Review and Recent Advances in PIC Modeling of Relativistic Beams and Plasmas*

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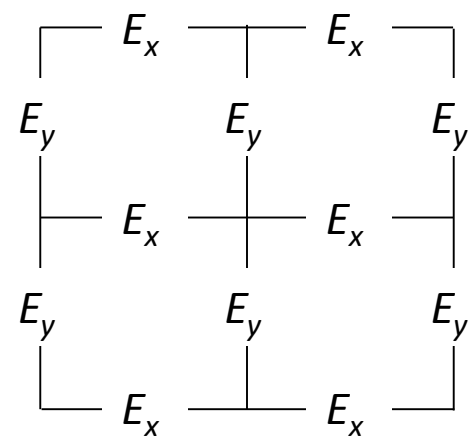
Particle-in-Cell Simulation Codes

- Solve Vlasov equation by computing particles' trajectories in their self-consistent fields
- Calculate particle trajectories from impulse forces
  - $\frac{dz}{dt} = v, \quad \frac{d\gamma v}{dt} = \sum_{n,l} F_l^n \, W(z - l\Delta z) \, \delta(t - n\Delta t)$
- Calculate currents by interpolation to space-time grid
  - $J_l^{n+½} = \sum_p v \, V(z - l\Delta z) \,|_{t=(n+½)\Delta t}$
  - W, V are interpolation functions (typically splines)
- Better yet, Esirkepov's charge-conserving algorithm
  - $\rho_{l+½}^{n+1} - \rho_{l+½}^{n} = \left(J_{l+1}^{n+½} - J_l^{n+½}\right) \frac{\Delta t}{\Delta z}$

Sample equations in 1D, generalization to 3D straightforward

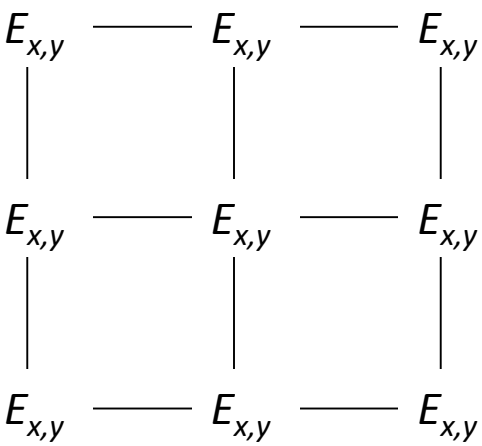
Finite Difference Time Domain Field Solver (FDTD)



- Calculate fields on "Yee" grid
  - B fields at cell centers, offset by $\Delta t/2$
  - Currents located with E, offset by $\Delta t/2$
  - 2D example at right
- Staggered fields give 2nd order accuracy (1D example)
  - $E_l^{n+1} = E_l^n - \left(B_{l+½}^{n+½} - B_{l-½}^{n+½}\right)\frac{\Delta t}{\Delta z} - J_l^{n+½}\Delta t$
  - $B_{l+½}^{n+½} = B_{l+½}^{n-½} - \left(E_{l+1}^n - E_l^n\right)\frac{\Delta t}{\Delta z}$
- More complex expressions yield improved dispersion
  - E. g., Cole-Karkkainen and Lehe algorithms

Pseudo-Spectral Time Domain Field Solver (PSTD)

- Fields advanced in Fourier space, but
  - 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 $^{\Delta t}/_{2}$



- Fields 2nd order accurate in time, exact in space
  - $\boldsymbol{E}^{n+1} = \boldsymbol{E}^{n} - i\boldsymbol{k} \times \boldsymbol{B}^{n+½}\Delta t - J_k^{n+½}\Delta t$
  - $\boldsymbol{B}^{n+½} = \boldsymbol{B}^{n-½} + i\boldsymbol{k} \times \boldsymbol{E}^{n}\Delta t$
- Full Spectral Field Solver bypasses spatial grid but requires Fourier transform at each particle position

Pseudo-Spectral Analytical Time Domain Field Solver (PSATD)

- Obtained by analytically integrating Maxwell's equations over Δt, assuming constant currents
- Fields exact in time and space (for constant currents)

$$\boldsymbol{E}^{n+1} = \boldsymbol{E}^{n} - 2iS_h \boldsymbol{k} \times \frac{\boldsymbol{B}^{n+½}}{k} - \frac{2S_h C_h \boldsymbol{J}^{n+½}}{k} + \frac{2S_h C_h}{k} \boldsymbol{k}\boldsymbol{k} \cdot \frac{\boldsymbol{J}^{n+½}}{k^2} - \boldsymbol{k}\boldsymbol{k} \cdot \frac{\boldsymbol{J}^{n+½} \Delta t}{k^2}$$

