Advanced simulation tools for next generation particle acceleration: PIC and beyond

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Speaker Profile

Dr Jonathan Smith is an application specialist working for Tech-X UK Ltd. He has 15 years professional experience in industry, academia and on government/national laboratory sites. His research focus has always been computational electromagnetics, principally the finite difference time domain (FDTD) technique and particle-in-cell (PIC) technique and is currently working mostly on novel acceleration techniques both with plasma and periodic dielectric structures. He has a wide experience using commercial and open-source simulation software in radio frequency vacuum electronics devices, particle accelerators and across plasma simulation of areas as diverse as space propulsion and plasma chambers for lithography and semiconductor processing.

Talk highlights:

- Fundamentals of plasma acceleration and future experiments (5 mins)
- Learn about the basics of the FDTD technique and PIC simulation (10mins)
- Have an overview of the simulation software landscape (5 mins)
- Understand the source of common numerical instabilities. (10 mins)
- Find out about cutting edge techniques to improve accuracy (15 mins)
  - Quiet loading, enhanced loading
  - Vay push
  - Beam Frame Poisson Solve
  - Smoothing
  - Controlled (sometimes 'Perfect' Dispersion)
- Find out about cutting edge techniques to improve speed (10 mins)
  - Envelope models (with or without phase tracking) & QSA.
  - Boosted frame
- Learn about cutting edge dielectric acceleration algorithms
- If time allows… A few words on controlled injection, computational infrastructure requirements, visualisation and future directions.

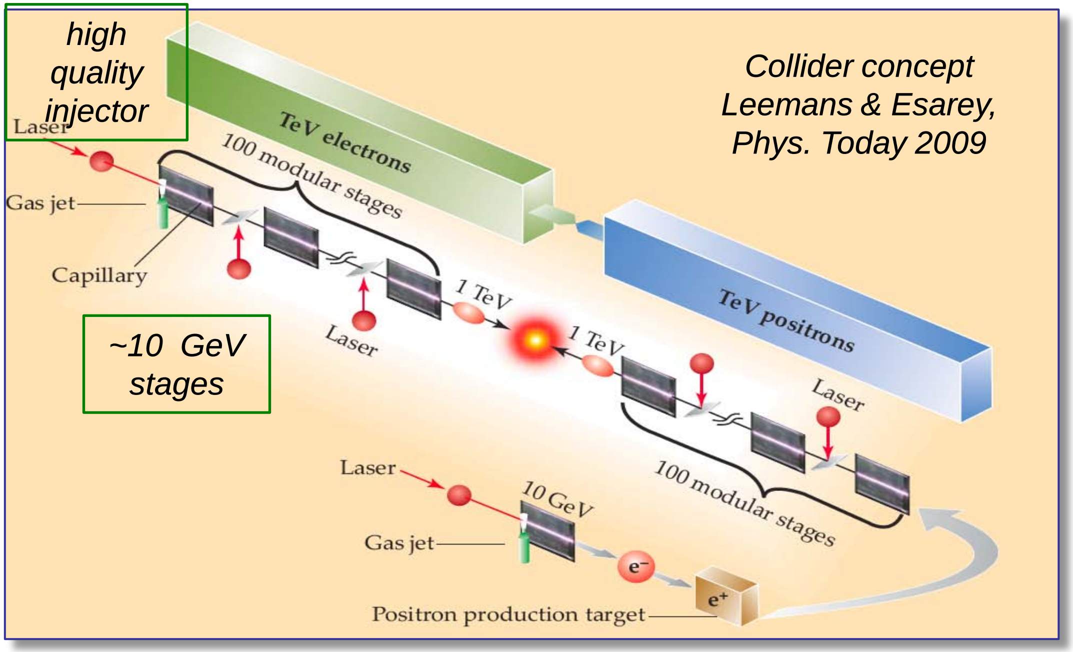
Plasma Acceleration: kinds

- PWFA: Plasma WakeField Acceleration
  - Theory late 1950s, Experiment Early 1970s
  - Electron beam driven (driver and tail of driver / driver witness)
- LWFA: Laser WakeField Acceleration
  - Tajima & Dawson ~1980
  - Use a laser to excite the plasma field
  - Self modulated scheme ($L > \lambda_p$, power $P > P_c$)
- LBWA: Laser Beat Wave Acceleration

Laser Plasma accelerators for table-top devices

- Ultra high accelerating gradient can be achieved with plasma accelerators:
- $E_0 = c m_e w_p / e \sim 0.96 n_0^{1/2}$ $[\mathrm{cm}^{-3}]$: **100GeV/m** for $10^{18}\mathrm{cm}^{-3}$ or $10^{24}\mathrm{m}^{-3}$
- Theoretical result ~3 orders of magnitude better than RF accelerators
- Plasma wake excited with ponderomotive force of laser pulse
- LPA experiments have been producing quasi-mono-energetic beams for many years (but not so good as RF)
- Beam energy and quality steadily improving bring interest in a wide range of applications

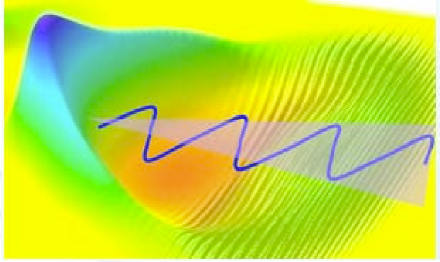
Next generation: new challenges



high quality injector

~10 GeV stages

Collider concept Leemans & Esarey, Phys. Today 2009



production of X-Rays, γ-Rays

- BELLA laser at LBNL will explore 10 GeV electron acceleration in a 1 m laser plasma accelerator
- Requires high quality injector
  - colliding pulse
  - ionization of high Z gases
- Requires preservation of low emittance beams
- Simulations challenging because of scale separation
  - $L_{acc} \sim 1$ m, $\lambda_{laser} \sim 1\ \mu$m
- Reduced models needed
  - envelope, boosted frame
- Improve simulations to reduce numerical noise
  - Beam Frame Poisson Solve

Fundamentals of plasma acceleration

What are we trying to achieve?

- Energy gain of particles, energy spread, proportion of electrons captured and accelerated, transverse momentum
- Emittance of particles (beam size), brightness
- Working out whether and which particles will be injected from the background
- Dispersion, dephasing (of laser and particles)
- Understand physical plasma instabilities: hosing, forward & reverse stimulated Raman scattering, self modulation, exciting ion modes, and other non-linear effects
- Depletion (laser loosing power as transfer of energy happens)
- **More accurate results, faster, easier (avoid numerical effects)**

Talk highlights:

