Numerical Stability of Pseudo-Spectral PIC Code Generalizations*

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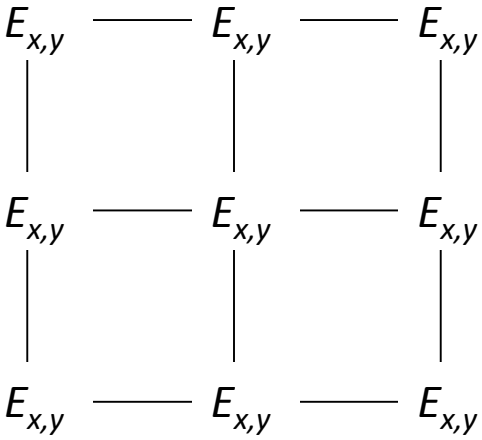
Pseudo-Spectral Time Domain Field Solver (PSTD)

- Fields advanced in Fourier space
  - $\boldsymbol{E}^{n+1} = \boldsymbol{E}^{n} - i\boldsymbol{k} \times \boldsymbol{B}^{n+½}\Delta t - J_k^{n+½}\Delta t$
  - $\boldsymbol{B}^{n+½} = \boldsymbol{B}^{n-½} + i\boldsymbol{k} \times \boldsymbol{E}^{n}\Delta t$
- Fields 2nd order accurate in time, exact in space
  - Fields applied to particles in real space
  - Currents also determined in real space
  - FFTs required at each time step
  - 2D sample mesh at right
  - B fields at cell corners, offset by $\Delta t/2$



- Somewhat restrictive Courant condition

PSTD Generalizations

- Sub-cycle field solver (relative to particle time-step) to relax PSTD restrictive Courant limit
  - Sub-cycling fields numerically straightforward
  - Analytically, if $F^{n+1} = M : F^n + S$ for N=1, then $F^{n+1} = M^N : F^n + \sum_{i=0}^{N-1} M^i : S$ for any N (*n* is particle time step)
  - PSTD in limit $N \to \infty$ becomes Haber's PSATD algorithm, *Proc. Sixth Conf. Num. Sim. Plasmas, USA, 46-48 (1973)*
- Reduce effective particle width by replacing *k* in PSTD algorithm by a finite-difference approximation
  - E.g., $k \Rightarrow \frac{\sin(k\,\Delta x/2)}{(k\,\Delta x/2)}$ (second-order approximation – has much in common with FDTD algorithm)
  - See *Lele, JCP* ***103****, 16 (1992)* for other approximations