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

- Many desirable traits but, like PSTD, requires global FFTs
  - Jean-Luc Vay's talk offers potential solutions

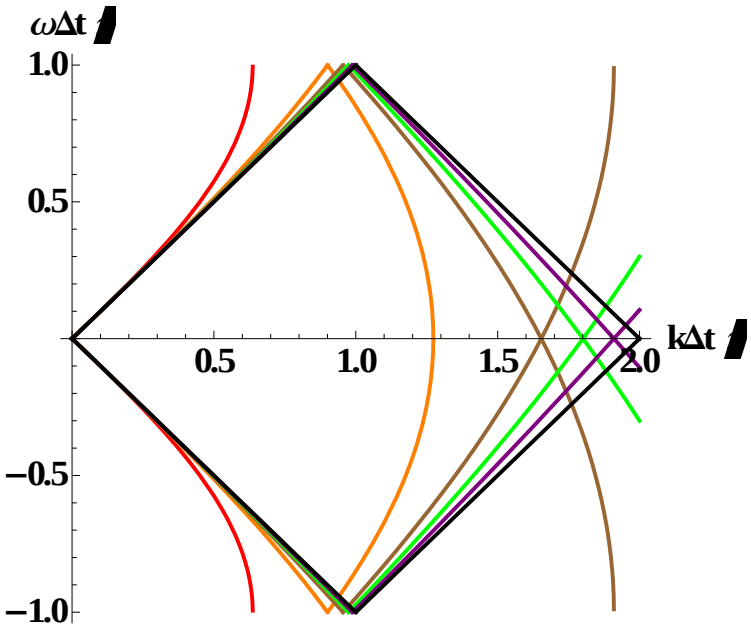
EM Field Sub-Cycling

- Advancing fields with short time step sometimes advantageous: $\Delta t_{field} = \Delta t_{part}/N$
  - Sub-cycling fields numerically is straightforward, of course
- Analytically, if $F^{n+1} = M : F^n + S$ for N=1, then

$$F^{n+1} = M^N : F^n + \sum_{i=0}^{N-1} M^i : S \text{ for any N}$$

(*n* is particle time step)

- Easily evaluated for PSTD
  - Useful for numerical analysis
  - PSATD obtained in limit $N \to \infty$
- Applications discussed in Jean-Luc Vay's talk



Courant Limit on Time Step

- EM dispersion relation: $\sin\frac{\omega\Delta t_{\text{part}}}{2N} = f(\Delta x_i)\frac{\Delta t_{\text{part}}}{2N}$
  - Field solver stable only for $\Delta t_{\text{part}} < 2N/f_{max}$
- Sample Courant limits (Δx_i equal; d - dimension)
  - PSTD $\Delta t_{\text{part}}/\Delta z < 2N/\pi\sqrt{d}$ {0.63, 0.45, 0.36}N
  - FDTD (Yee) $\Delta t_{\text{part}}/\Delta z < N/\sqrt{d}$ {1.00, 0.70, 0.57}N
  - FDTC (C-K) $\Delta t_{\text{part}}/\Delta z < N$
  - PSATD no limit
- But, EM dispersion, as seen by particles, distorted for $\Delta t_{\text{part}}/\Delta z > 1/\sqrt{d}$ (more or less)
  - Creates practical limit of $\Delta t_{\text{part}}/\Delta z < 1.5$

Note: finite plasma density makes Courant limit more restrictive

Sources of Inaccuracy

- Small number of particles per cell
  - Numerical noise
- Particle, field solvers typically second-order accurate
  - Errors of order $(\omega\Delta t)^2$, $(k\Delta z)^2$, with ω, k the frequency, wavenumber of physical phenomena of interest
- Particles support more wavenumbers than fields do
  - Numerical aliases $k_P = (k_F + 2\pi m/\Delta z)$ integer m
  - Aliases cause instabilities (e.g., Landau growth)
- Mismatch between Eulerian field solver, Lagrangian particle pusher
  - Spurious mode coupling: numerical Cherenkov instability

PIC Linear Theory in Two Slides (1)

- Linearize Vlasov equation from particle equations
  - $\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial z} = -\frac{\partial f^0}{\partial v}\sum_{n,l} F_l^n\, W(z - l\Delta z)\,\delta(t - n\Delta t)$
- Fourier transform linearized Vlasov equation
  - $f = i\frac{\partial f^0}{\partial v}\frac{F_k^\omega W_{-k'}}{\omega' - k'v}$ with $\omega' = \omega + n\frac{2\pi}{\Delta t}$, $k' = k + m\frac{2\pi}{\Delta z}$
- Integrate over f to obtain current
  - $J_k^\omega = i\int dv\,\frac{\partial f^0}{\partial v}\, v\sum_{n,m}(-1)^n\frac{V_{k'}F_k^\omega W_{-k'}}{\omega' - k'v}$
- Simplify by performing sum over n
  - $J_k^\omega = i\int dv\,\frac{\partial f^0}{\partial v}\, vF_k^\omega\sum_m V_{k'}W_{-k'}\cot\left[(\omega - k'v)\frac{\Delta t}{2}\right]\frac{\Delta t}{2}$