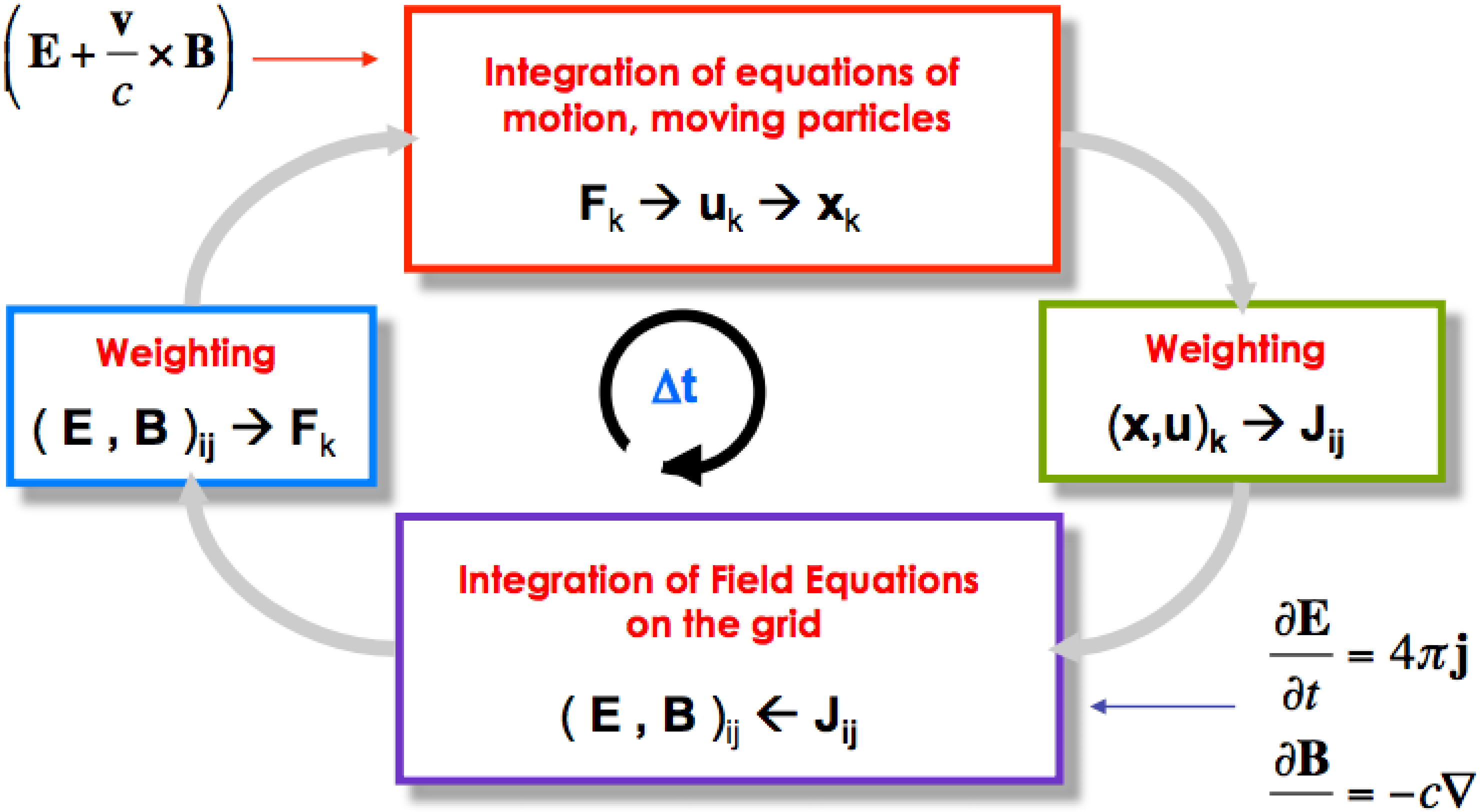
- Fundamentals of plasma acceleration and future experiments (5 mins)
- Learn about the basics of the FDTD technique and PiC simulation (10mins)
  - Commonalities to all codes
  - Some popular codes for laser plasma wakefield acceleration
  - Understanding the basics of instabilities
- Have an overview of the simulation software landscape (5 mins)
- Understand the source of common numerical instabilities. (10 mins)
- Find out about cutting edge techniques to improve accuracy (15 mins)
- Find out about cutting edge techniques to improve speed (10 mins)
- Learn about cutting edge dielectric acceleration algorithms
- If time allows… A few words on computational infrastructure requirements, visualisation and future direction.

Commonalities:

- Grid
- Parallel Decomposition
- Fields (EmField/MultiField – includes basic Yee leap-frog scheme in different dimensionalities)
  - Boundary Conditions
    - Current Sources (SumRhoJ) external+particles
    - PML/MAL/Open
    - Magnetic/Electric Conductor
  - Updates with time
  - Order of update
- Particles (Species - macroparticles)
  - Properties, relativistic pushers, tagging, variable weighting, tracking
  - Sources/Sinks – loaders (from other formats, gridded, pseudorandom) emitters, boundary conditions
- Fluids (reduces computation for many particle-per-cell)
- Interactions (monte carlo - Fields/Particles/Fluids – Ionizations, Collisions)
  - Cross sections, rate of reaction, external libraries
- Diagnostics (History)
- Depositors (Vector/Scalar), Interpolators built into fields.
- Basic properties, verbosity, timestepping, restarts, moving window (part of grid), control of I/O

Basic PIC method

$$\frac{d\mathbf{p}}{dt} = q\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right)$$



Integration of equations of motion, moving particles

$F_k \rightarrow u_k \rightarrow x_k$

Weighting

$(x,u)_k \rightarrow J_{ij}$

Integration of Field Equations on the grid

$(E, B)_{ij} \leftarrow J_{ij}$

Weighting

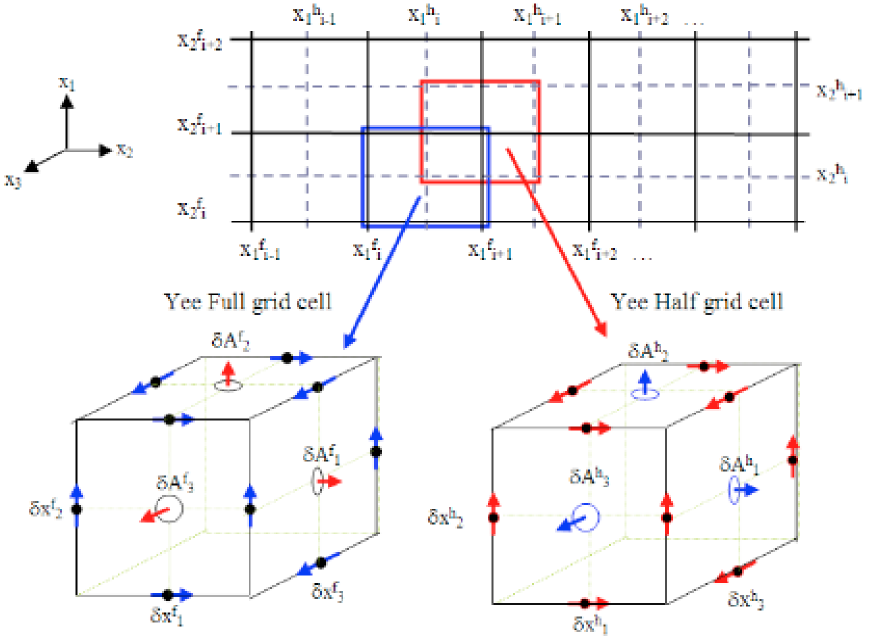
$(E, B)_{ij} \rightarrow F_k$

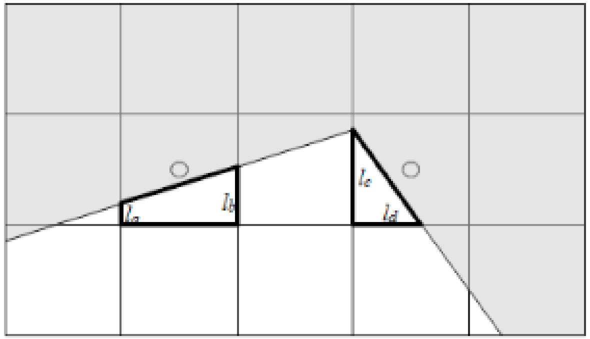
Δt

$$\frac{\partial \mathbf{E}}{\partial t} = 4\pi \mathbf{j} - c\nabla \times \mathbf{B}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$

Fields 1: Yee algorithm

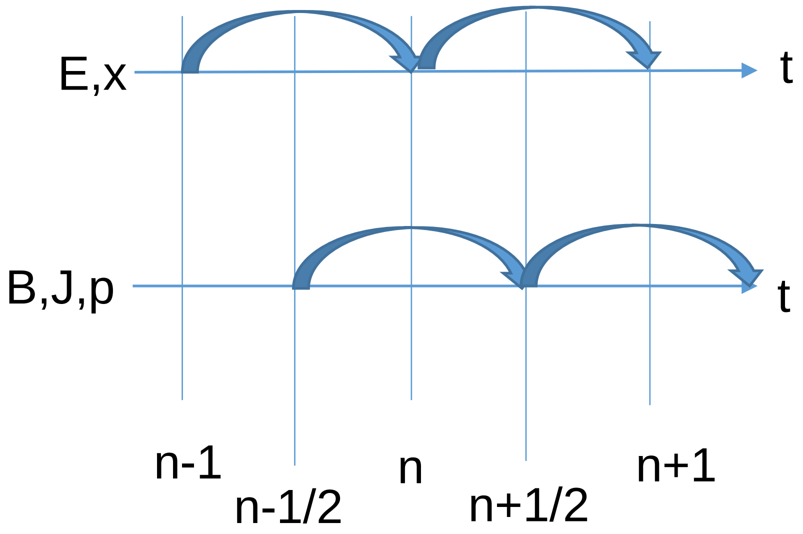




- Offset grids – one holds B fields, one holds E fields.
- Sum of currents around loop gives exact flux through surface. (Kelvin-Stokes theorem)
- Have special algorithms for handling cut cells and/or dielectrics

Taflove & Hagness: “The Finite-Difference Time-Domain Method, Third Edition”

Fields 2: Leapfrog



- Leapfrog used both for particle pushes as well as for fields.
- More numerically stable
- Discussion about (in)stability later.