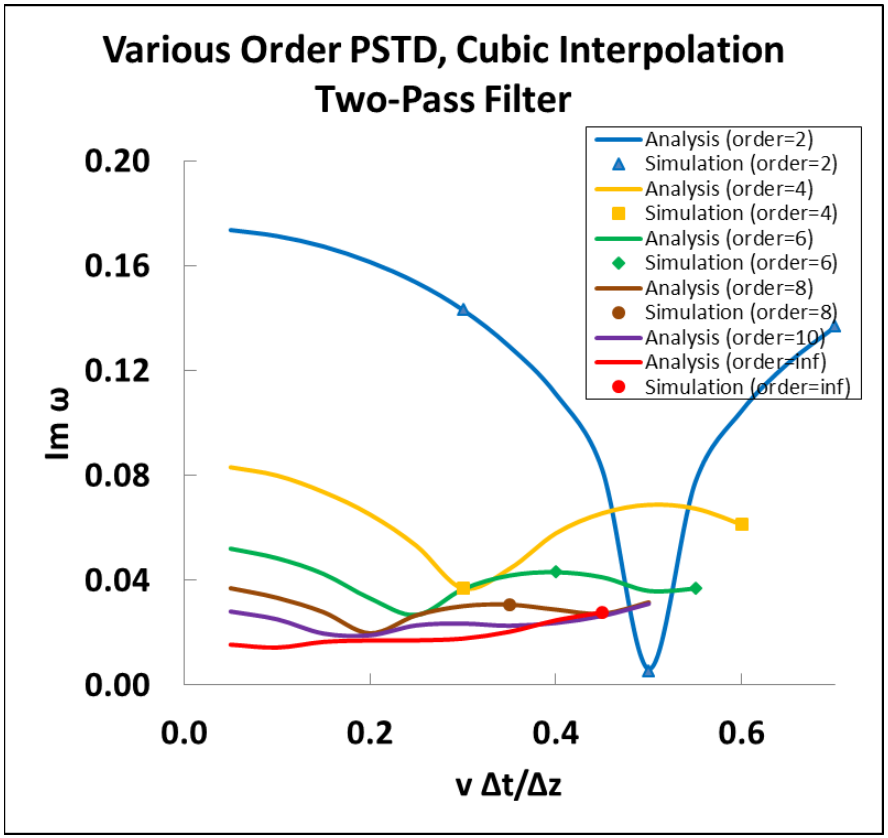
Numerical Cherenkov Instability

- Serious issue in 2D, 3D relativistic beam simulations
  - Growth rates a large fraction of $\left(\omega_p{}^2 k_\perp{}^2 \Delta z\right)^{1/3}$
- High- γ dispersion relation

$$C_0 + \omega_p{}^2 \sum_m C_1 \csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]$$
$$+\omega_p{}^2 \sum_m C_{2x} \csc\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]^2 = 0$$
$$\text{with } k_z' = k_z + m\frac{2\pi}{\Delta z} \qquad \text{(aliases)}$$

- Beam modes associated with C_1, C_{2x} are numerical artifacts, trigger numerical Cherenkov instability

Numerical Instability Growth Rates Often Large



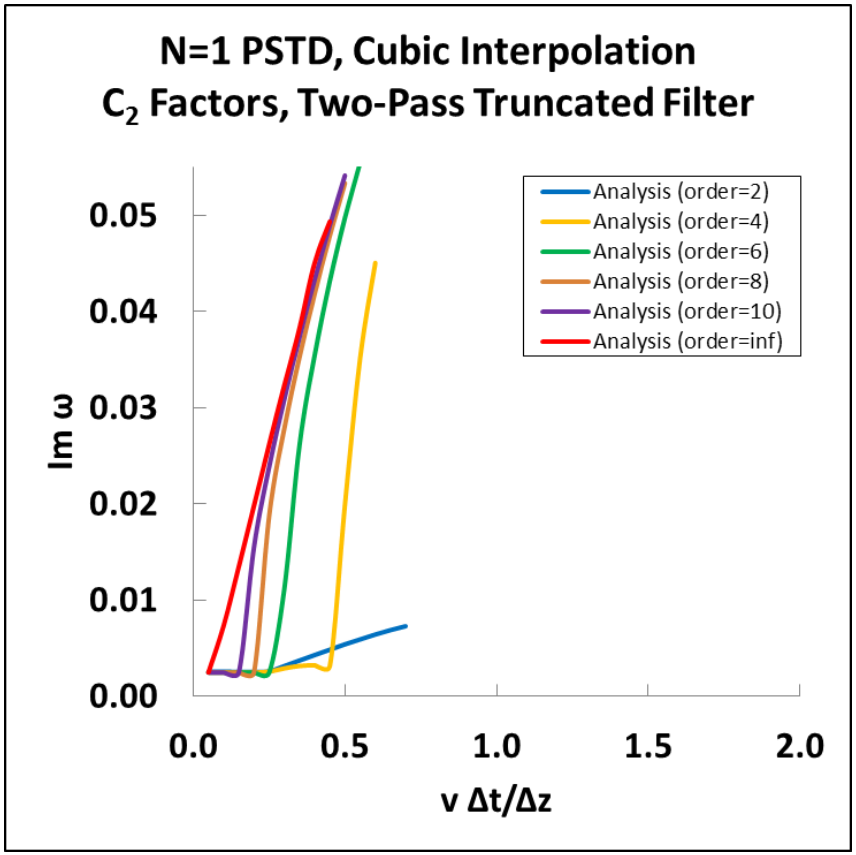
- N=1, various orders
- PSTD is "infinite order"
- $\omega_p = 1, \gamma = 130$
- $\Delta z = \Delta x = 0.3868$
- Single bilinear digital filter of fields, currents
- Cubic interpolation