PIC Linear Theory in Two Slides (2)

- Fourier transform FDTD EM equations on space-time grid and insert J to obtain dispersion relation
  - $$\left[\frac{\sin(\omega\Delta t/2)}{\Delta t/2}\right]^2 - \left[\frac{\sin(k\Delta z/2)}{\Delta z/2}\right]^2 = \int dv \frac{\partial f^0}{\partial v}\, v \cdot$$
    $$\left[\frac{\sin(\omega\Delta t/2)}{\Delta t/2} - \frac{\sin(k\Delta z/2)}{\Delta z/2} v\right] \sum_m \frac{V_{k'} W_{-k'} \frac{\Delta t}{2}}{\tan\left[(\omega - k'v)\frac{\Delta t}{2}\right]}$$
  - Numerous simplifications but qualitatively correct
  - Similar expressions for PSTD, PSATD field solvers
- Numerical instabilities can arise from
  - $(\omega - k'v)$ modes interacting with EM modes
  - $V_{k'} W_{-k'}$ coefficient with wrong sign
  - Courant condition violation

Various Ways to Control Numerical Instabilities

- Filter short wavelength modes
  - Numerical instabilities usually at short wavelengths
  - Field, current smoothing (with (¼,½,¼) stencil for FDTD)
- Use higher order interpolation
  - $V_{k'}W_{-k'}$ decreases as k'^{-4} with linear interpolation, as k'^{-8} with cubic interpolation
- Choose simulation parameters wisely
  - E.g., numerical Cherenkov instability "magic time steps"
- Modify algorithm
  - Helps to know numerical growth rates in advance