Particle pushes

- Lorentz force is applied to particles
- Together a Vlasov-Maxwell system
- Boris Algorithm
  - Leapfrog schemes work, otherwise particles spiral out of control. Better and quicker than Runge-Kutta integrator, or forward Euler.
  - J. P. Boris, Relativistic plasma simulation-optimization of a hybrid code, Proceedings of the Fourth Conference on Numerical Simulations of Plasmas, 1970.
- More recently J-L Vay, “Simulation of beams or plasmas crossing at relativistic velocity” Phys. Plasmas **15**,056701 (2008);
  - http://dx.doi.org/10.1063/1.2837054

So what's so complicated?

- Geared toward high-energy colliders: meter-scale stages
- Linear dephasing length scales as $\lambda_p^3/\lambda^2 \Rightarrow$ use low plasma density, ~ 10^{23} m^{-3}
    - Physical parameters: λ_p = 106 µm, λ = 800 nm
- Some reasonable simulation parameters
    - Global domain sizes: $L_x = 3\lambda_p$, $L_y = L_z = 6\lambda_p$
    - Resolution: $\Delta x = \lambda/24$, $\Delta y = \Delta z = \lambda/3 \Rightarrow c\Delta t$ = 33 nm
    - Resulting grid sizes: N_x = 9540, $N_y = N_z$ = 2385
    - # of time steps = $3.0\text{x}10^7$, $1.7\text{x}10^{18}$ total updates
    - Estimate ~$3\text{x}10^9$ CPU hours required
- There can often be subtle and complex differences between actual physics and the numerical implementation of a model
    - We want quantitative accuracy, not just qualitative understanding

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Codes:

- VSim (VORPAL)
  - (scaling 100k cores+)
  - http://www.txcorp.com/home/vsim/vsim-pa
- OSIRIS
  - UCLA/IST + Large collaboration (scaling 100k cores+)
  - https://plasmasim.physics.ucla.edu/codes/
- QuickPIC
  - UCLA/IST QSBA, PGC (envelope), QSBA link as above
- EPOCH
  - http://ccpforge.cse.rl.ac.uk/gf/project/epoch/
- XOOPIC
  - http://ptsg.eecs.berkeley.edu/pub/codes/xoopic/
- LCODE
  - Fluid RZ, AWAKE deck, ‘kinetic’ plasma
  - http://www.inp.nsk.su/~lotov/lcode/
- Calder & Calder-Circ
  - V Malka (Ecole Polytechnique, France)
  - Lifschitz A F, Davoine X, Lefebvre E, Faure J, Rechatin C and Malka V 2009 J. Comput. Phys. 228 1803–14
- WARP
  - Renewed development work by J-L Vey
  - http://iopscience.iop.org/1749-4699/5/1/014019
- VLPL
  - http://www.tp1.uni-duesseldorf.de/~pukhov/
- PIConGPU
  - HZDR http://picongpu.hzdr.de (github for developers)
  - https://github.com/ComputationalRadiationPhysics/picongpu
- MANDOR
  - Lebedev Physics Institute (Bychenkov) once U of Alberta
  - http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.93.215004
  - http://core.kmi.open.ac.uk/display/20048281
- HiPACE
  - DESY, Quasi Static PIC.
  - http://iopscience.iop.org/0741-3335/56/8/084012/
- Inf&rno
  - 2DRZ PIC/Fluid (envelope/QSB)
  - https://accelconf.web.cern.ch/accelconf/PAC2011/papers/mop082.pdf
  - Scales to ~4k cores
- WAKE, Tristan MP, ILLUMINATION others…

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Understand the source of common numerical instabilities:

- Leap-frog vs Euler
- The Courant condition (Courant Friedrichs Lewy)
- Numerical Cerenkov Radation (Smoothing, Perf Dispersion)
- Grid instability (Higher order particle shapes, better loading)
- Plasma wavelength
- Laser/RF wavelengths
- The Debye length
- The plasma period
- Geometric features (though cut cell technologies exist)
- Particle movement
- Careful about losing low frequencies/long wavelengths

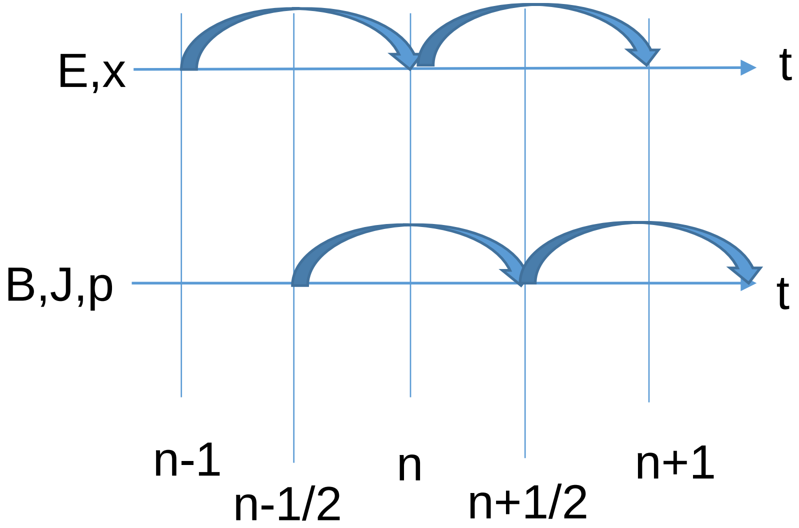
Leap-Frog vs Euler

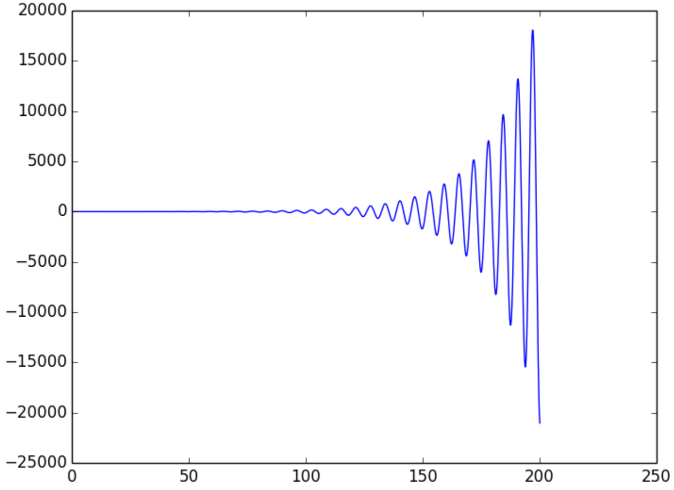
- Leap-frog technique like Yee is more stable.
- Try it yourself!
- Consider simple harmonic oscillator with (ω=1)

$$x + \ddot{x} = 0$$

$x_{t=0}=0$, $v_{t=0}=1$, vary Δt

Euler rapidly reaches 1.5e43, 5.5e194, answer =1!





Courant condition 1: Wave Equation

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}-\frac{\partial^2}{c^2\partial t^2}\right)\Psi=0 \qquad \Psi(x,y,z,t)=\Psi_0 e^{(j[\omega t-k_x x-k_y y-k_z z])}$$

In discrete form: $\Psi^n(I,J,K)=\Psi_0 e^{(j[\omega n\Delta t-k_x I\Delta x-k_y J\Delta y-k_z K\Delta z])}$

$$\begin{aligned}
&\frac{\Psi^n(I+1,J,K)-2\Psi^n(I,J,K)+\Psi^n(I-1,J,K)}{\Delta x^2}\\
+&\frac{\Psi^n(I,J+1,K)-2\Psi^n(I,J,K)+\Psi^n(I,J-1,K)}{\Delta y^2}\\
+&\frac{\Psi^n(I,J,K+1)-2\Psi^n(I,J,K)+\Psi^n(I,J,K-1)}{\Delta z^2}\\
=&\frac{\Psi^{n+1}(I,J,K)-2\Psi^n(I,J,K)+\Psi^{n-1}(I,J,K)}{c^2\Delta t^2}.
\end{aligned}$$

Courant condition 2: Solution

$$\frac{1}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right)+\frac{1}{\Delta y^2}\sin^2\left(\frac{k_y\Delta y}{2}\right)+\frac{1}{\Delta z^2}\sin^2\left(\frac{k_z\Delta z}{2}\right)=\left(\frac{1}{c\Delta t}\sin\left[\frac{\omega\Delta t}{2}\right]\right)^2$$

Note: as Δx,y,z,t → 0, free space wave equation emerges.
Rearrange for ω, realise we need real solution, and max of sin=1.

