PPPS-2013: Topic 1.2

NUMERICAL STABILITY OF THE PSEUDO-SPECTRAL EM PIC ALGORITHM*

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Pseudo-spectral methods, which advance fields in Fourier space, offer a number of advantages over more common Finite Difference Time Domain (FDTD) PIC algorithms. In particular, Haber's Pseudo-Spectral Analytical Time-Domain (PSATD) algorithm[1] exhibits dispersion-free propagation and no Courant limit in vacuum. Moreover, Vay's recent research[2] suggests that it can be parallelized about as well as FDTD algorithms. As the research presented here shows, it also has superior numerical stability properties, at least for relativistic beam transport.

Typically the most serious numerical instability in PIC simulations of particle beams is the numerical Cherenkov instability[3], arising from coupling between electromagnetic and nonphysical beam modes. Due to its improved dispersion properties, the PSATD algorithm is less prone to this instability. Nonetheless, the instability still occurs, either directly for time steps larger than the FDTD Courant limit or through nonphysical beam mode aliases at any time step. In this talk we derive the PSATD numerical dispersion relation, present illustrative numerical solutions of it, and compare them with simulation results from the WARP-FFT PIC code. Additionally, we compare these findings with our recent analysis of numerical instabilities in FDTD PIC beam codes[4] and, as time permits, with stability properties of other pseudo-spectral algorithms.

1. I. Haber, R. Lee, H. Klein, and J. Boris, "Advances in Electromagnetic Simulation Techniques", Proceedings of the Sixth Conference on Numerical Simulation of Plasmas, Berkeley, CA, July 16-18, 1973, pp. 46-48.
2. J.-L. Vay, I. Haber, and B. B. Godfrey, "A Domain Decomposition Method for Pseudo-Spectral Electromagnetic Simulations of Plasmas", Journal of Computational Physics, to be published.
3. B. B. Godfrey, "Numerical Cherenkov Instabilities in Electromagnetic Particle Codes", Journal of Computational Physics 15, 504-521, 1974.
4. B. B. Godfrey and J.-L. Vay, Numerical Stability of Relativistic Beam Multidimensional PIC Simulations Employing the Esirkepov Algorithm, arXiv:1211.0232, November 1, 2012.

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Pseudo-Spectral "Analytical" Time Domain (PSATD) Algorithm*

- Numerical Cherenkov instability largely eliminated for PSATD relativistic beam simulations
- Numerical stability software collection at http://hifweb.lbl.gov/public/BLAST/Godfrey/
  - Content meager at present
- Algebra omitted from this talk available at http://arxiv.org/abs/1305.7375v2
- 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.*, paper 1B-1, PPPS 2013

Generalized PSATD Algorithm

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

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

with $\boldsymbol{B}^{n} = \frac{\left(\boldsymbol{B}^{n+½}+\boldsymbol{B}^{n-½}\right)}{2C_h}$, $S_h = \sin\frac{k\Delta t}{2}$, $C_h = \cos\frac{k\Delta t}{2}$

- $\boldsymbol{\zeta} = \mathrm{diag}\left(\zeta_z, \zeta_x, \zeta_y\right)$ - free parameters
- $\boldsymbol{J}$ assumed to conserve charge
  - *e.g.*, Esirkepov algorithm or standard current correction

2-D High-γ Dispersion Relation

$$C_0 + n\sum_m C_1 \csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]$$
$$+n\sum_m C_2 \csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]^2 = 0$$

with $C_0 = \sin\left(\omega\frac{\Delta t}{2}\right)^2 - \sin\left(k\frac{\Delta t}{2}\right)^2$, $k_z' = k_z + m\frac{2\pi}{\Delta z}$

- Dispersion relation reduces to $\omega^2 - k^2 - n = 0$ in continuum limit (n is density divided by γ)
- Beam modes are numerical artifacts, trigger numerical Cherenkov instability
  - May have other deleterious effects

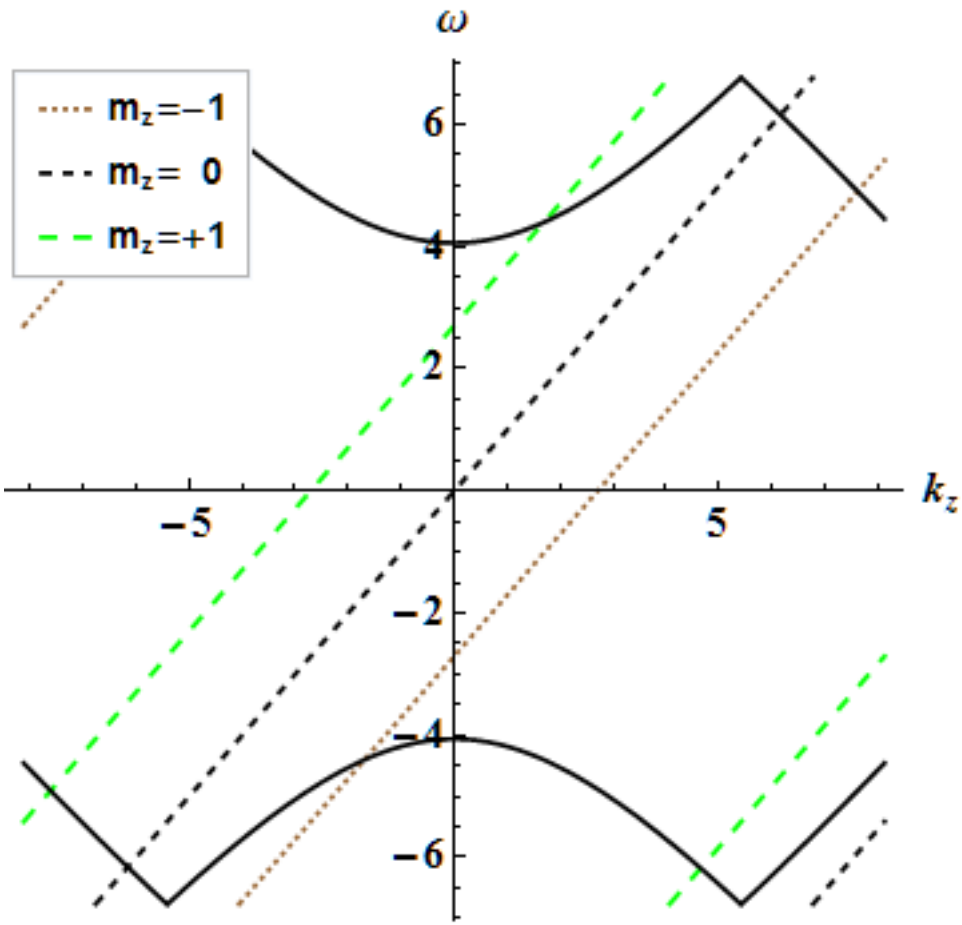
ζ_z Can Reduce Instability

- Option (a) - $\zeta_z = k_z \frac{\Delta z}{2} \cot\left(k_z \frac{\Delta z}{2}\right)$