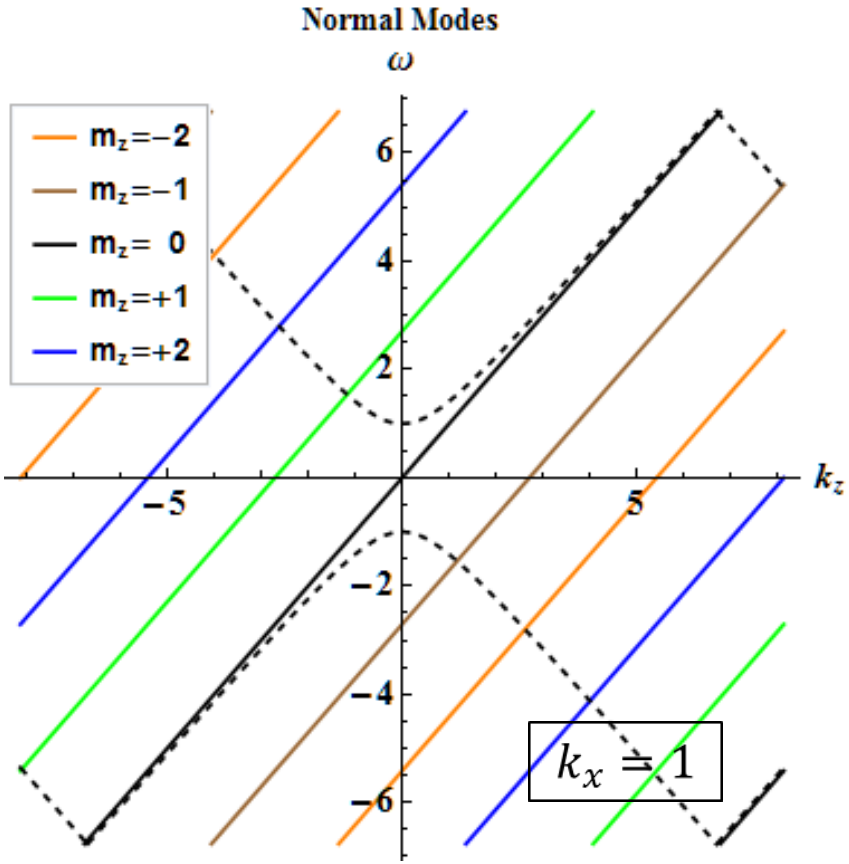
Numerical Cherenkov Instability

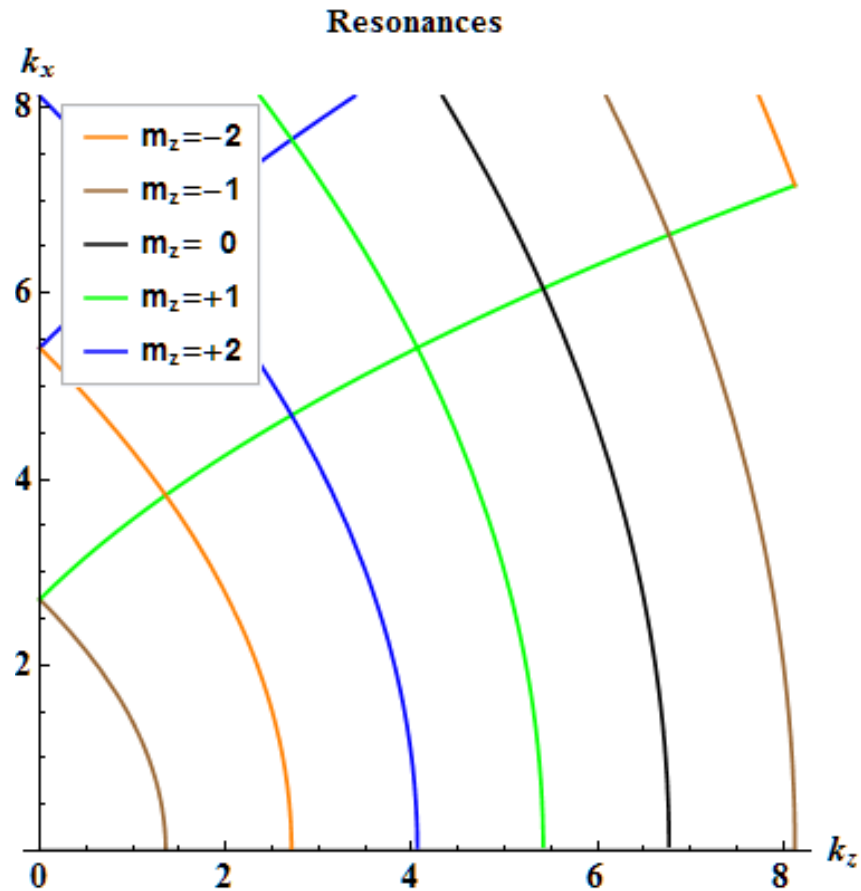
- Serious issue in 2D, 3D EM PIC simulations of relativistic beams (accelerators, astrophysics, *etc.*)
  - Growth rates a large fraction of $\left(\omega_p{}^2 k_\perp{}^2 \Delta z\right)^{1/3}$
- High- γ dispersion relation