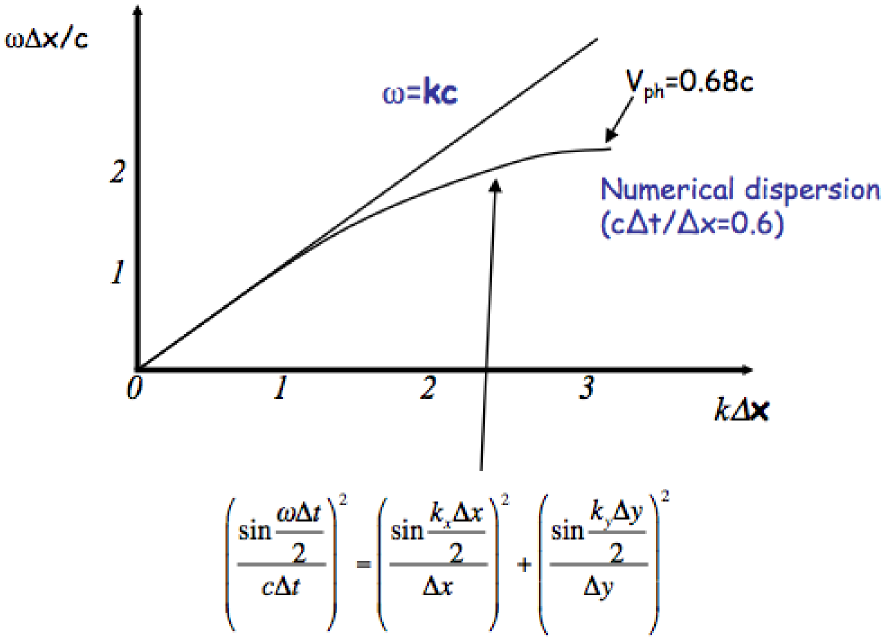
$$\boxed{\omega=\frac{2}{\Delta t}\sin^{-1}\left(c\Delta t\sqrt{\frac{1}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right)+\frac{1}{\Delta y^2}\sin^2\left(\frac{k_y\Delta y}{2}\right)+\frac{1}{\Delta z^2}\sin^2\left(\frac{k_z\Delta z}{2}\right)}\right)}$$

$$c\Delta t\sqrt{\frac{1}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right)+\frac{1}{\Delta y^2}\sin^2\left(\frac{k_y\Delta y}{2}\right)+\frac{1}{\Delta z^2}\sin^2\left(\frac{k_z\Delta z}{2}\right)}\leq 1$$

$$\boxed{\Delta t\leq\frac{1}{c\sqrt{\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2}}}}$$

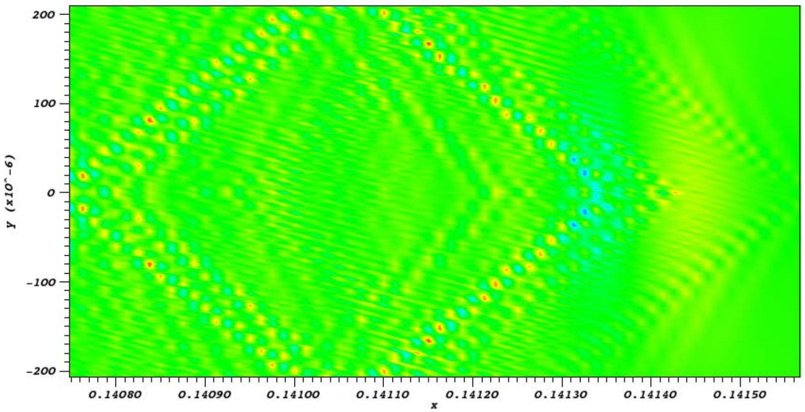
Numerical ‘Cerenkov’ radation

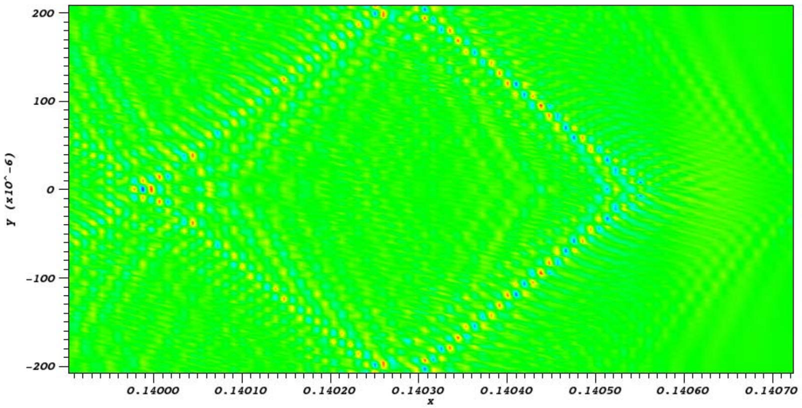
- Dispersion on a structured mesh is neither the same in all directions, nor is it the same as in free space.
- Particles can travel faster than fields on the grid – leading to a ‘Cerenkov’ like effect
- Some codes (like VSim) have advanced algorithms for controlling dispersion
- ‘Smoothing’ is another approach.

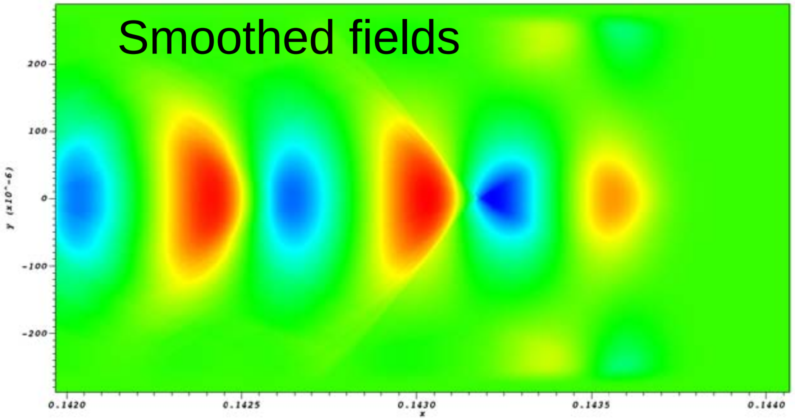


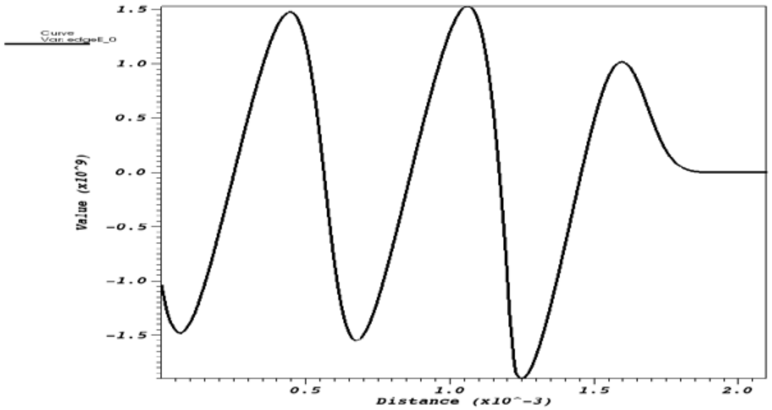
$$\left(\frac{\sin\frac{\omega\Delta t}{2}}{c\Delta t}\right)^2=\left(\frac{\sin\frac{k_x\Delta x}{2}}{\Delta x}\right)^2+\left(\frac{\sin\frac{k_y\Delta y}{2}}{\Delta y}\right)^2$$