  $\zeta_x = k_x \frac{\Delta x}{2} \cot\left(k_x \frac{\Delta x}{2}\right)$
- Option (b) - $\zeta_z = \zeta_x = 1$
- Option (c) - ζ_z to suppress $m = 0$ instability
  - Choose ζ_z so that $C_2 = 0$ at resonance
  - Verify $\zeta_z \to 1$ as $k \to 0$ (it does)
  - Set $\zeta_z = 0$ when it falls outside $1 \geq \zeta_z \geq 0$
  - Choose any reasonable ζ_x – here, $\zeta_x = \zeta_z$

In general, $1 \geq \zeta \geq 0$ necessary to avoid new instabilities

PSATD Normal Modes



Normal Modes

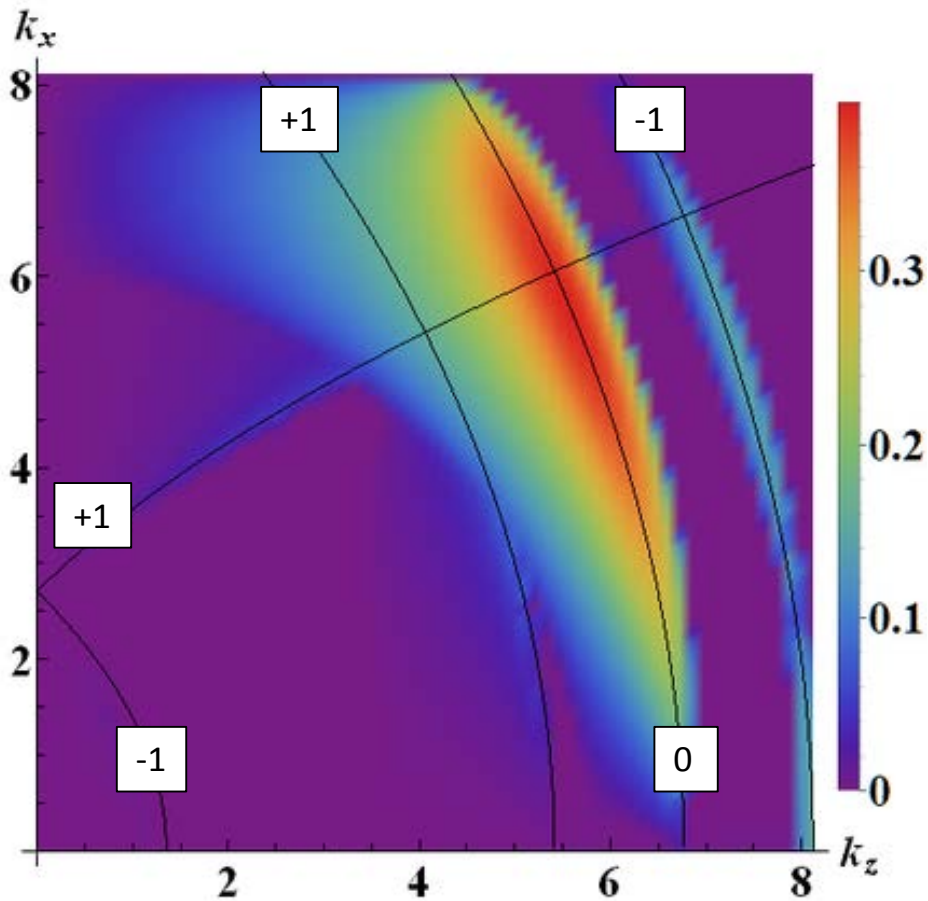
- $\omega = \pm \mathrm{Mod}\left[k, \frac{2\pi}{\Delta t}\right]$
- $\omega = \mathrm{Mod}\left[k_z, \frac{2\pi}{\Delta t}\right]$

Parameters

- $\frac{v\Delta t}{\Delta z} = 1.2, v \approx 1$
- $k_x = ½ \frac{\pi}{\Delta z}$
- $\Delta z = \Delta x = .3868$

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

Full Dispersion Relation Growth Rates

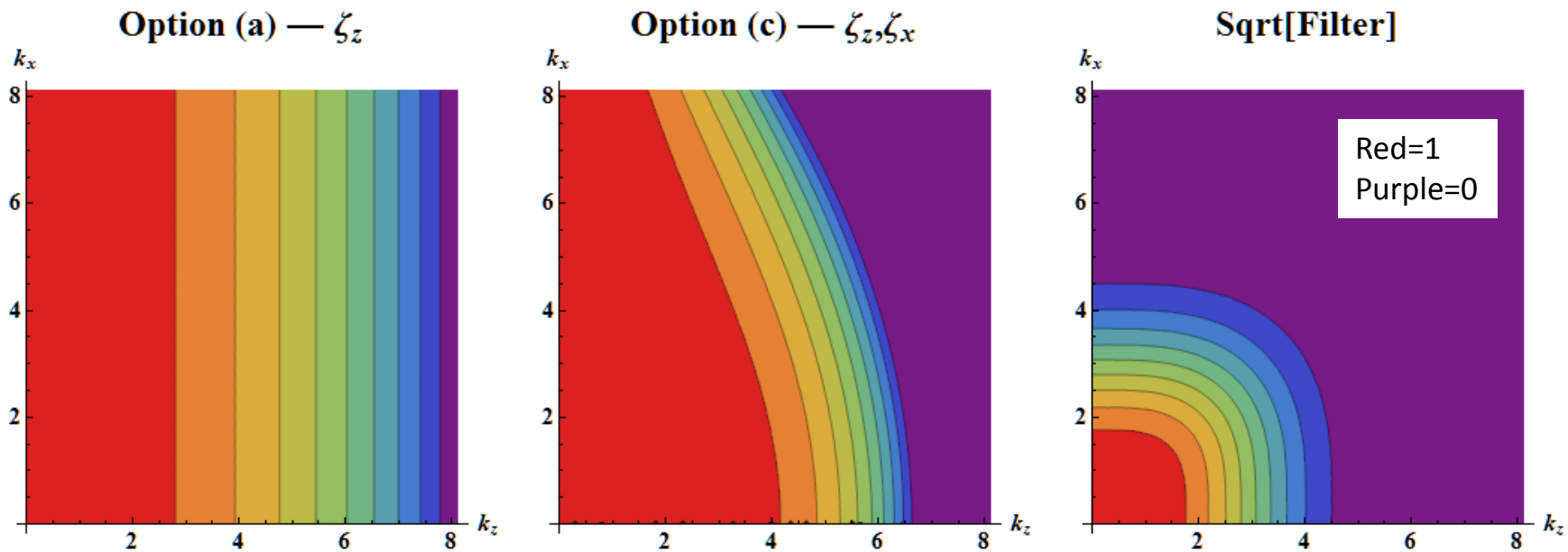


- Peak growth rates at resonances
  - $m = 0$ dominates for $\frac{\Delta t}{\Delta x} > 2\left(\frac{\Delta x}{\Delta t_c} - \frac{\Delta z}{\Delta x}\right)$
  - $m = -1$ dominates otherwise
- Parameters
  - $\frac{v\Delta t}{\Delta z} = 1.2, v \approx 1$
  - Option (a)