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

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

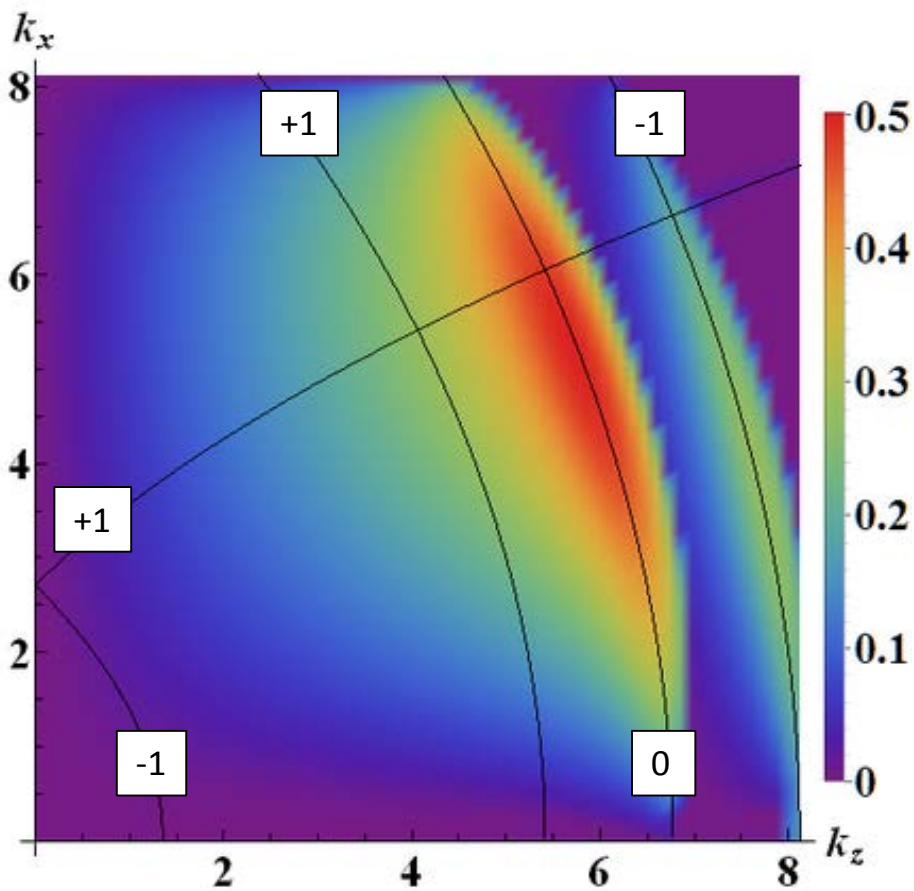
PSATD Normal Modes, Resonances





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

Full Dispersion Relation Growth Rates



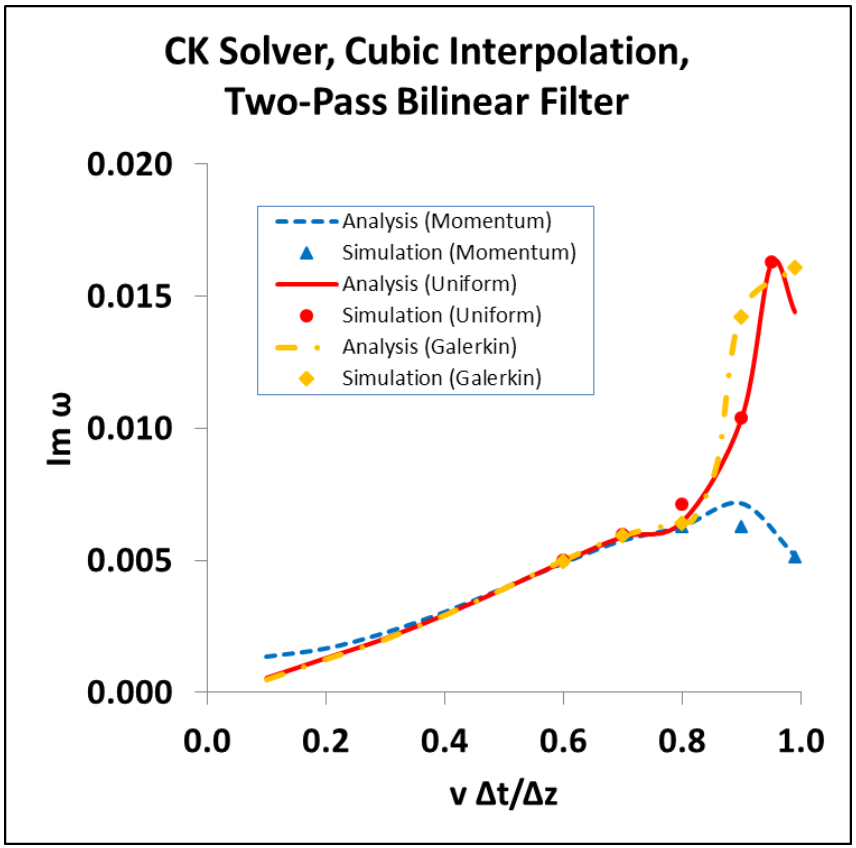
- Peak growth rates at resonances
  - $m = 0$ dominates for $\frac{\Delta t}{\Delta x} > 2\left(\frac{\Delta x}{\Delta t_c} - \frac{\Delta z}{\Delta x}\right)$
  - $m = -1$ dominates otherwise
- Parameters
  - PSATD
  - $\frac{v\Delta t}{\Delta z} = 1.2, v \approx 1$
  - Linear interpolation