Cerenkov



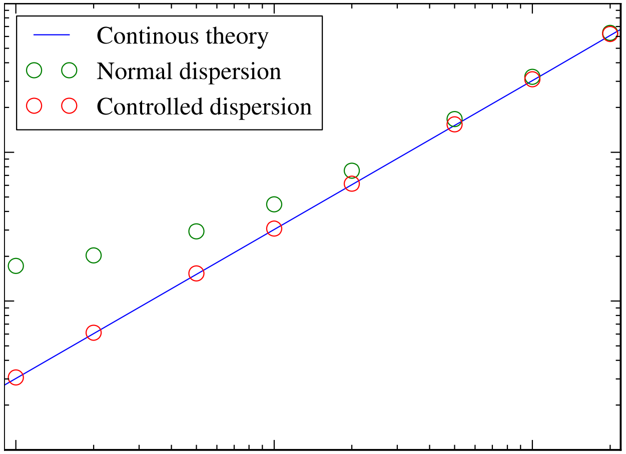


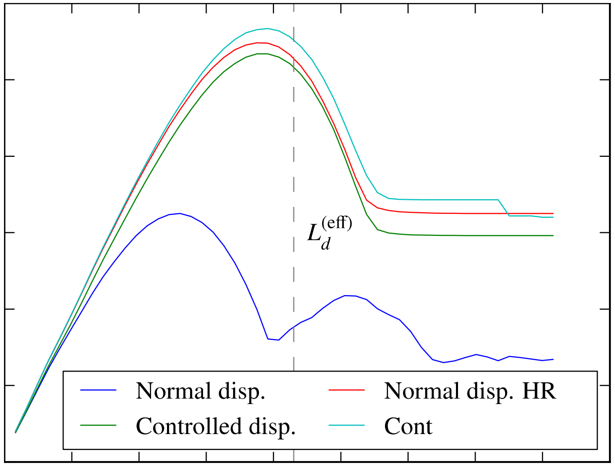

Smoothed fields



Controlled dispersion algorithm allows more accurate modeling of beam

- Accuracy in LPA simulations requires correct group velocity of laser pulse
- Standard FDTD update known to exhibit numerical dispersion for waves propagating along one axis
- Use generalized method to achieve much more accurate dispersion for on-axis waves
  - generalized to arbitrary aspect ratios and benchmarked
  - fields are smoothed for computational curl in directions transverse to the derivative
- Nearly eliminates dispersion error in linear channel propagation tests
- Produces better converged results in quasi-linear stage tests
- Gets correct dephasing length, more accurate final energy for accelerated electron beam





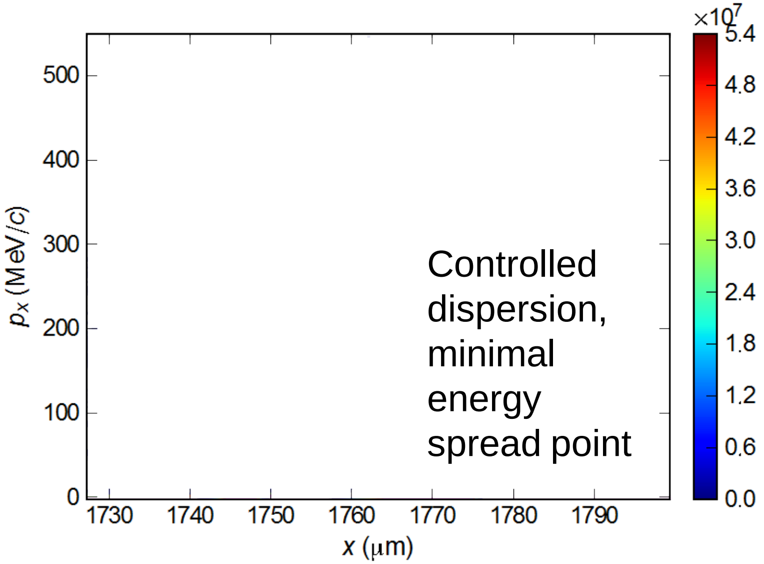
[1] A. J. Pukhov, J. Plasma Phys. **61** (1999)

[2] M. Kärkkäinen *et al.*, Proc. ICAP 2006

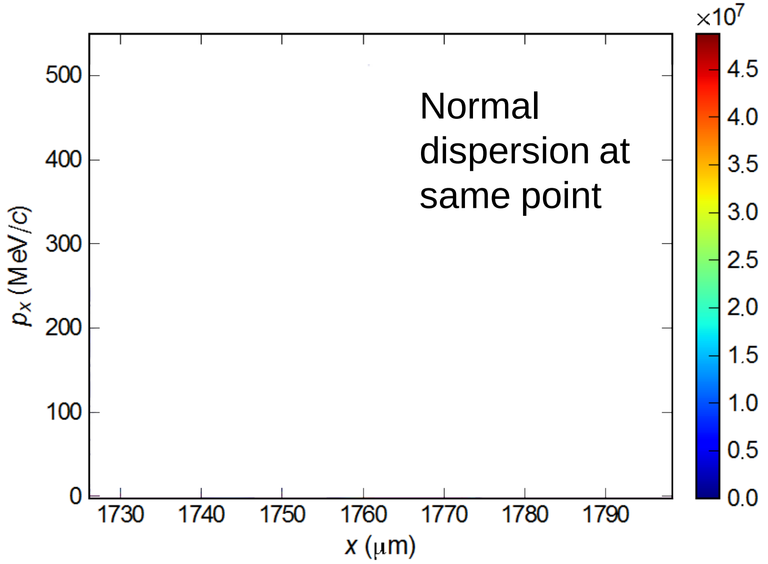
[3] B. Cowan *et al.*, PRST-AB (2012)

Controlled dispersion represents more correctly self-injected e- beam

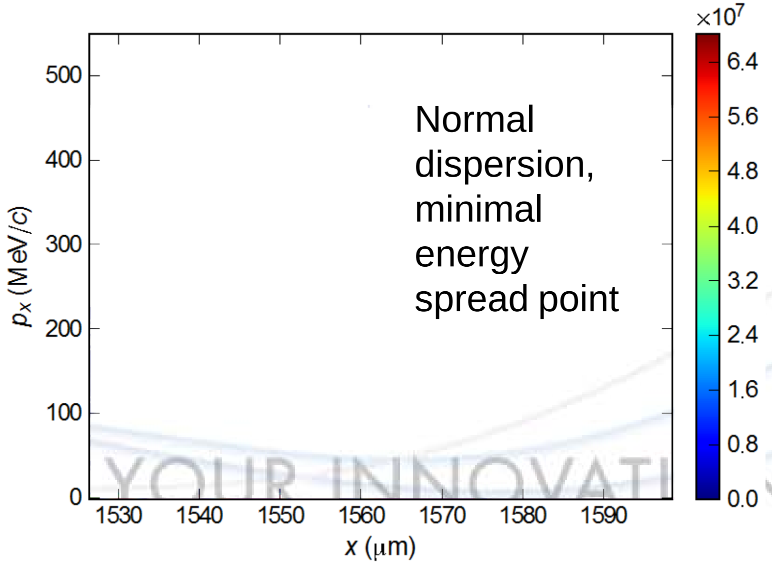
- With controlled dispersion, injected beams dephases more slowly, gains more energy



