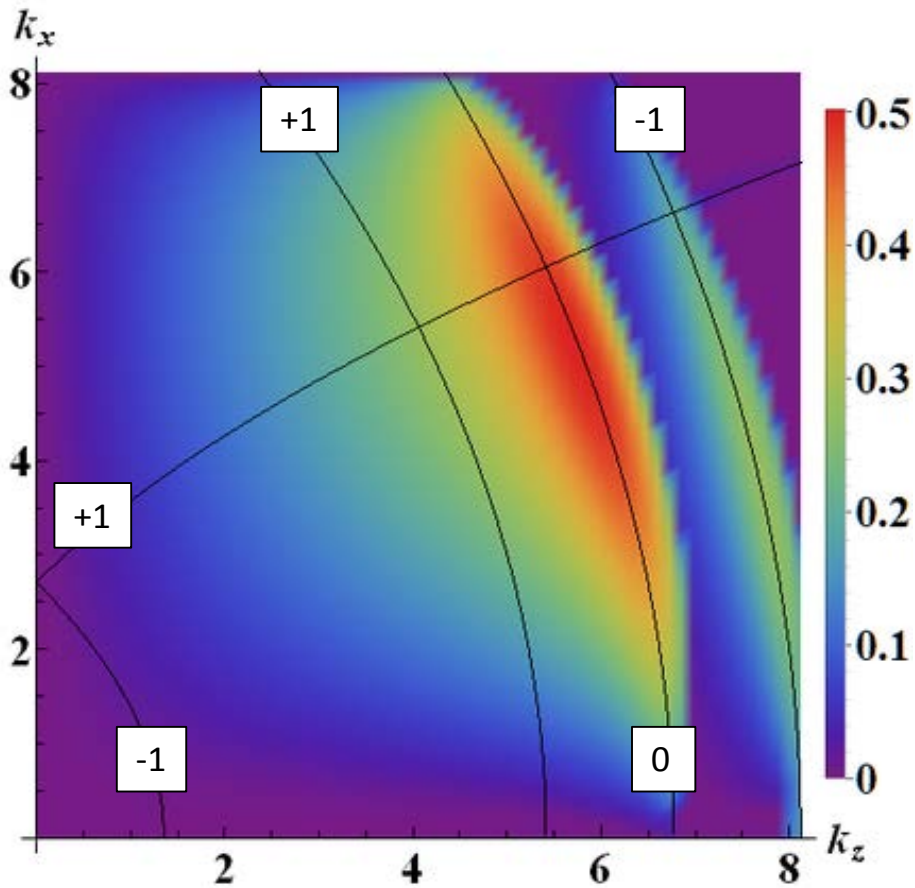
$$C_0 + n\sum_m C_1 \csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]$$
$$+n\sum_m \left(C_{2x} + \frac{C_{2z}}{\gamma^2}\right)\csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]^2$$
$$+n\sum_m C_{3x}\frac{C_{3z}}{\gamma^2}\csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]^3 = 0$$