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

Instability Suppression Strategy

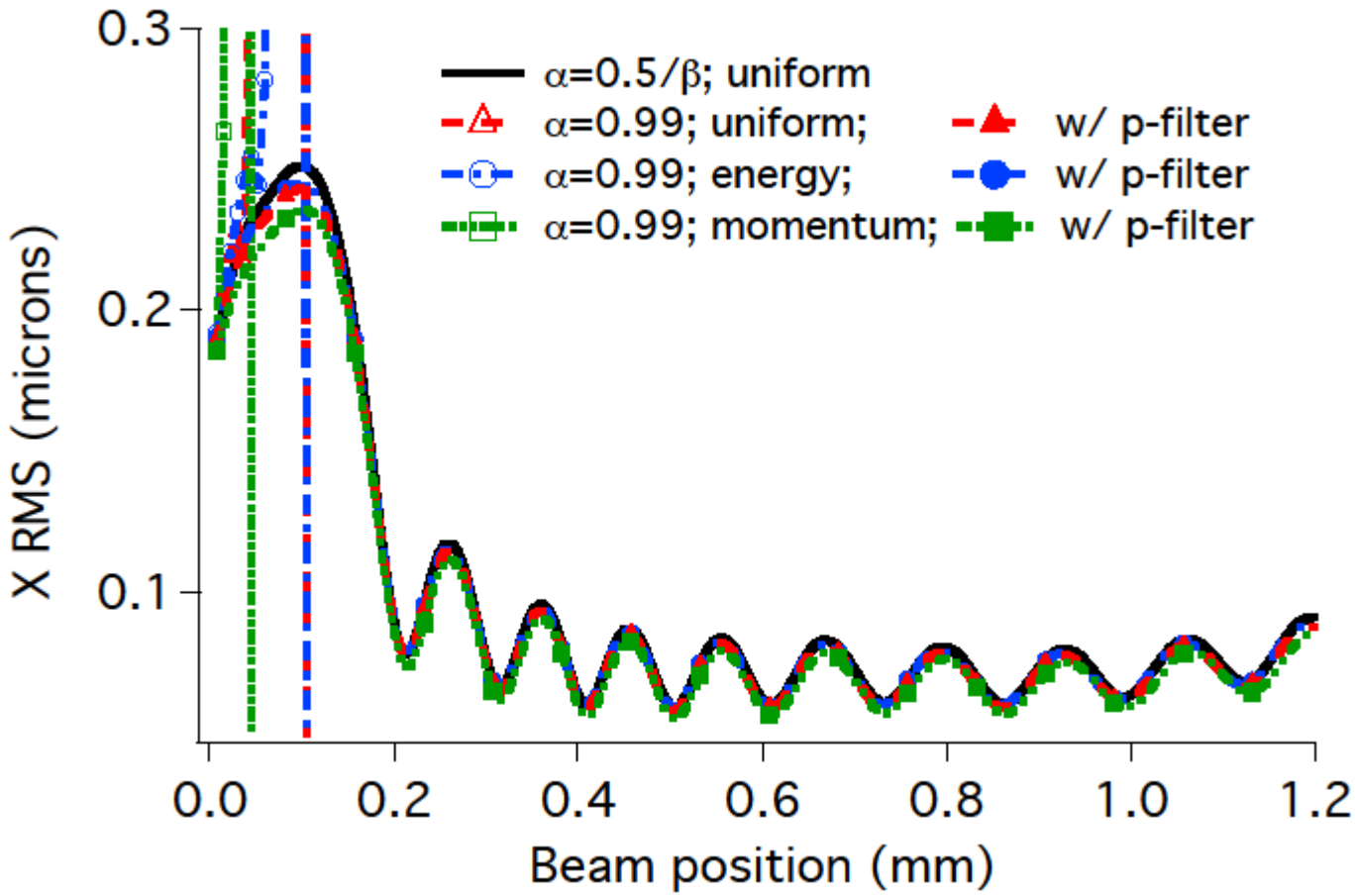
- Filter to eliminate resonant instabilities at large k
  - Multi-pass bilinear filter, or
  - Sharp-cutoff filter, $k < \alpha\, Min\left[\frac{\pi}{v\,\Delta t}, \frac{\pi}{\Delta z}\right]$, or
  - Interpolate current on 2x mesh in *z*, discard upper half of k_z (effective but more expensive)
- Modify fields or currents to suppress $m = 0$ non-resonant instabilities at smaller k
  - Set $C_{2x} = 0$ at $\omega = k_z$, or
  - Various other options; see references on final slide