Numerical Cherenkov instability dominant resonances typically lie at large $k_z \Delta t/2$

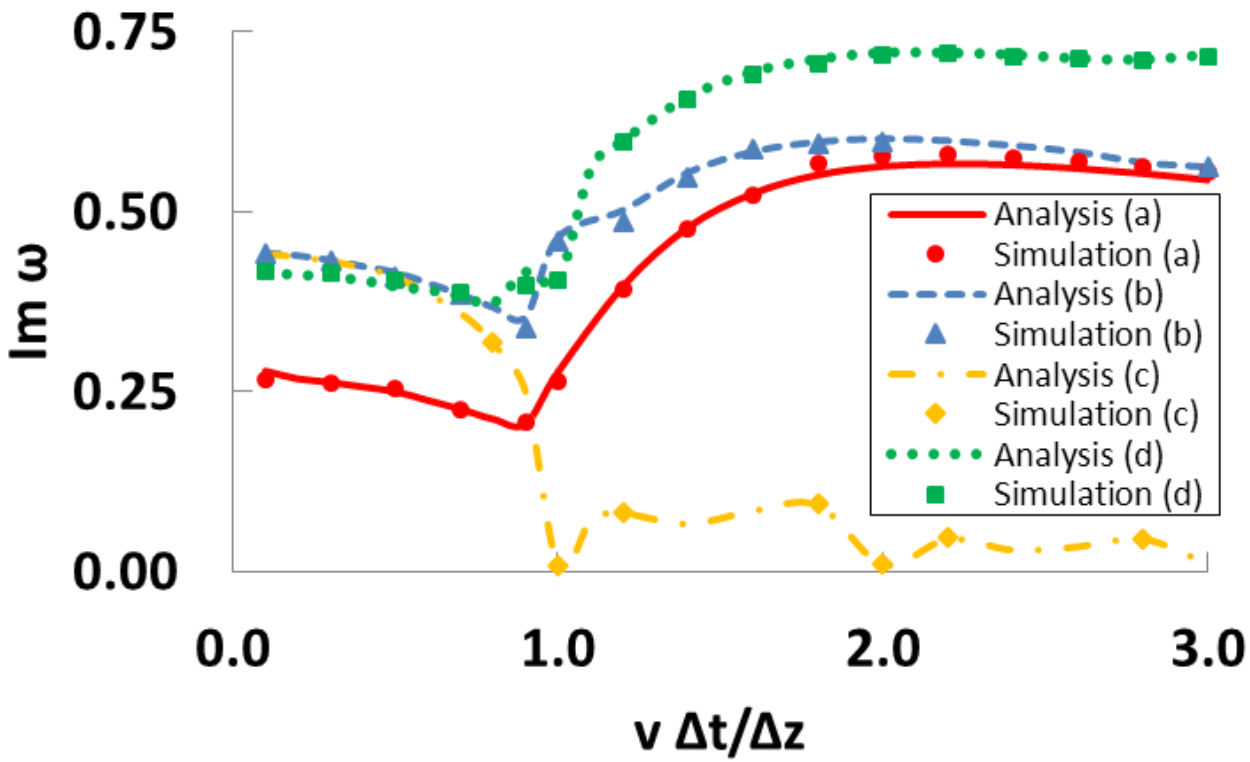
ζ_z, ζ_x and Digital Filter Plots

- Evaluated for $\frac{\Delta t}{\Delta z} = 1.2$
- Ten-pass bilinear filter shown for comparison



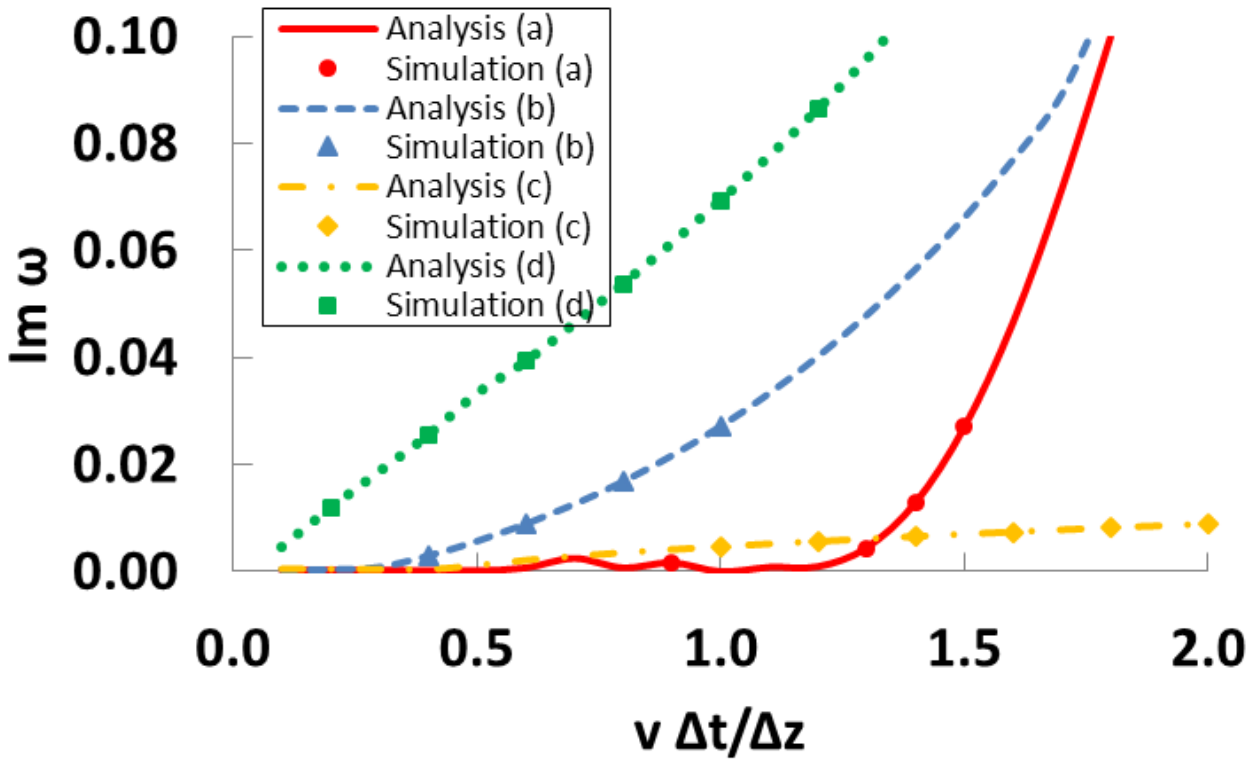
ζ_z, ζ_x filter transverse current components only