with n the beam density divided by γ

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

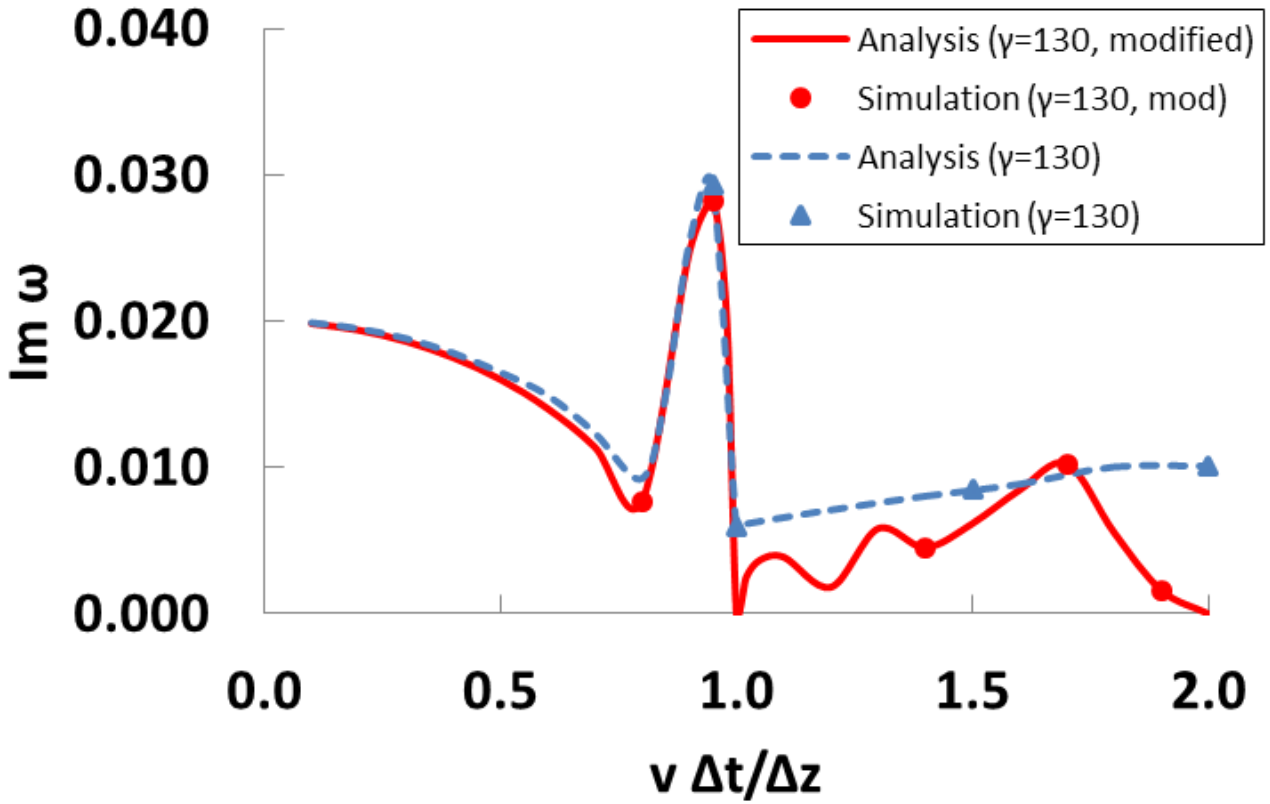
Full Dispersion Relation Growth Rates



- 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
  - $\frac{v\Delta t}{\Delta z} = 1.2, v \approx 1$
  - Linear interpolation

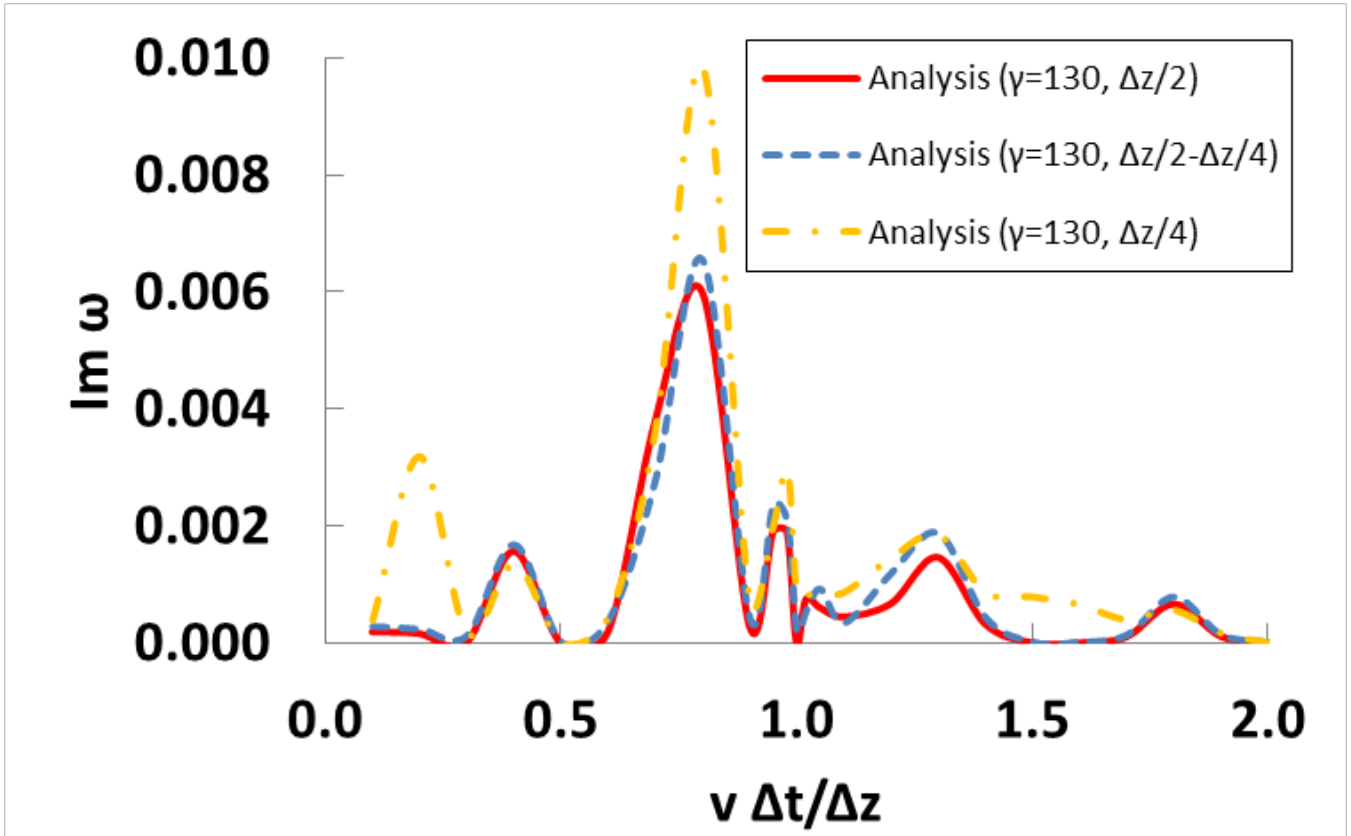
Use digital filtering to eliminate m=0,-1 resonant instabilities
Select free parameters to suppress nonresonant instabilities