Two-Pass Filter, Field Correction Yield Good FDTD Stability



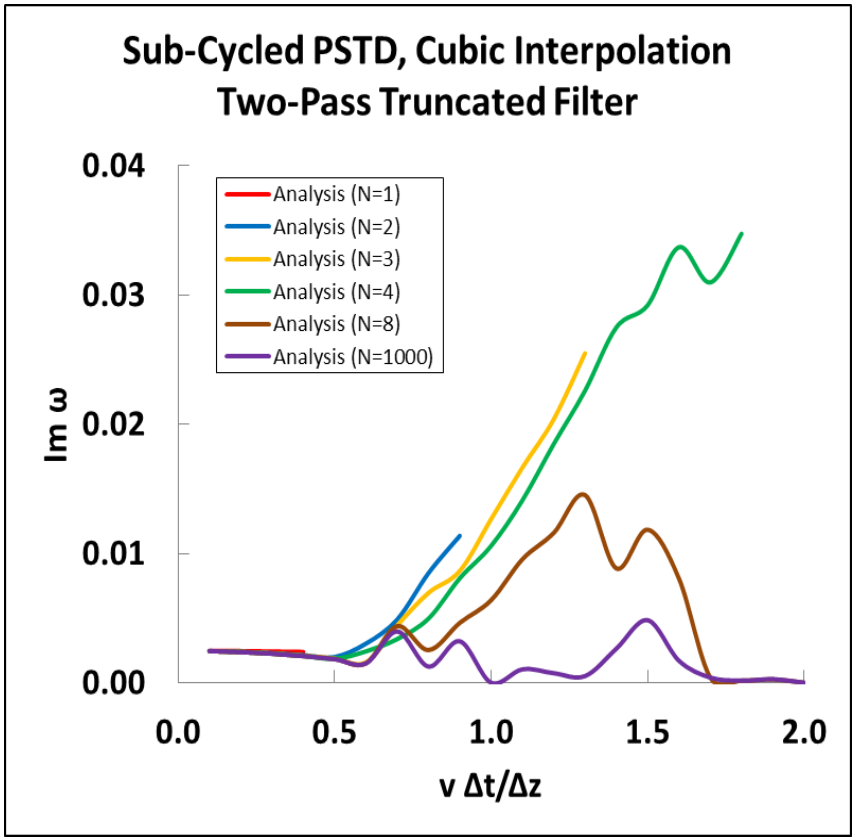
- Scale $E_\perp$ by ψ_E, $B_\perp$ by ψ_B
  - As seen by particles
- Choose $\frac{\psi_E}{\psi_B}$ to set $C_{2x} = 0$ (in *k*-space)
- Approximate by 4th order ratio of polynomials in $\sin^2\left[\frac{k_z \Delta z}{2}\right]$
- Set ψ_E to numerator, ψ_B to denominator of ratio
- Implement $\sin^2\left[\frac{k_z \Delta z}{2}\right]$ using (-¼,½,-¼) stencil in *z*

Field Correction, One-Pass Filter Stabilize WARP FDTD LPA Simulations



Same simulations without field correction severely unstable, produce meaningless results (Uniform interpolation simulation stable at "magic time step" $v\Delta t/\Delta z = 0.5$)

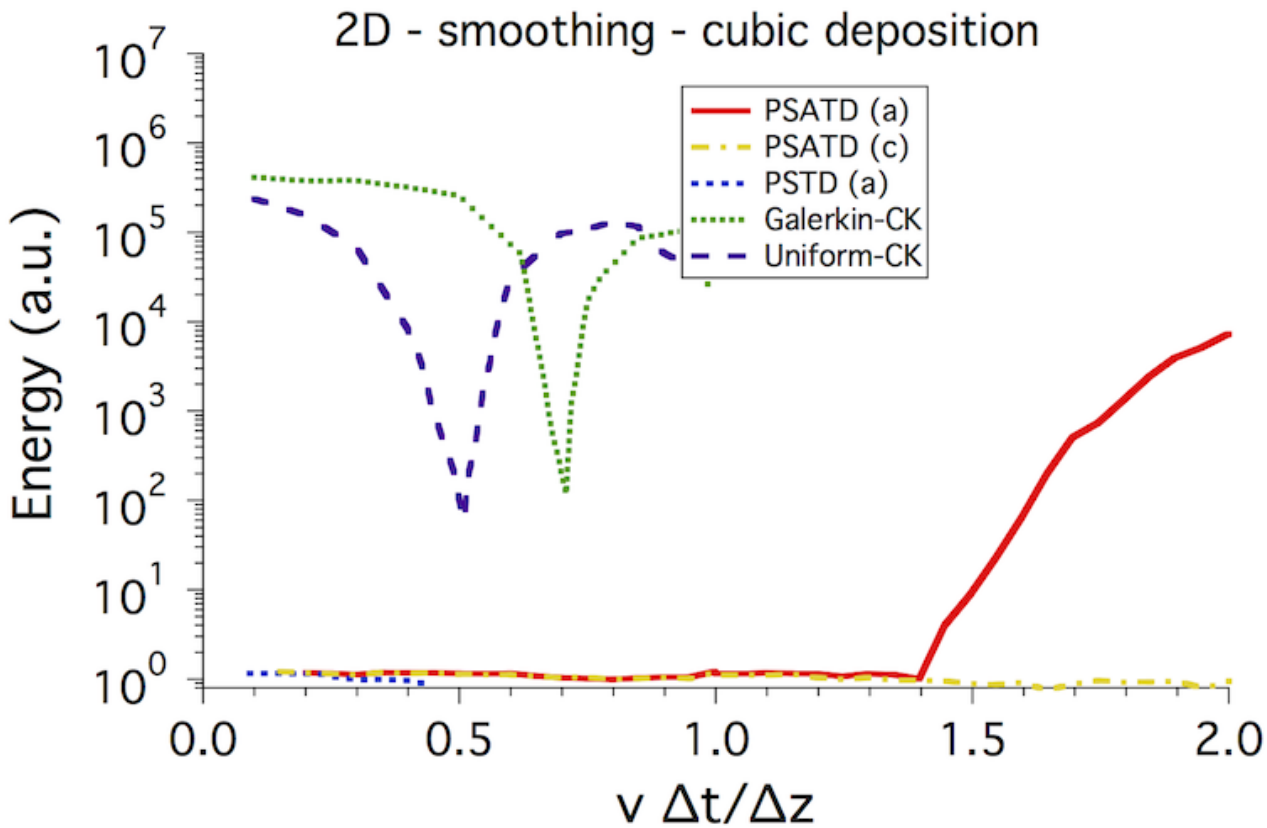
Two-Pass Truncated Filter, Field Correction Yields Acceptable Sub-Cycled PSTD Stability