Linear Interpolation, No Filter, γ=130



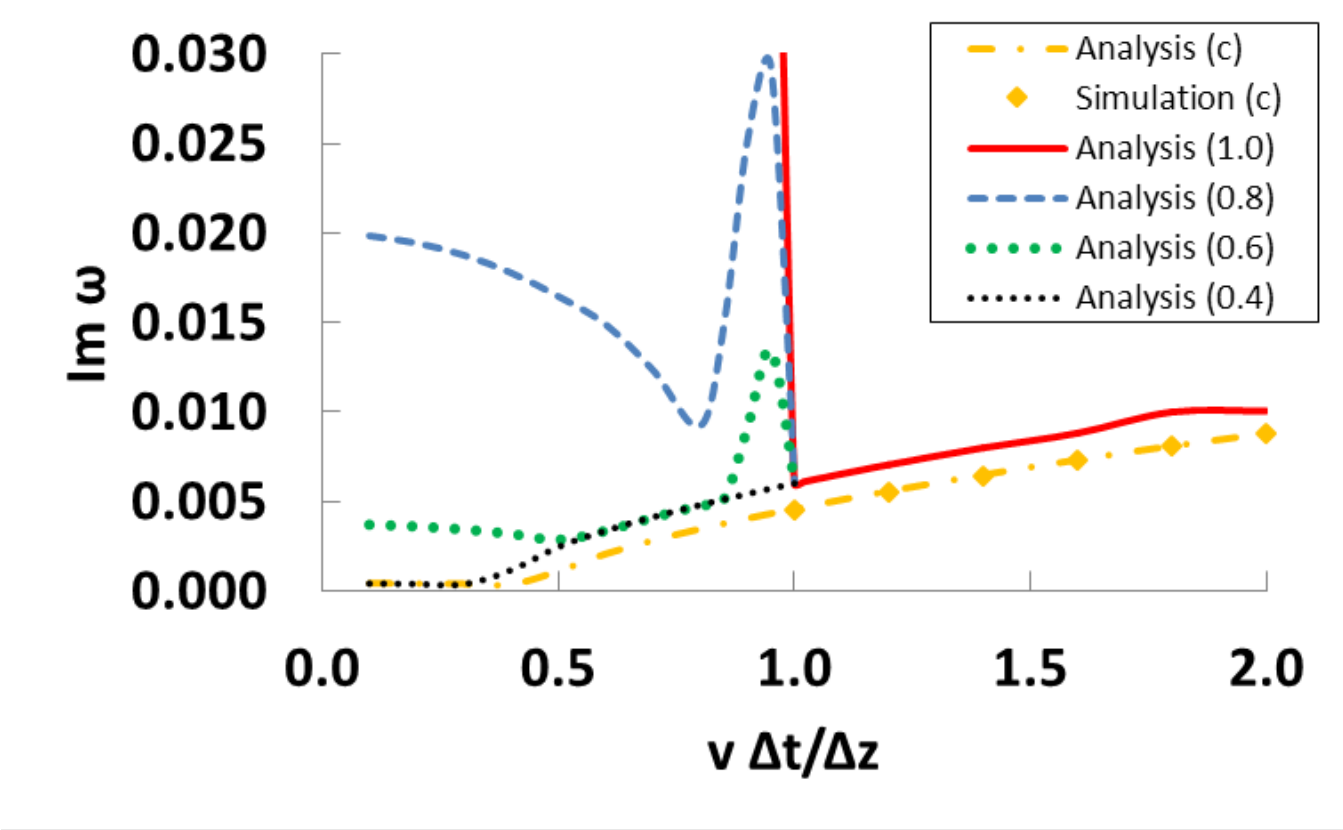
- Option (c) suppresses $m = 0$ instability only
- Option (d) – conventional current deposition and correction – included for comparison

Cubic Interpolation, Filter, γ=130



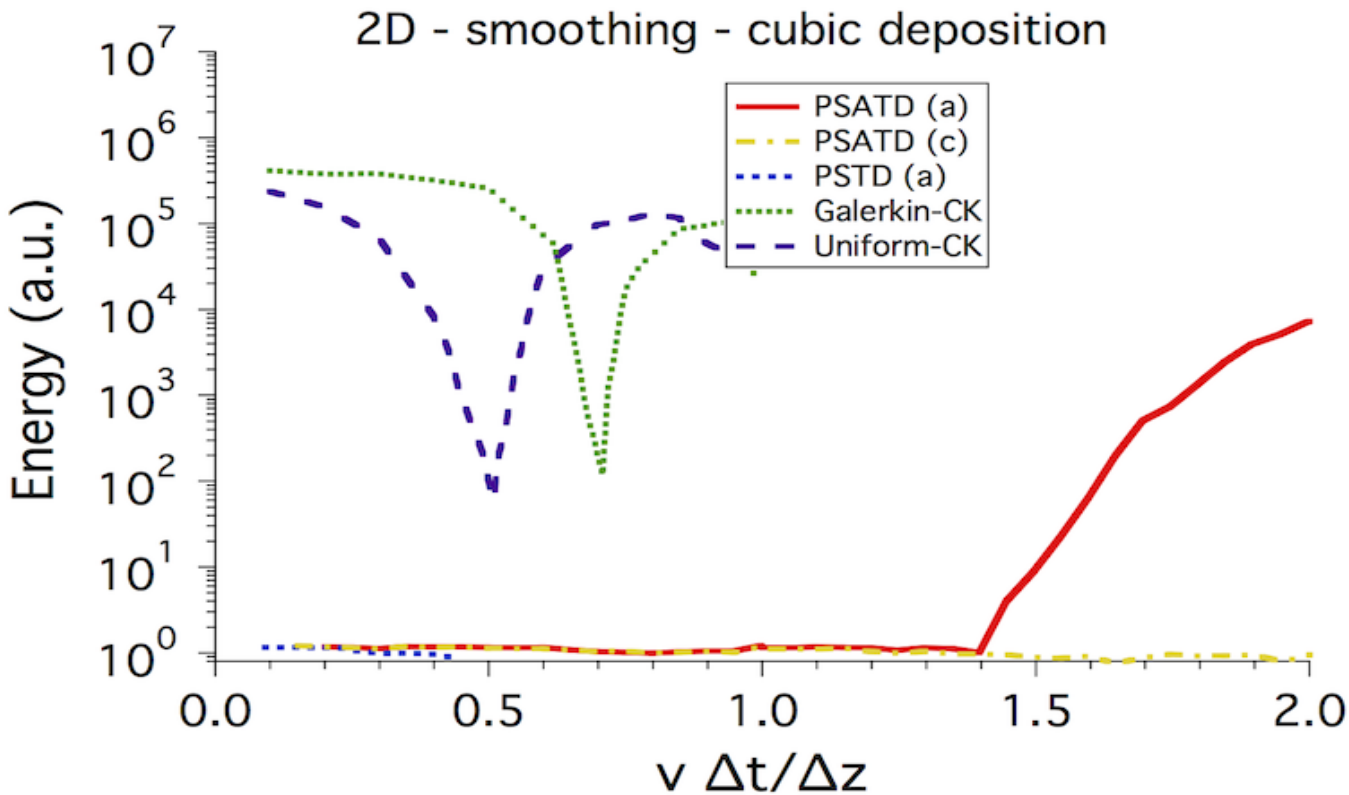
- Numerical Cherenkov instability largely eliminated
- Option (c) residual growth a finite-γ effect