Appropriate ζ, Cubic Interpolation, Filtering: Good Stability for $v\Delta t/\Delta z \geq 1$



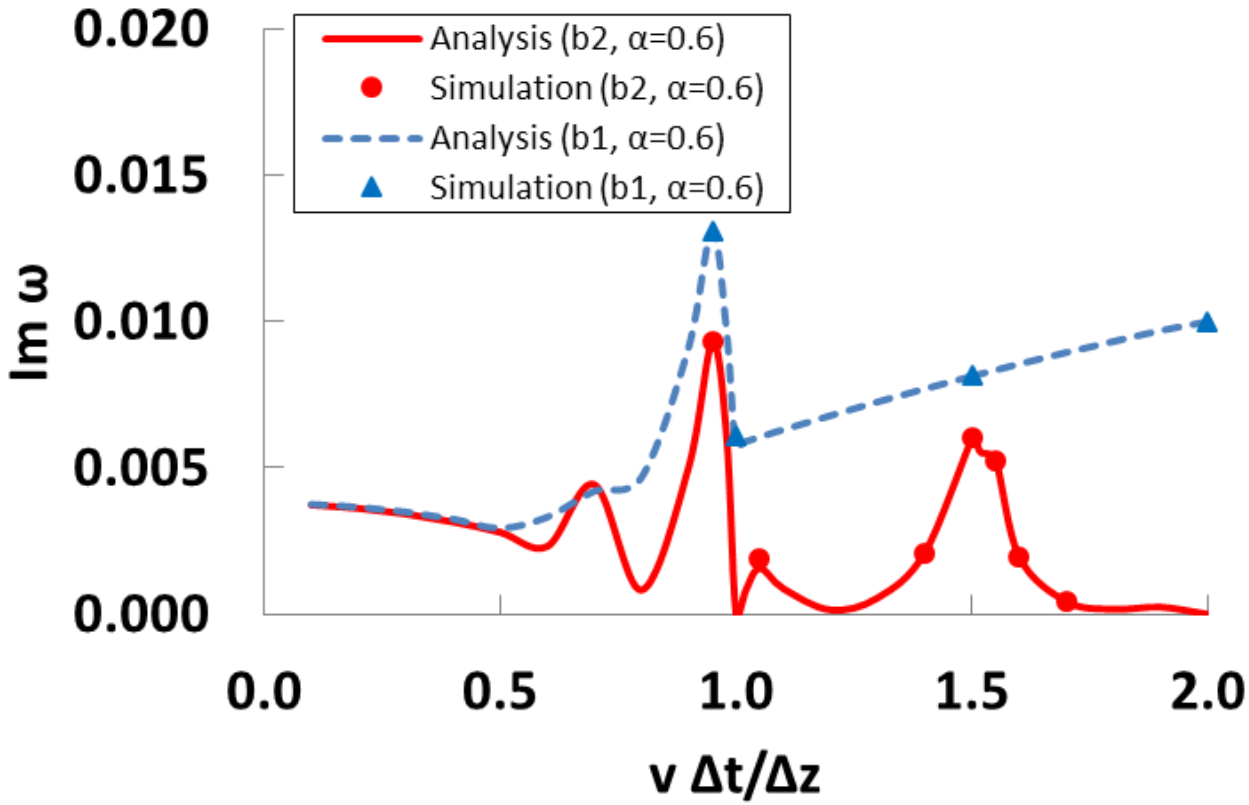
- Choose ζ to set $C_2 = 0$, multiply by $sin^{1/6}(k_z \Delta z/2)$
- Residual instability at $v\Delta t/\Delta z$>1 from $m = \pm 2$ aliases