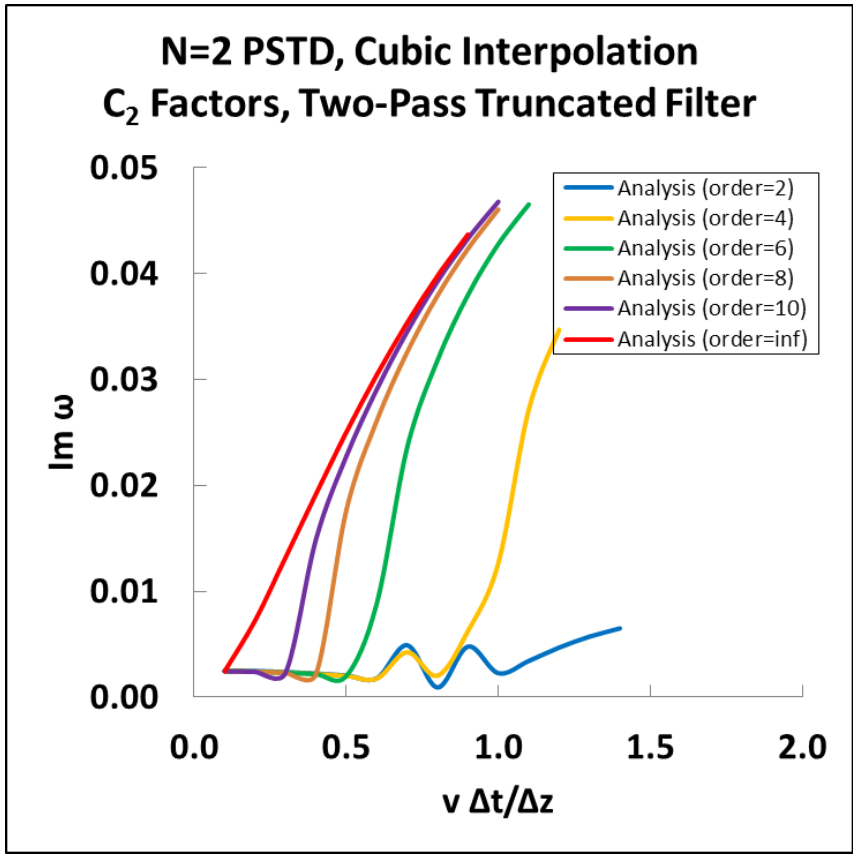
Second-order curve has characteristic FDTD shape, including "magic time step", *Godfrey and Vay, JCP* ***248****, 33-46 (2013)*

Instability Suppression Strategy

- Filter to eliminate resonant instabilities at large k
  - Multi-pass bilinear filter, and/or
  - Sharp-cutoff filter, $k < \alpha\, Min\left[\frac{\pi}{v\,\Delta t}, \frac{\pi}{\Delta z}\right]$, or
  - Interpolate current on 2x mesh in *z*, discard upper half of k_z (effective but more expensive)
- Modify fields slightly to suppress $m = 0$ non-resonant instabilities at smaller k
  - Set $C_{2x} = 0$ at $\omega = k_z v$
  - Other options, developed for PSATD, do not work well here
- Combination of bilinear filter, $\alpha = 0.6$ cutoff, C_{2x} field modification factors used below