Controlled dispersion, minimal energy spread point



Normal dispersion at same point

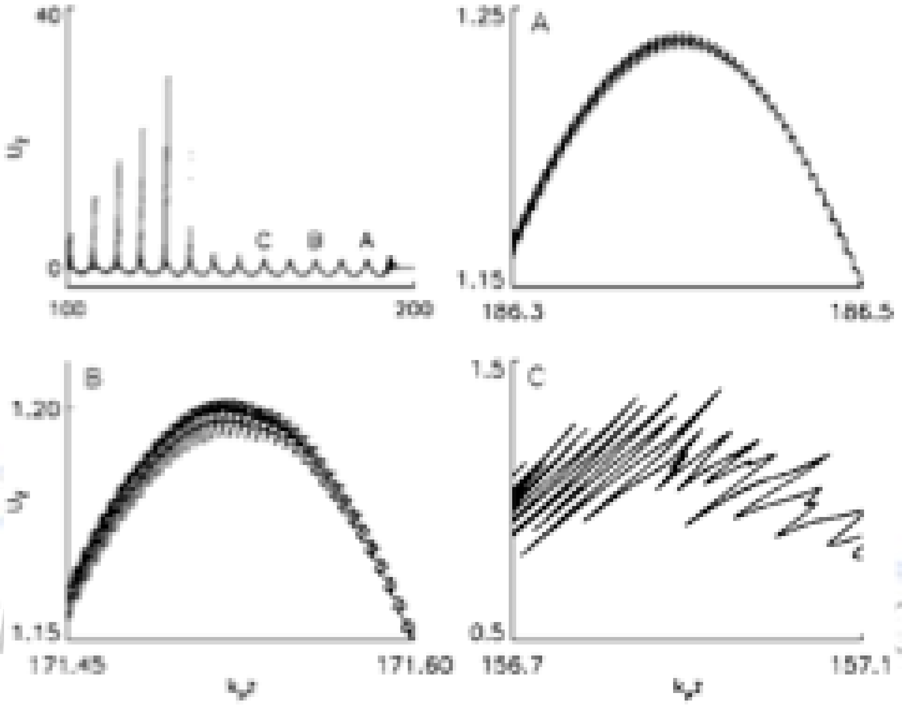


Normal dispersion, minimal energy spread point

B. Cowan *et al.*, J. Plasma Phys **78**, 469 (2012)

Grid Instability 1: Particle noise

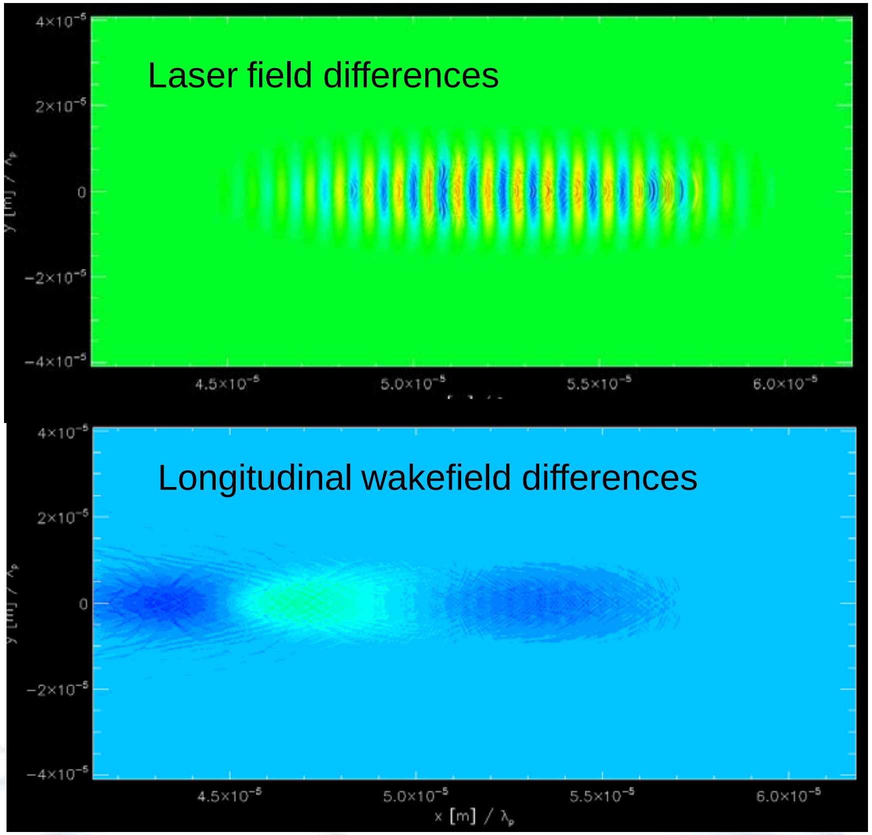
- Discretization of fields on a grid leads to numerical errors
    - Interpolation of gridded fields to particle positions
    - Computation of gridded currents from particle trajectories
- Leads to numerical noise – “grid heating”
- Can even cause unphysical trapping in LPA simulations!



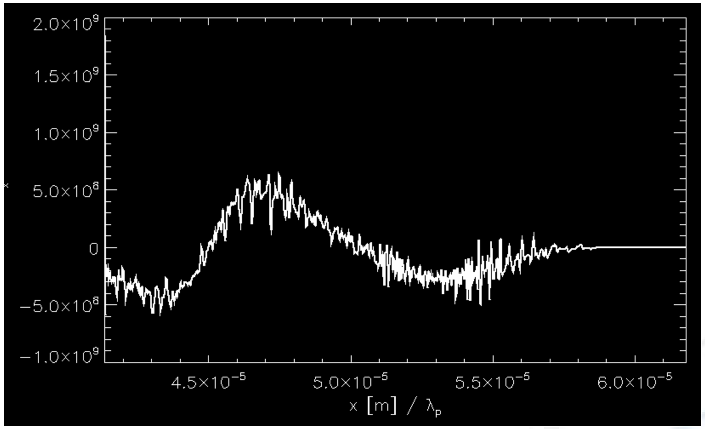
1D simulation of LPA with an initially cold plasma, $\lambda_p/\lambda = 10$, and $a_0 = 2$ — below wave-breaking threshold, but trapping is seen anyway.

From E. Cormier-Michel et al., “Unphysical kinetic effects in particle-in-cell modeling of laser wakefield accelerators,” Phys. Rev. E **78**, 016404 (2008).

Grid instability 2: Higher order particles



- Comparison of 1st- and 3rd-order particles shows reduced noise for 3rd-order
- Fluid models reduce noise even further
  - But no kinetic effects, such as trapping, can be modeled



Wavelengths: Resolve these

- Undersampling leads to lost physics
- $\Delta x < \lambda_p/4$ (or better – better resolution-> better results)
- $\Delta x < \lambda_{laser}/4$ (…much better for good results)
- $\Delta x < \lambda_{rf}/4$ (…or better)
- $\Delta x < \lambda_D/3$ (or better – fluid cold plasma approximation excluded)
- $\Delta x < \langle$size of smallest features in geometry$\rangle$
- $\Delta x < v\Delta t$
- Insufficient absorbtion at PMLs
- Low frequencies lost by size of simulation box (not necessarily LPA)

We'd better have some good tricks

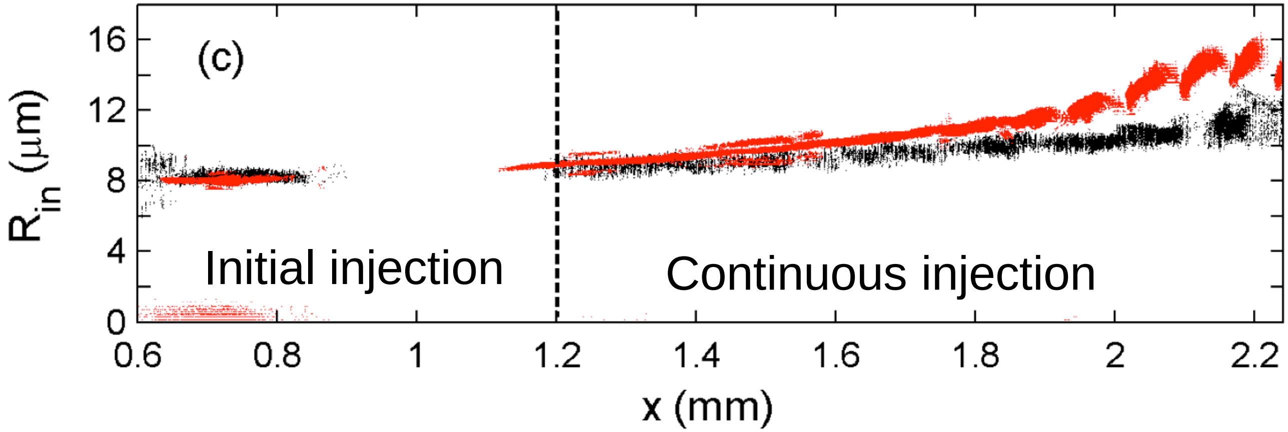
- ~~Higher order particle shapes (instability prevention)~~
- ~~Smoothing (instability prevention)~~
- ~~Controlled (sometimes 'Perfect' Dispersion) (accuracy/instability)~~
- Quiet loading, enhanced loading (more accurate)
- Vay push (more accurate)
- Beam Frame Poisson Solve (more accurate)
- Improved plasma chemistry (more accurate)
- Envelope models (with or without phase tracking) (faster)
- Boosted frame (faster)
- Quasi-Static beam (no longer self-consistent) (faster)