Previous Slide's Option with Odd Aliases Eliminated Gives Excellent Results



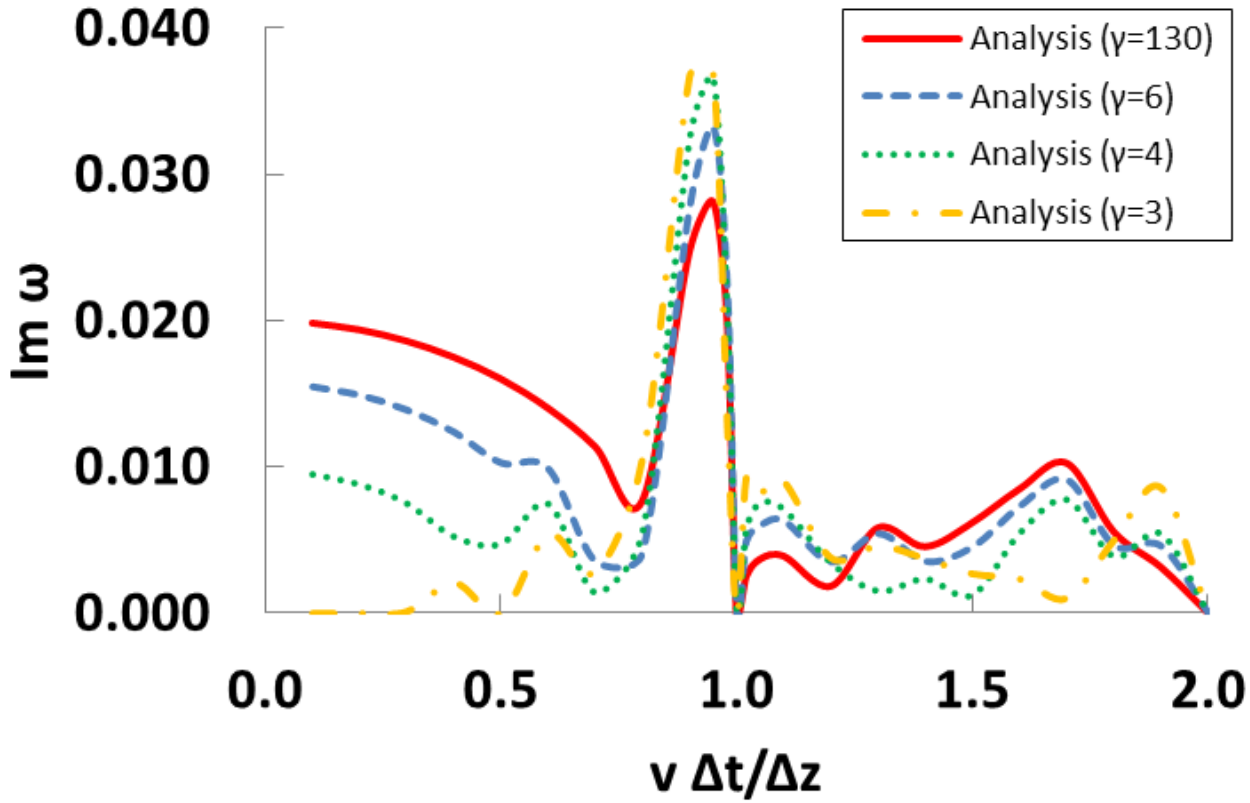
- Collect currents with twice usual resolution, discard upper half of k_z, use rest to push fields
- Interpolation scale-length modestly impacts stability