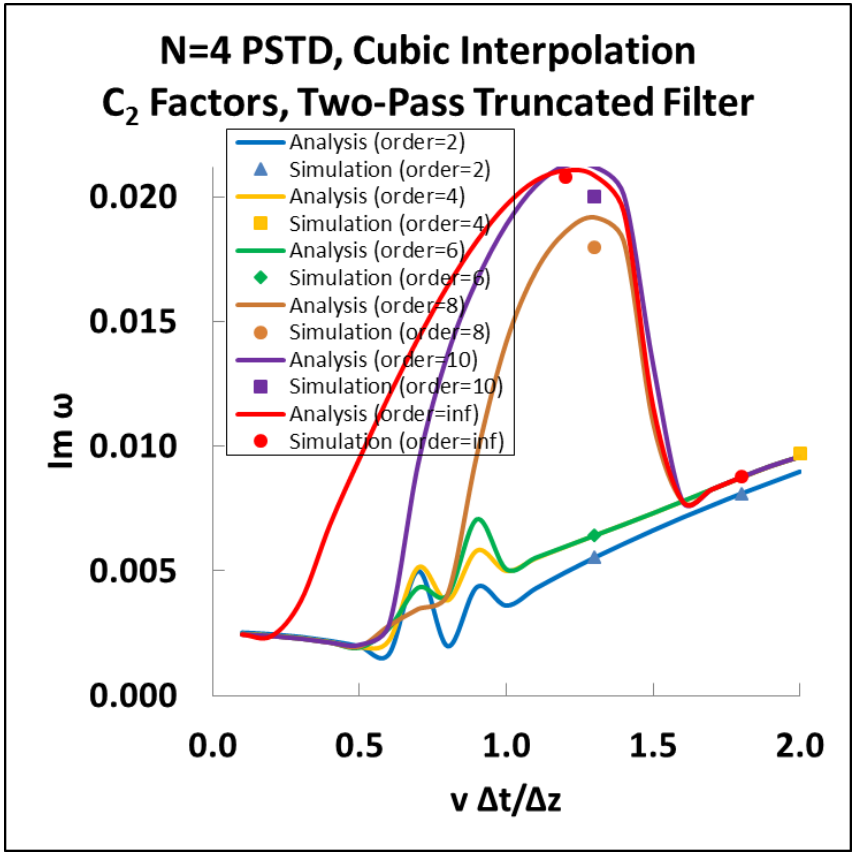
Peak Growth Rates for N=1, 2

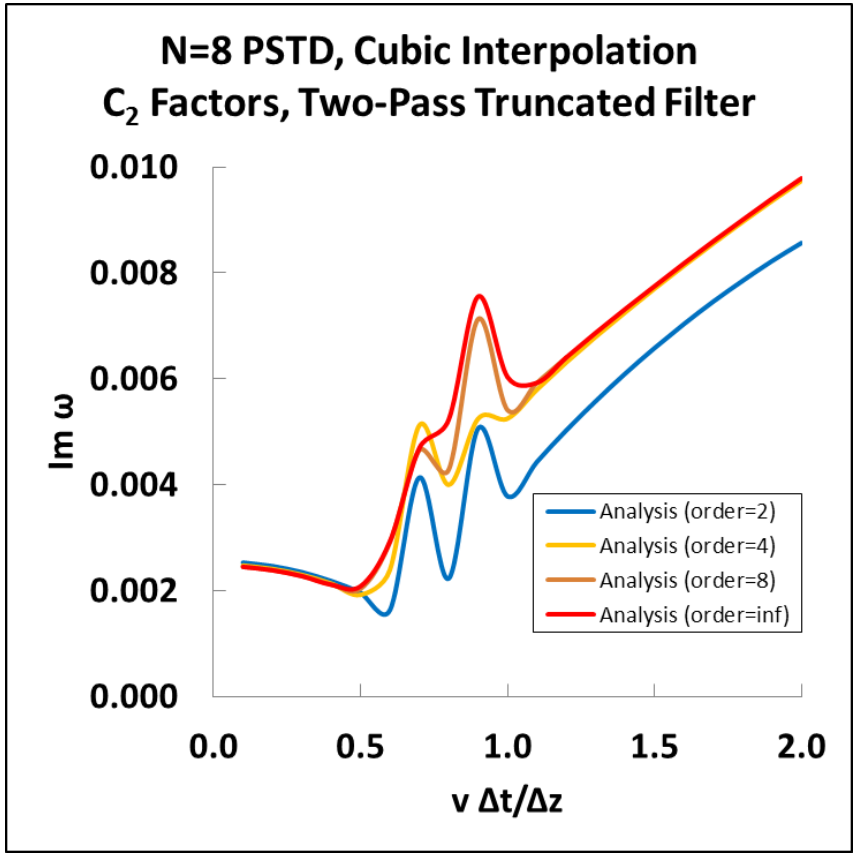




Weaker numerical instabilities for larger N, smaller order

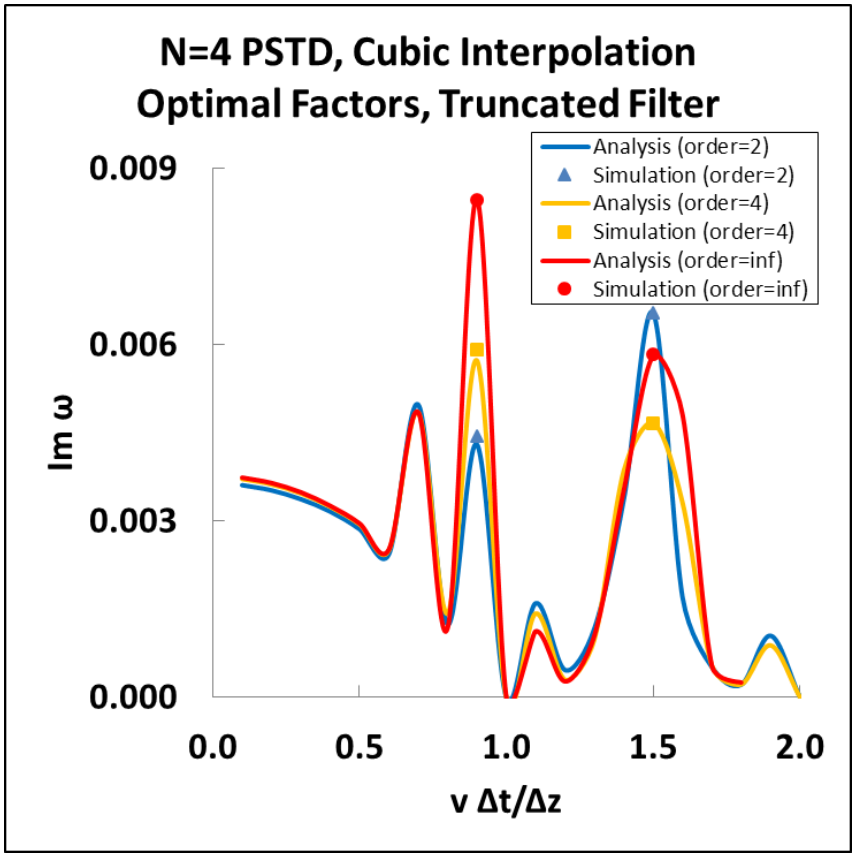
Peak Growth Rates for N=4, 8





Weaker numerical instabilities for larger N, smaller order

Even Better Scheme in Development



- Small, numerically determined field correction factors from full dispersion relation
- Completely suppresses $m = 0$ instability
- $\alpha = 0.6$ cutoff filter controls higher m modes
- No bilinear filter
- Good agreement with WARP simulations

Peak growth rates relatively insensitive to N, order

Summary

- Generalized PSTD Numerical Cherenkov instability suppressed fairly well by C_{2x} field-correction factors
  - (combined with cubic interpolation, modest bilinear filtering, $\alpha = 0.6$ cutoff)
- C_{2x} correction: scale interpolated $B_\perp$ by Ψ_B
  - $$\Psi_B = \frac{\sin^2\left(\frac{\theta\,\Delta t}{2}\right)\frac{\sin(k_Z\,\Delta t)}{k_Z\,\Delta t}}{\sin^2\left(\frac{k_Z\,\Delta t}{2}\right)\left[\frac{\sin(\theta\,\Delta t)}{N}\csc\left(\frac{\theta\,\Delta t}{N}\right)-1\right]+\sin^2\left(\frac{\theta\,\Delta t}{2}\right)}$$

    with $$\sin\left[\frac{\theta\Delta t}{2N}\right] \equiv \frac{k\Delta t}{2N}$$
- Even better correction factors in development

Software and Slides

- Software and other supporting material at http://hifweb.lbl.gov/public/BLAST/Godfrey/
  - **FDTD** – Solves FDTD numerical dispersion relation
  - **Resonances** – Plots normal modes and resonances
  - **RatIntCoef** – Computes FDTD ψ polynomials
  - *Mathematica CDF Player* needed (free)
  - Contact Brendan.Godfrey@ieee.org
- Various references also available there
  - Including these slides
- More material to be added over next several months