Option (c), Cubic Interpolation, Variable Width Sharp Filter, γ=130



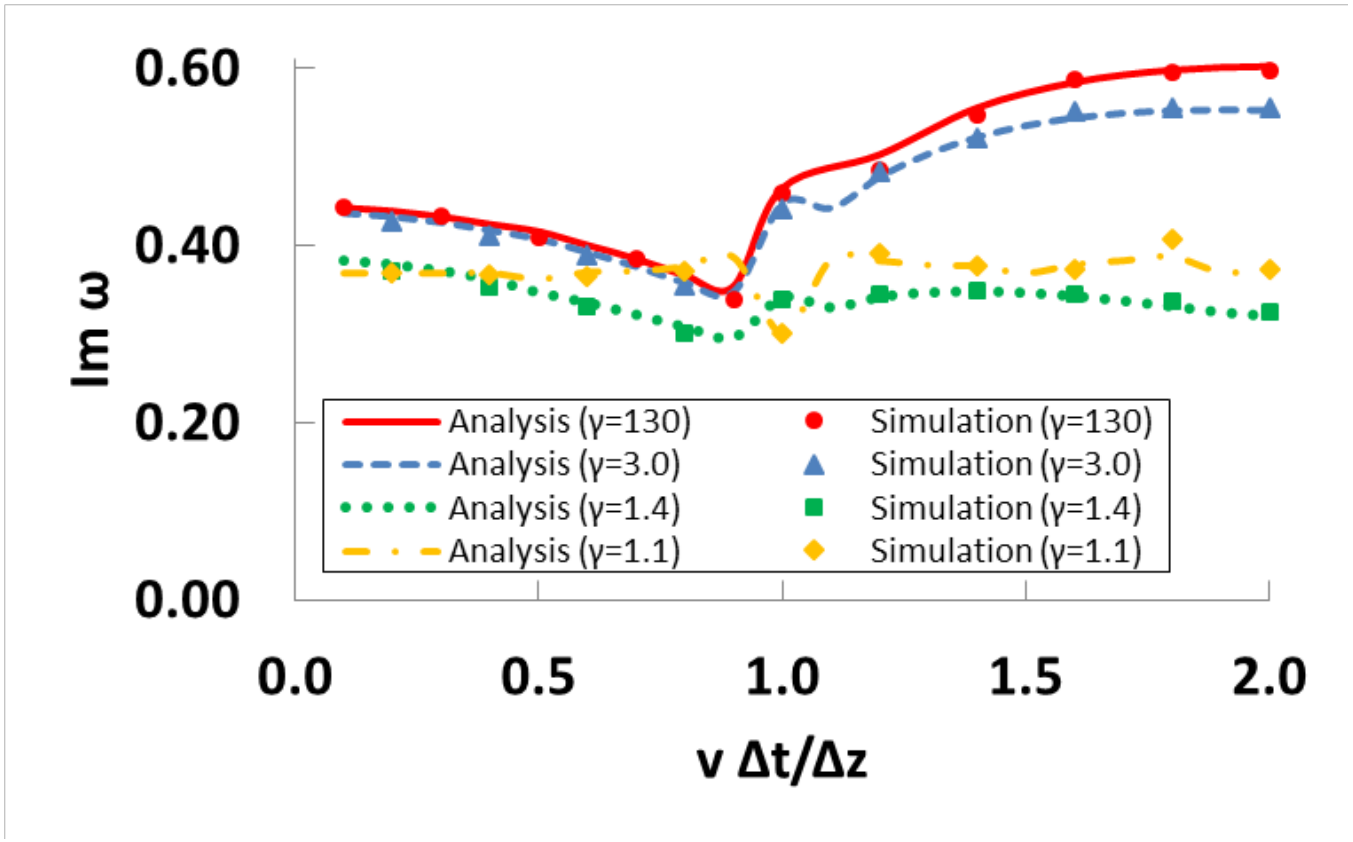
- $\boldsymbol{J} = 0$ for $k > \alpha \min\left[\frac{\pi}{\Delta t}, \frac{\pi}{\Delta z}\right]$, α values in legend
- Option (c) filter from last slide kept as baseline

WARP Simulations Confirm Numerical Cherenkov Instability Suppression



- Numerical energy growth in 3 cm, γ=13 LPA segment
- FDTD-CK simulation results included for comparison

Analysis Also Valid at Low γ



- Performed to identify errors not visible at high γ
- Electrostatic numerical instability dominates at low γ
- Option (b) used

PSATD with Potentials
(Use for Pushing Canonical Momenta)

$$\boldsymbol{A}^{n+3/2} = 2\boldsymbol{A}^{n+½} - \boldsymbol{A}^{n-½}$$
$$+\boldsymbol{k}\left(4{S_h}^2\boldsymbol{k}\cdot\frac{\boldsymbol{A}^{n+½}}{k^2} - i\left(\Phi^{\boldsymbol{n+1}} - \Phi^{\boldsymbol{n}}\right)\Delta t\right)$$
$$+\frac{4{S_h}^2 C_h \boldsymbol{\zeta}:\boldsymbol{J}^{n+½}}{k^2} - \frac{4{S_h}^2 C_h}{k^2}\boldsymbol{kk}\cdot\frac{\boldsymbol{\zeta}:\boldsymbol{J}^{n+½}}{k^2} + \boldsymbol{kk}\cdot\frac{\boldsymbol{J}^{n+½}\Delta t}{k^3}$$

$$\boldsymbol{E}^n = -\left(\boldsymbol{A}^{n+½} - \boldsymbol{A}^{n-½} - i\boldsymbol{k}\Phi^{\boldsymbol{n}}\Delta t\right)/(2S_h/k)$$

$$\boldsymbol{B}^{n+½} = -i\boldsymbol{k}\times\boldsymbol{A}^{n+½}$$

- Gauge invariance: One of four potentials $\{\boldsymbol{A}, \Phi\}$ can be specified arbitrarily