Using ψ Instead of ζ Also Gives Excellent Results



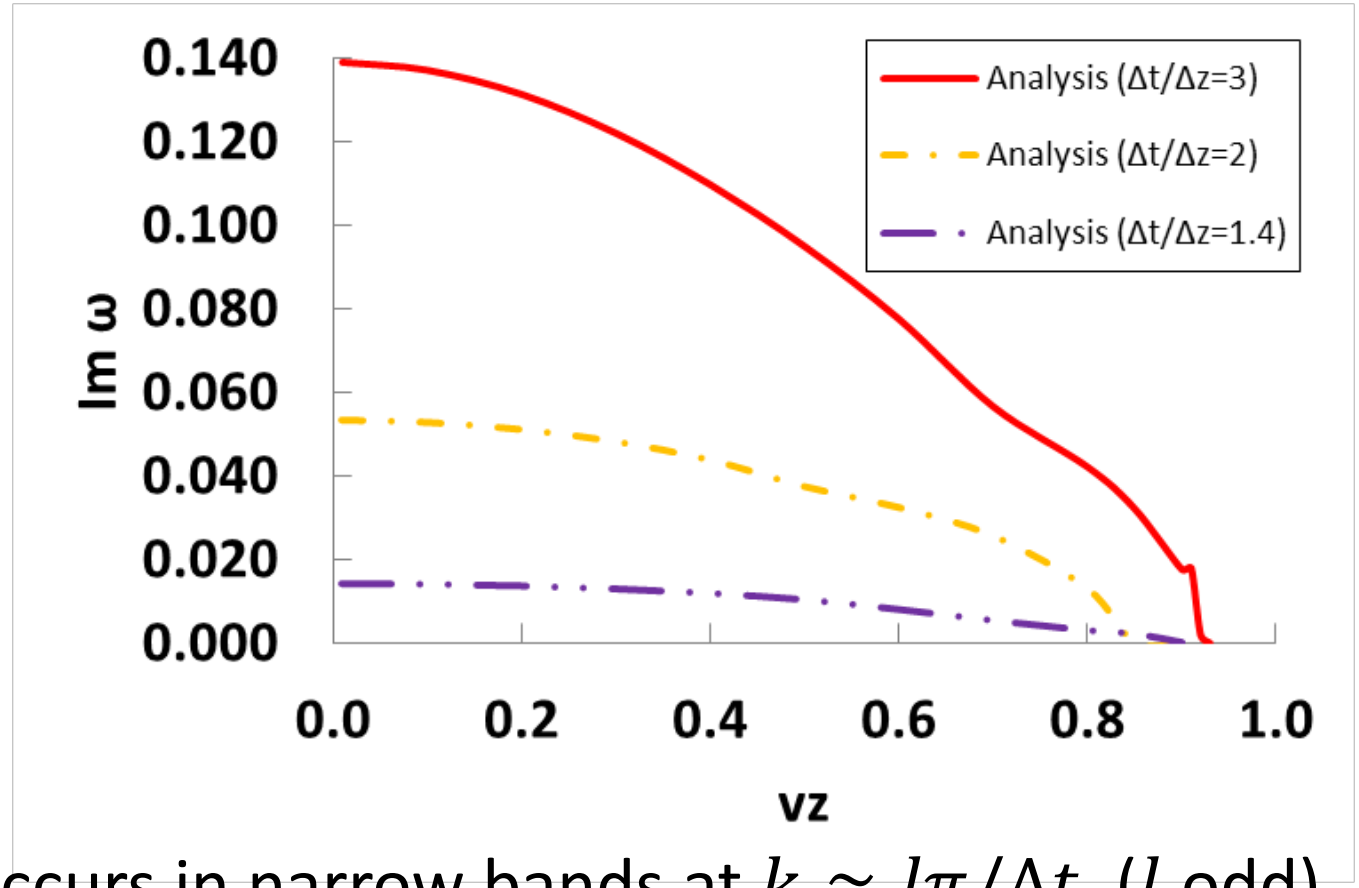
- Choose ζ to set $C_{3x} = 0$ (finite-γ third-order pole)
- No need to eliminate odd aliases (lower cost)

ζ-based Option with E_z Shifted by $\Delta z/2$ Suppresses Low-γ Instability



- Superior at high γ , equally effective at low γ as "energy-conserving" algorithms (which also shift E_z)
- ψ-based options presumably also work well