- Scale $E_\perp$ by ψ_E, $B_\perp$ by ψ_B
- $\psi_E = \frac{k_z v \Delta t}{2} \cot\left[\frac{k_z v \Delta t}{2}\right]$
- $\psi_B = \frac{k \Delta t}{2} \cot\left[\frac{\theta \Delta t}{2}\right] \sec\left[\frac{\theta \Delta t}{2N}\right]$

  with $\sin\left[\frac{\theta \Delta t}{2N}\right] \equiv \frac{k \Delta t}{2N}$
- Several alternative PSTD, PSATD stabilization options
  - Instability growth 10x larger without stabilization

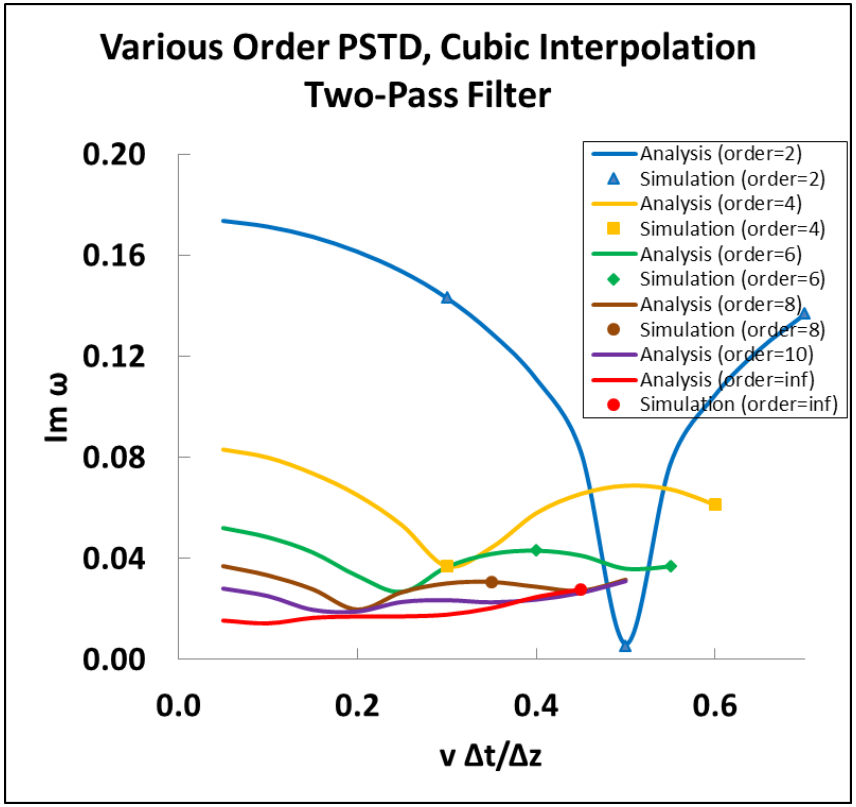
Current Correction, Eight-Pass Filter Stabilize WARP PSTD, PSATD Simulations



$\gamma = 13$ PSTD, PSATD energy conservation simulations with cubic interpolation

FDTD "magic time step" results provided for comparison

Pseudo-Spectral Arbitrary Order Time Domain Algorithm (PSAOTD)



- Research underway on PSTD with arbitrary order approximation to spatial derivatives
- Sub-cycling included
- Stabilization straight-forward but not yet analyzed

Hear Jean-Luc Vay's talk for details and applications

Summary

- PIC simulations a power tool for particle beam, microwave source, plasma research
- History of steady progress
  - PIC basics well established since early 70's (see text by Birdsall and Langdon)
  - Continuous advances to the present (e.g., Esirkepov's current conservation algorithm)
  - Numerical instabilities largely eliminated
- Advanced accelerator concepts stimulating new research in PIC methodology

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

References

(by no means complete)

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