First Attempt Partly Successful

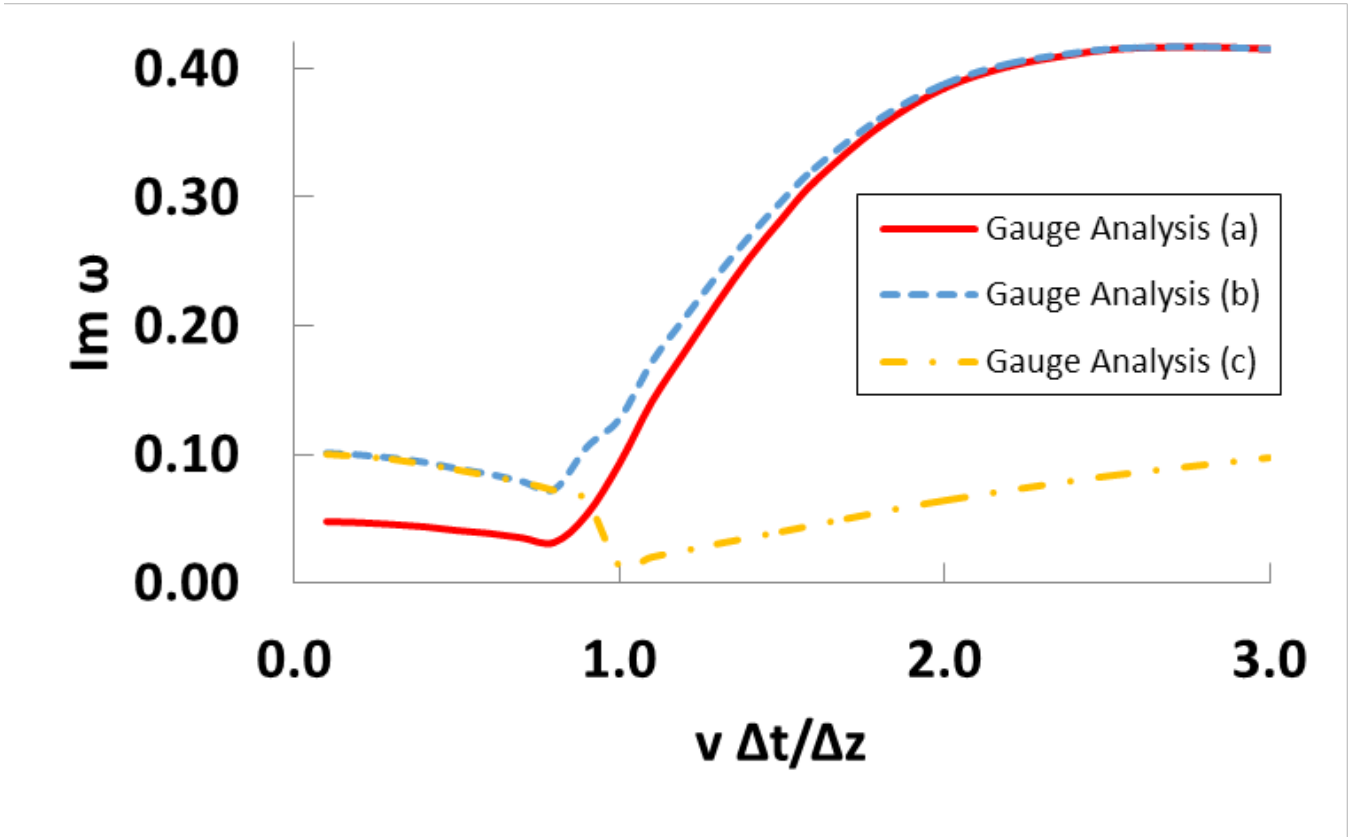
- Choose gauge $\Phi = vA_z \cos\left(\omega \frac{\Delta t}{2}\right)$
- Resulting high-γ dispersion relation:

$$C_0 \sin\left(\omega \frac{\Delta t}{2}\right)\left[\sin\left(\omega \frac{\Delta t}{2}\right) - \frac{k_z \Delta t}{2}\cos\left(\omega \frac{\Delta t}{2}\right)\right]$$
$$+ n\sum_m \widetilde{C_0} + n\sum_m \widetilde{C_1} \csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right] = 0$$

- Reduces order of spurious beam mode from 2 to 1
- Introduces spurious vacuum mode

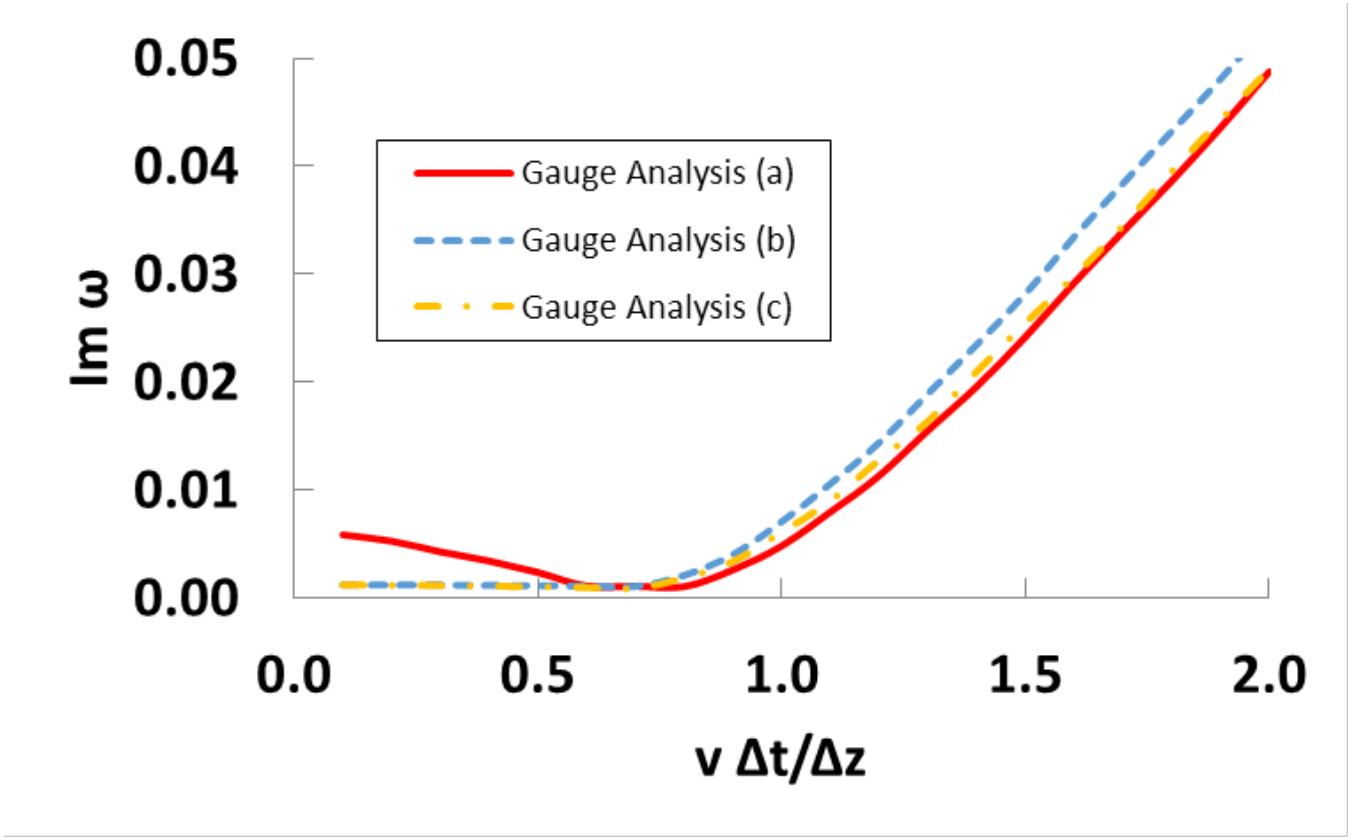
$$\tan\left(\omega \frac{\Delta t}{2}\right) = \frac{k_z \Delta t}{2}$$