Instability Predicted by Birdsall-Langdon is Price of no Courant Limit

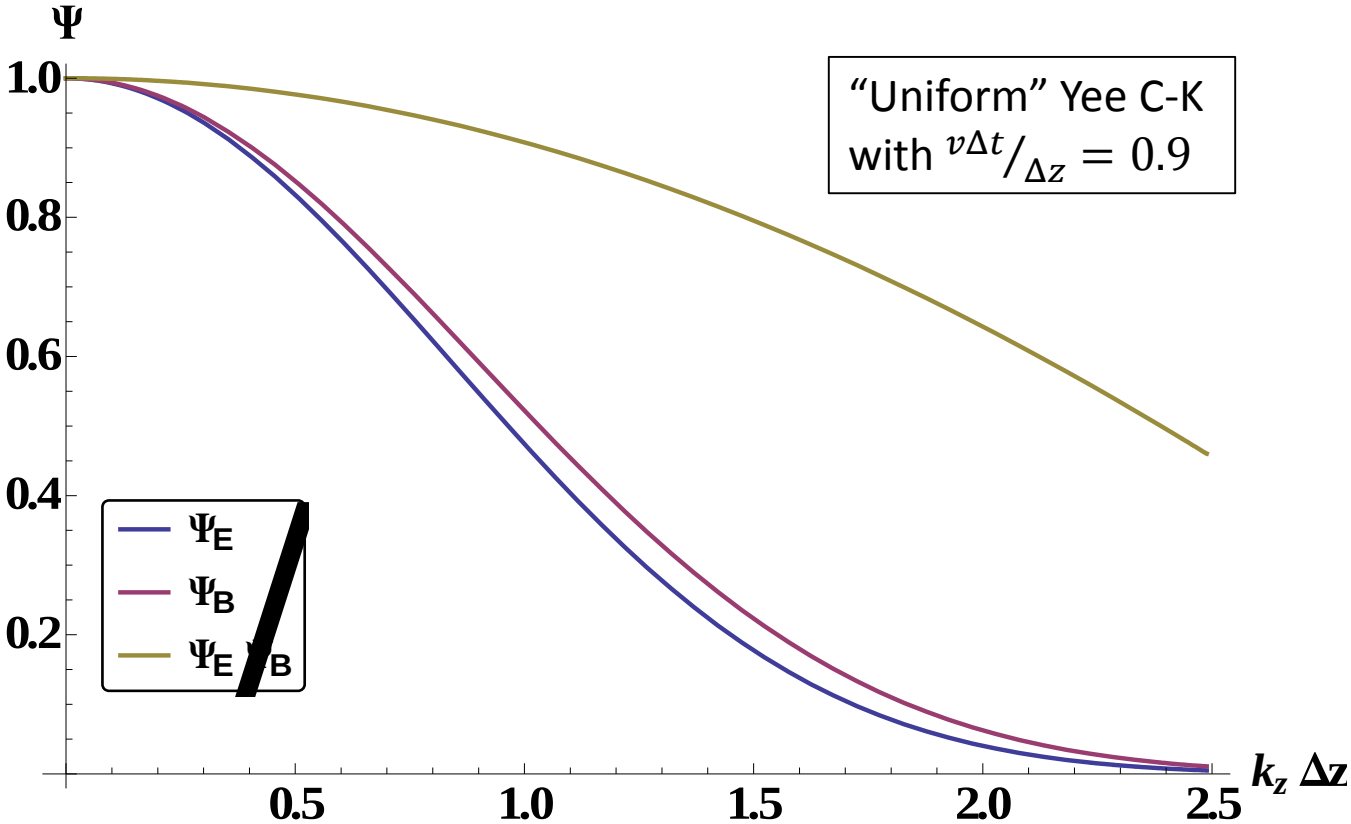


- Occurs in narrow bands at $k \approx l\pi/\Delta t$ (l odd)
- Insignificant at relativistic energies
- Plot parameters: ζ-based option, no odd aliases

Ψ-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 ψ_E to numerator, ψ_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 ψ_E to ratio, ψ_B to 1 also possible but requires matrix inversion, more filtering at larger $^{v\Delta t}/_{\Delta z}$