Quiet/enhanced loading

- Quiet load: load in a grid
  - Delays onset of grid instability
- Enhanced load: load more in a grid in particular places
  - You may not need the same resolution (of phase space) everywhere

Collection volumes

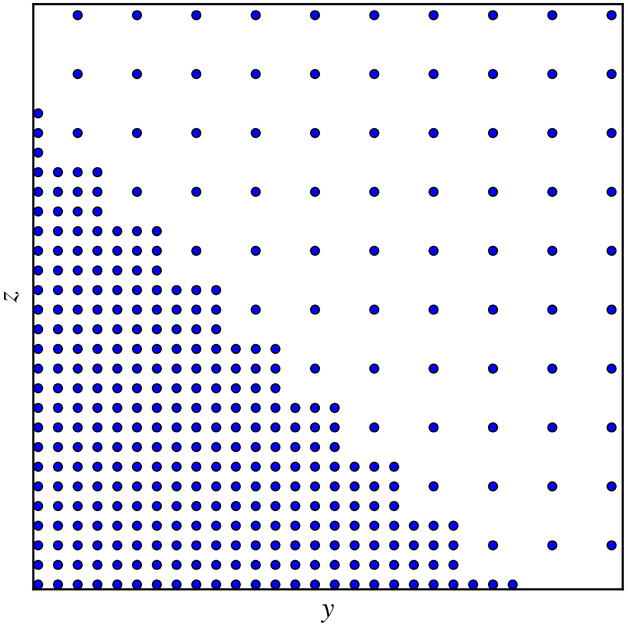
- We can enhance particle statistics with *a priori* knowledge from an initial simulation
- We use the *collection volume* — the range of initial positions of injected electrons



From B. Cowan *et al*., “Computationally efficient methods for modelling laser wakefield acceleration in the blowout regime,” J. Plasma Phys. **78**, 469 (2012)

Enhanced statistics in the collection volume

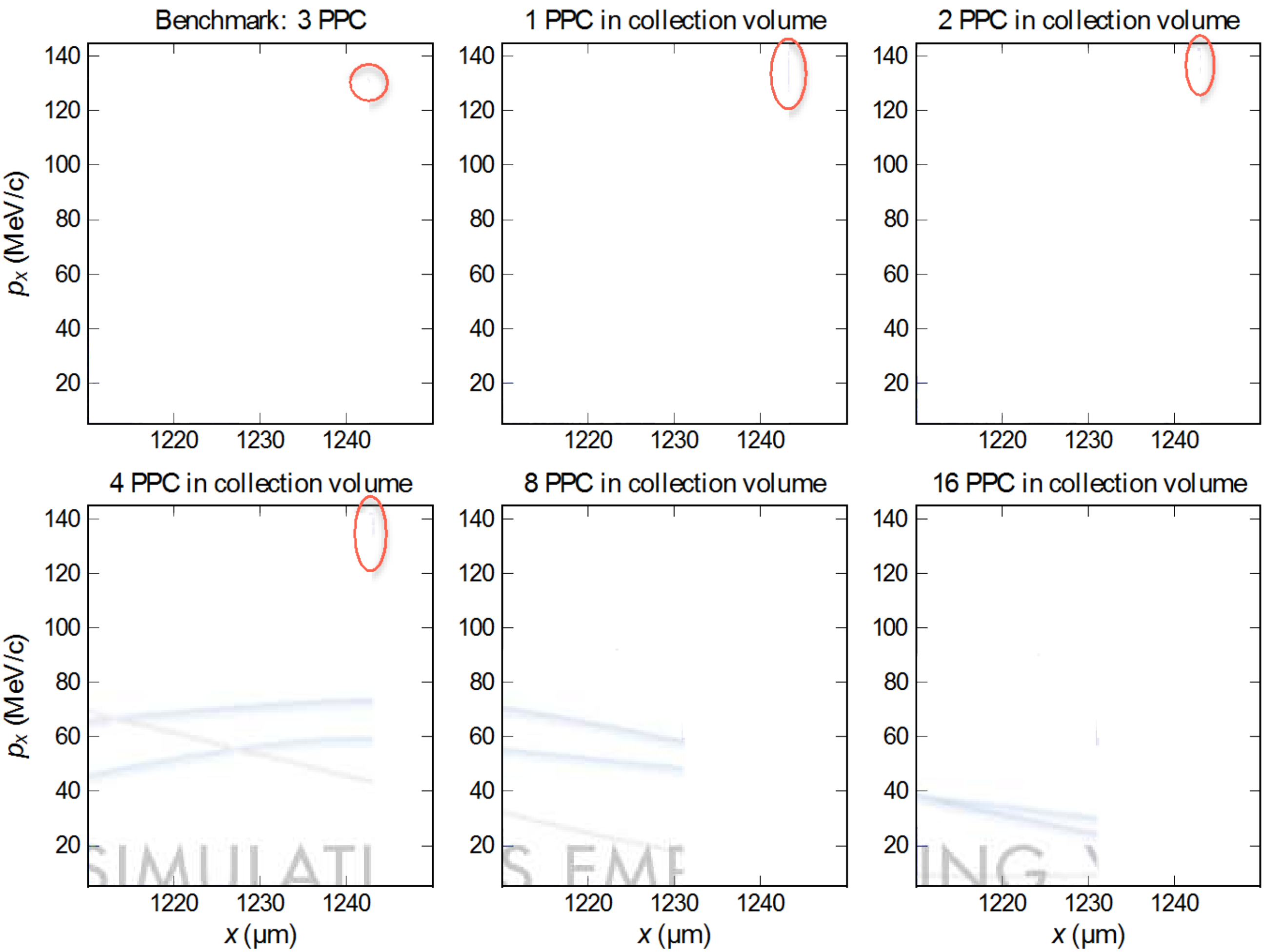
- The collection volume forms an annular region around the axis
- We load a larger number of particles per cell in that region
- With grid loading, we enhance on a cell-by-cell basis
  - Preserves quiet start
  - Loading is enhanced if the cell center is in the collection volume
  - Load on a uniform grid within each cell