Linear Interpolation, No Filter, γ=130



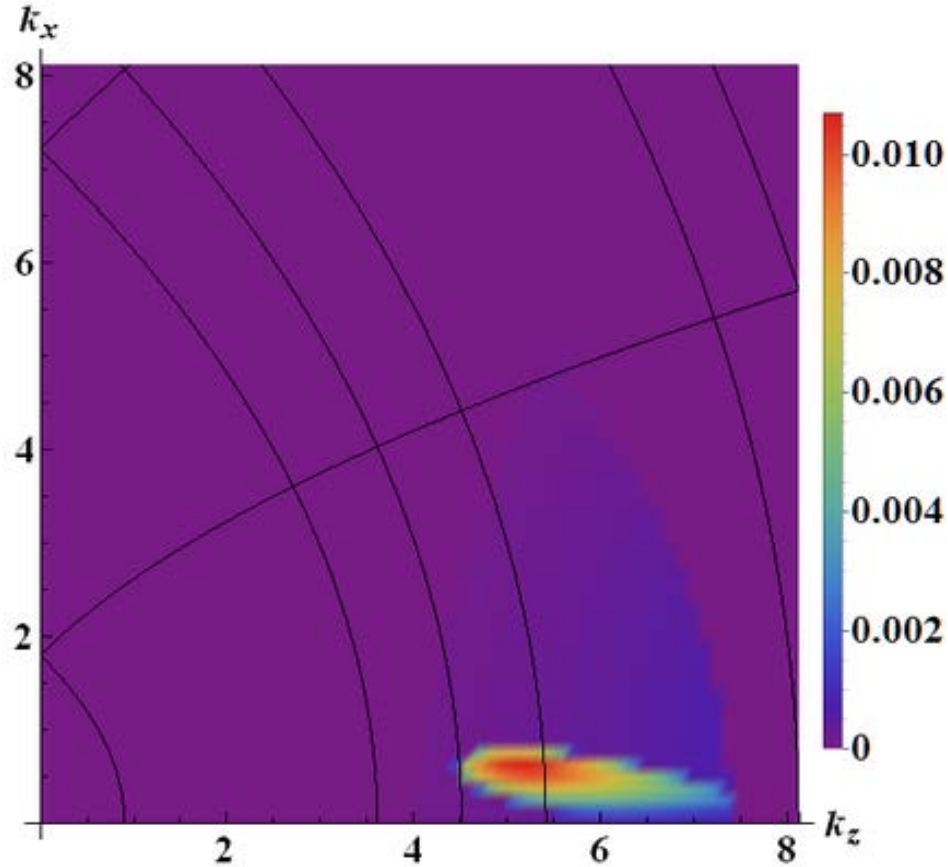
- Growth reduced by ¼ at small $v\Delta t/\Delta z$, by ½ otherwise
- Options defined as before, but details of (c) differ

Cubic Interpolation, Sharp Filter, γ=130



- $\boldsymbol{J} = 0$ for $k > \alpha \min\left[\frac{\pi}{\Delta t}, \frac{\pi}{\Delta z}\right]$, $\alpha = 1$
- New instability dominates (but vanishes for $\alpha < 0.6$)

New, but Weak, Instability Occurs



- Low growth rate
- Small k range
- Bad location
- $\omega \approx k_z v$
- Also occurs in PSTD
- Parameters
  - $\frac{v\Delta t}{\Delta z} = 1.2, \gamma = 130$
  - Option (b)
  - Sharp filter, $\alpha = 1$

Next Steps

- Obtain Option (c) ζ_z, ζ_x for finite γ
- Implement $\Phi = vA_z$ algorithm in WARP, validate results
- Understand, suppress new instability
- Explore other PSATD variants
- Generalize to FDTD