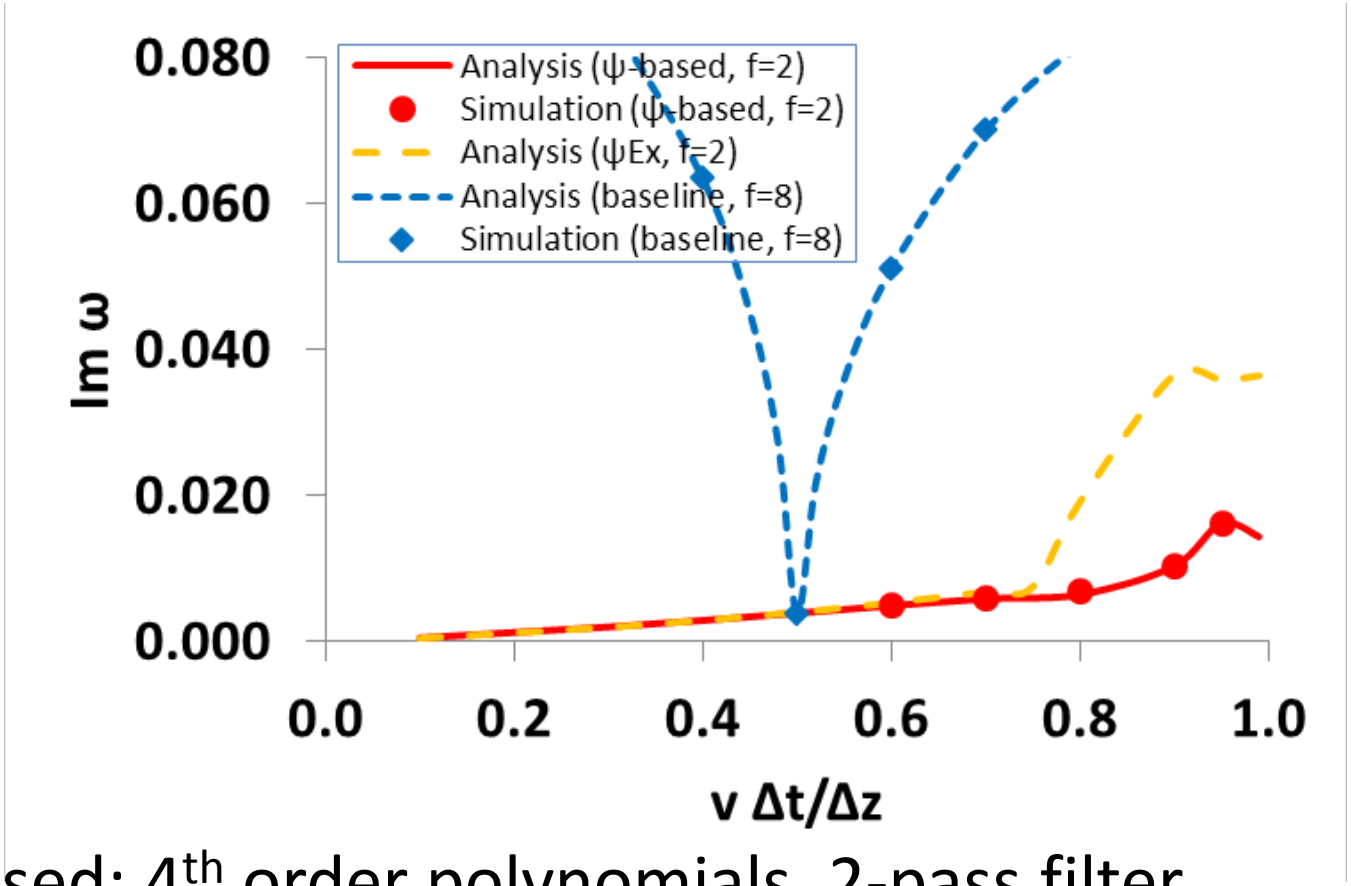
Sample Ψ-Based Multipliers



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

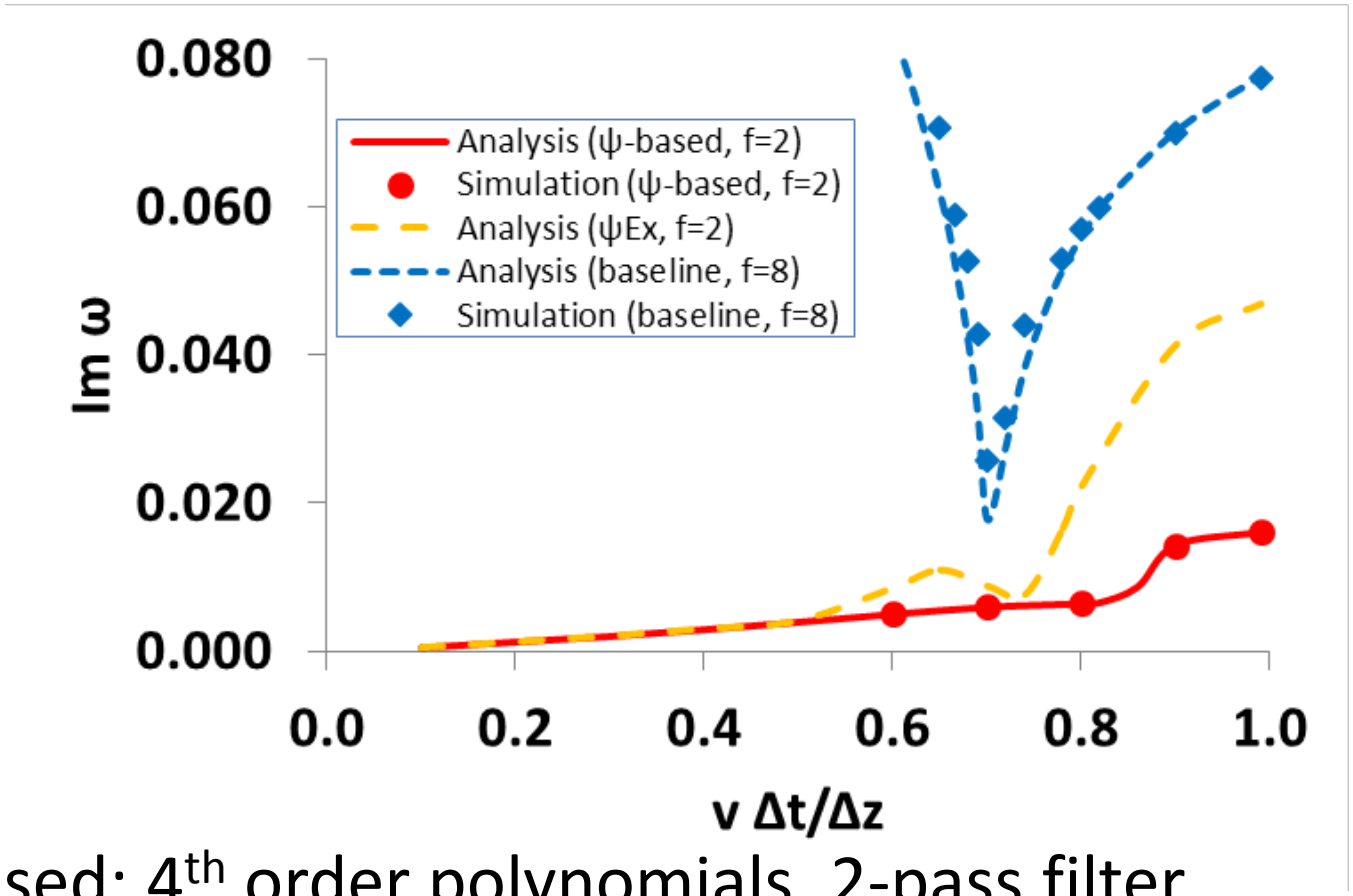
$$\alpha_E = \{-2.92128, 3.04729, -1.31363, 0.187765\}$$
$$\alpha_B = \{-2.54796, 2.20374, -0.709955, 0.054882\}$$

"Uniform" Yee C-K Interpolation



- Ψ-based: 4th order polynomials, 2-pass filter
- Ψ_{Ex}: ratio of 4th order polynomials (E_x only), 2-pass filter
- Baseline: cubic interpolation, 8-pass filter

"Galerkin" Yee C-K Interpolation



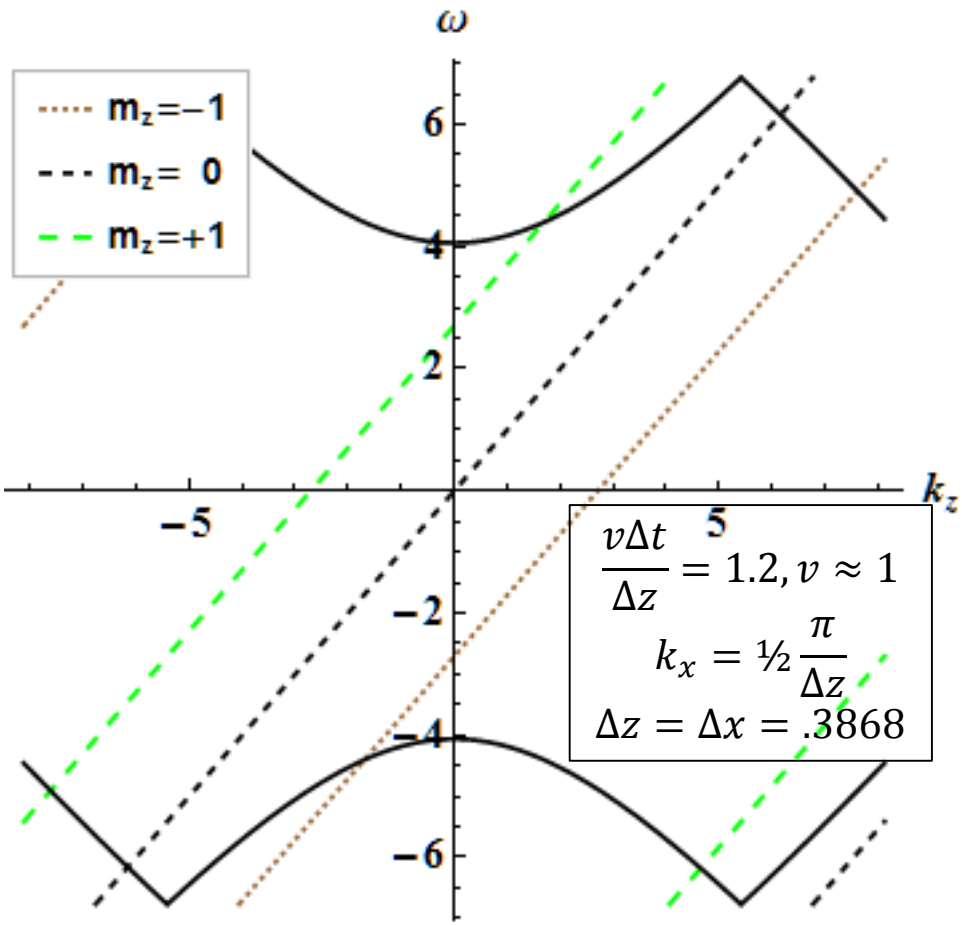
- Ψ-based: 4th order polynomials, 2-pass filter
- Ψ_{Ex}: ratio of 4th order polynomials ($E_x$only), 2-pass filter
- Baseline: cubic interpolation, 8-pass filter

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

- $\omega = \pm \mathrm{Mod}\left[k, \frac{2\pi}{\Delta t}\right]$

Spurious beam modes

- $\omega = \mathrm{Mod}\left[k'_z, \frac{2\pi}{\Delta t}\right]$

Intersections trigger numerical Cherenkov instability

EM modes fold over when $\Delta t > \Delta t_c = (\Delta z^{-2} + \Delta x^{-2})^{-½}$