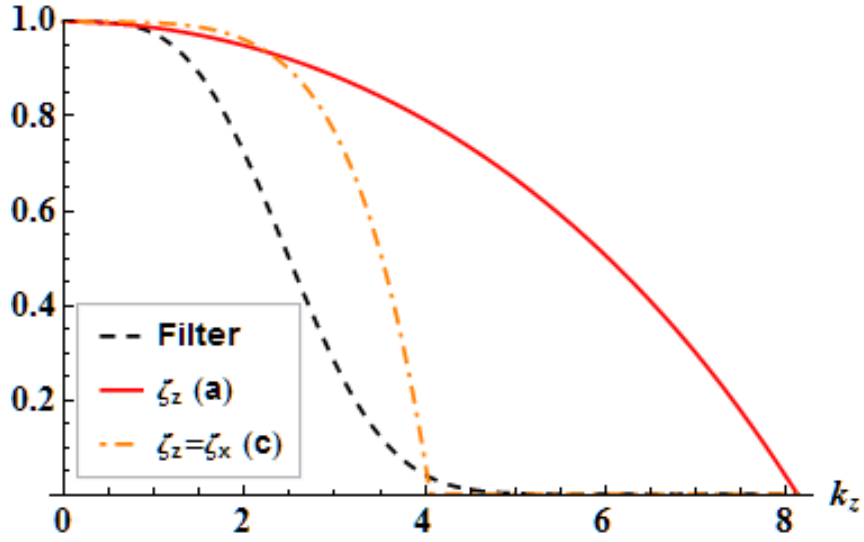
BACKUP

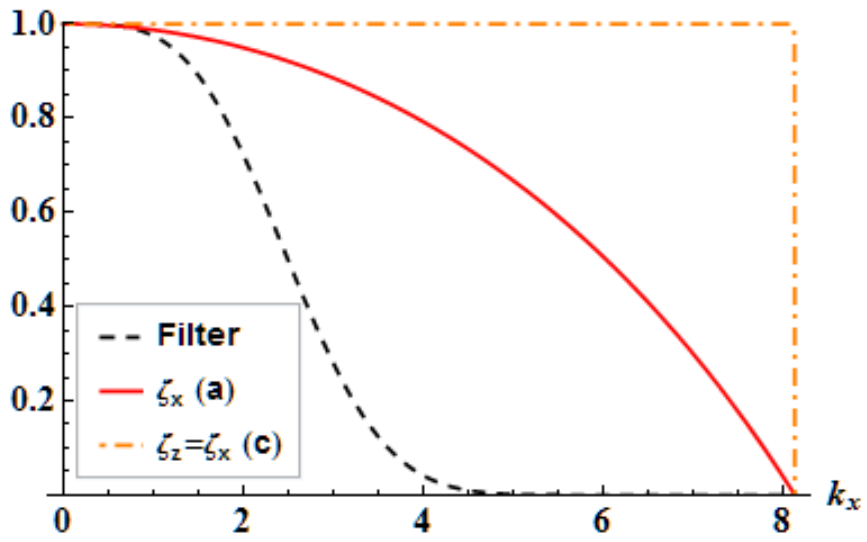
Analytical Approximations Available

- Resonant instability - $\Gamma \approx \left|\frac{nC_2\Delta t}{4k_z}\right|^{1/3} / \Delta t$
  - Typically so strong it must be filtered digitally
  - But, not difficult to do
- Nonresonant instability - $\Gamma \approx \frac{\sqrt{4nC_0C_2 - n^2{C_1}^2}}{C_0\Delta t}$
  - Not so strong, but often lies at small $k_z\Delta t/2$
  - Filtering more difficult to accomplish
  - So, combine filtering with making $n{C_1}^2 > C_0C_2$
- Eliminating nonresonant instability the focus of talk

ζ_z, ζ_x and Digital Filter Plots

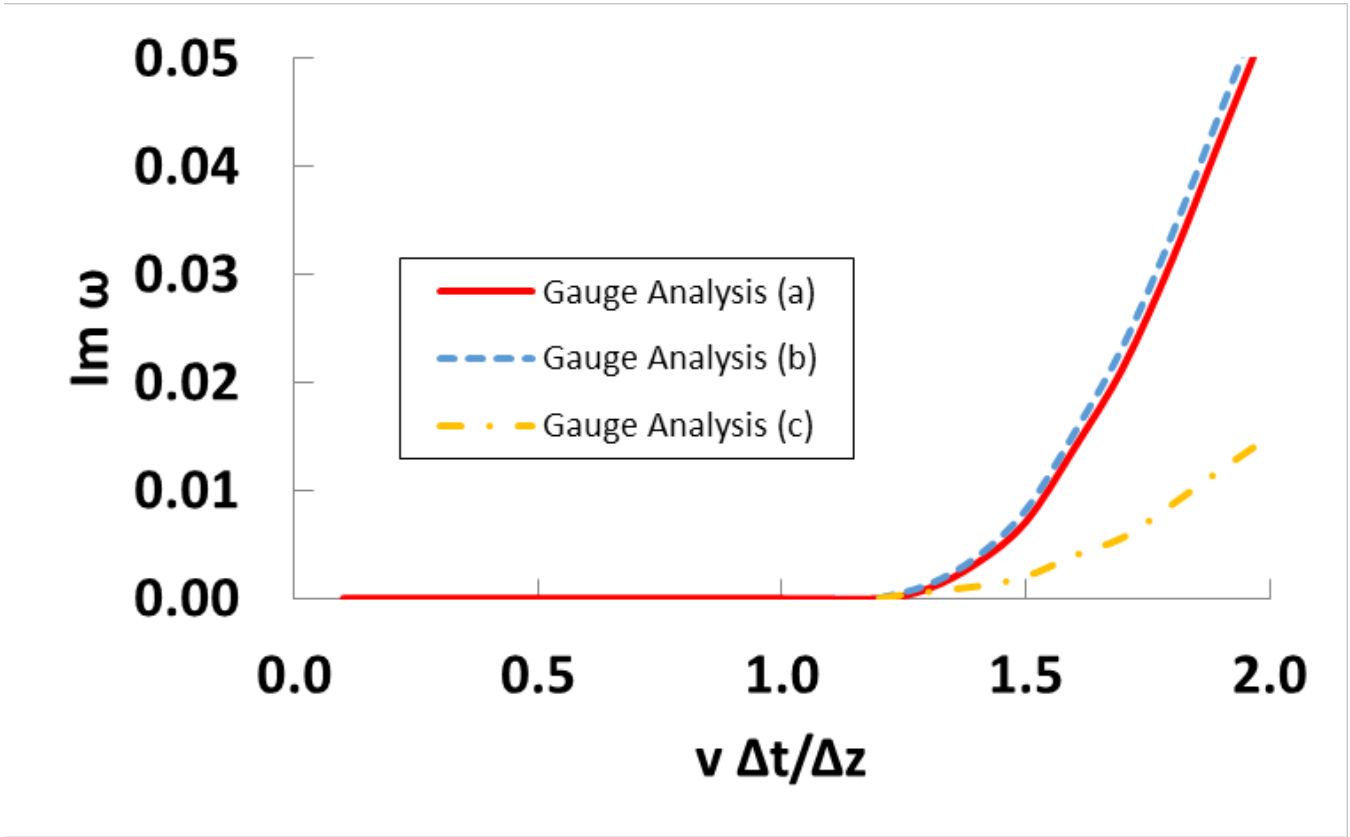
- ζ_z at $k_x = 0$ on left, ζ_x at $k_z = 0$ on right
- Ten-pass bilinear filter shown for comparison
- Evaluated for $\frac{\Delta t}{\Delta z} = 2$





ζ_z, ζ_x filter transverse current components only

Cubic Interpolation, Filter, γ=130



- Growth infinitesimal for $v\Delta t/\Delta z < 1.3$
- New instability increases option (c) growth at larger $v\Delta t/\Delta z$, but still very small