Transition between unenhanced and enhanced regions

2D results: Longitudinal phase space

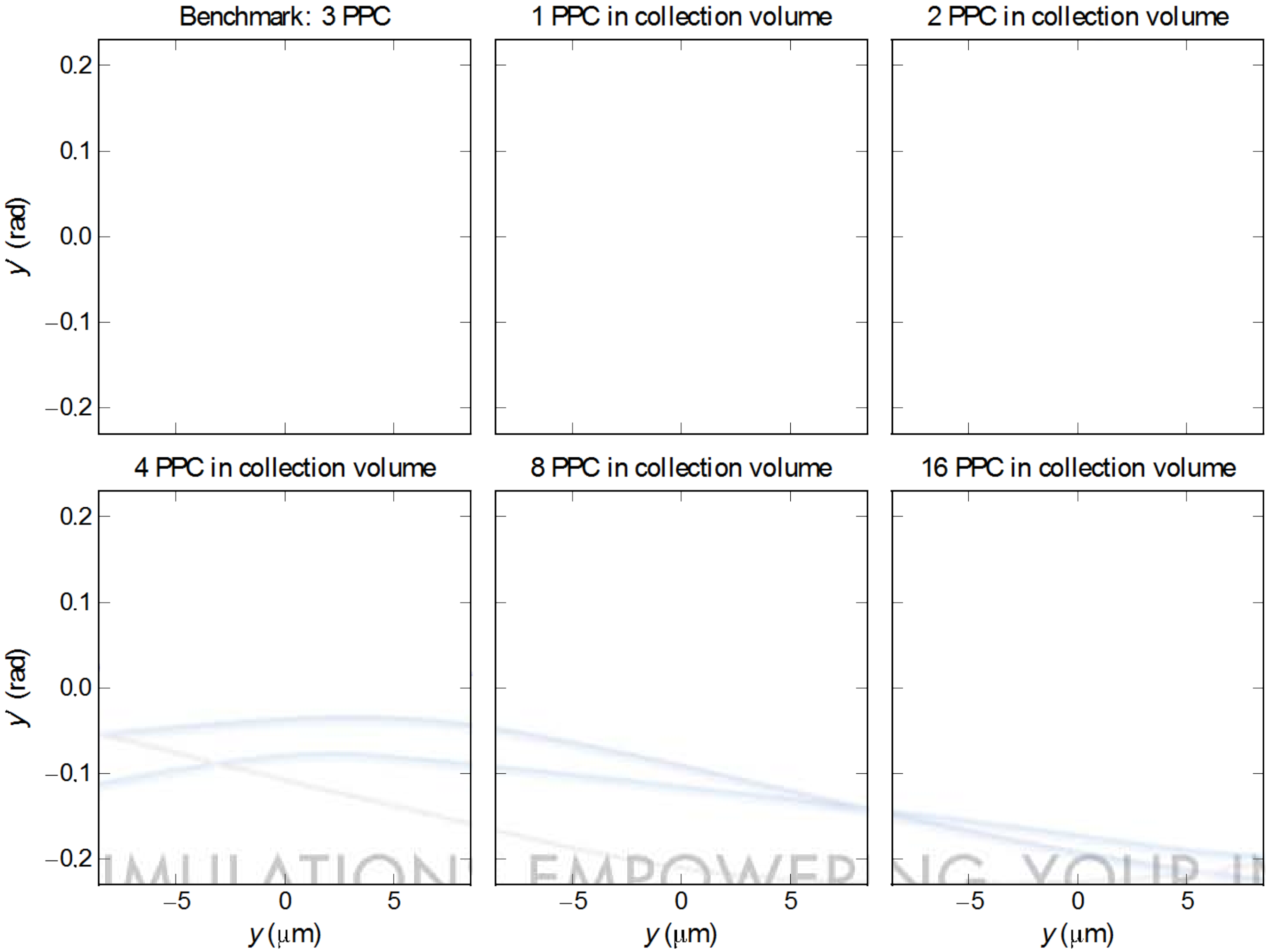
- Ran tests with 1, 2, 4, 8, and 16 PPC in collection volume and 1 PPC outside, as well as benchmark with 3 PPC everywhere



- Observed at point of minimal energy spread
- Up to 4 PPC (including benchmark) shows small injection in first bucket
- Conclusion: Injection in first bucket due to statistical noise, and more than 4 PPC required to eliminate it

2D results: Transverse phase space

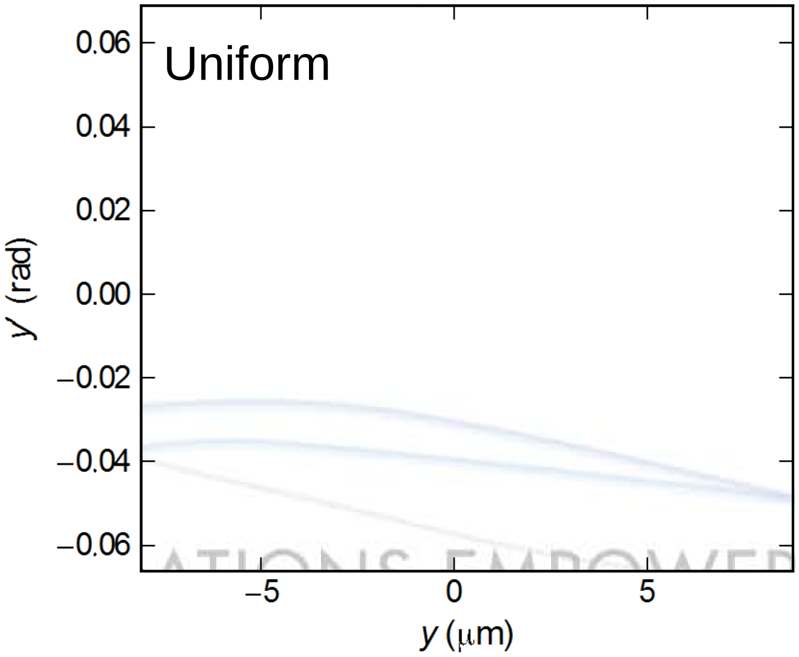
- Enhanced loading reveals, clarifies features

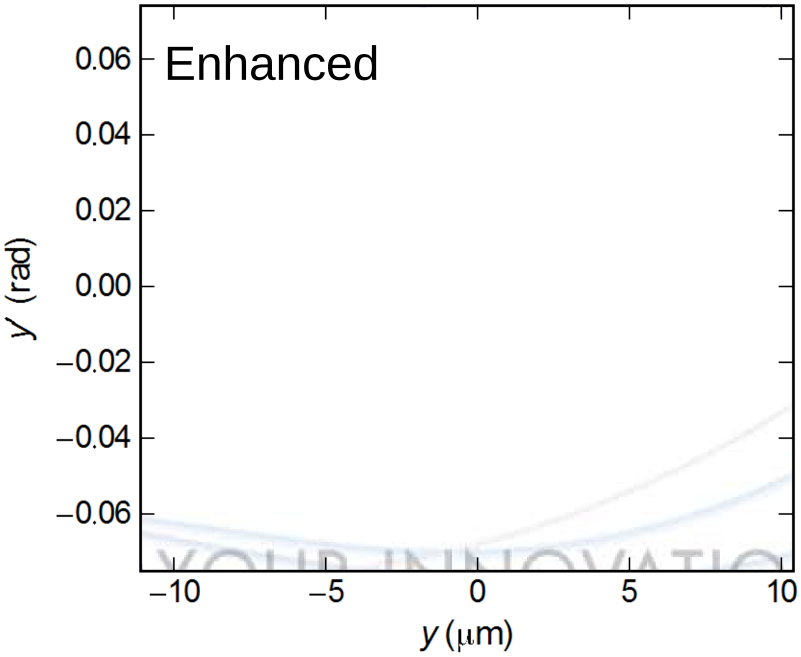


- Halo around core of beam phase space more clearly defined with enhanced loading
- Spiral pattern reveals nonlinear effects
- At 16 PPC, additional spiral pattern visible even within core

3D comparison

- For uniform loading, used 4 PPC everywhere
- For enhanced loading, used 16 PPC (1 x 4 x 4) inside collection volume (radius 7–10 μm), 1 PPC outside
- Compared transverse phase space
  - Better definition of halo for enhanced loading
  - Cleaner resolution of Gaussian core





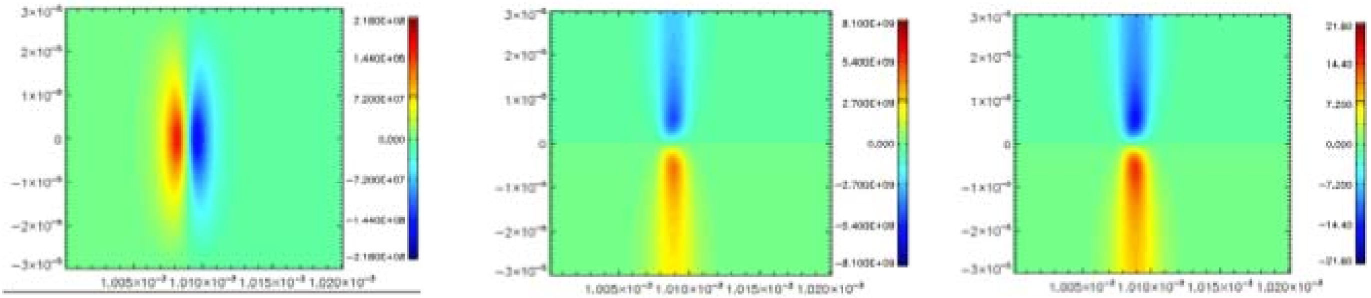
Vay push

- Vay push improves calculation of forces on a particle. By breaking up how the fields are stored and calculated it may be possible to improve calculation accuracy.
- It is a bad idea (numerically) to subtract a big floating point number from a big number – leads to rounding errors.
- Exists in VSim, WARP, probably some others.
- more recently J-L Vay, “Simulation of beams or plasmas crossing at relativistic velocity” Phys. Plasmas **15**,056701 (2008)

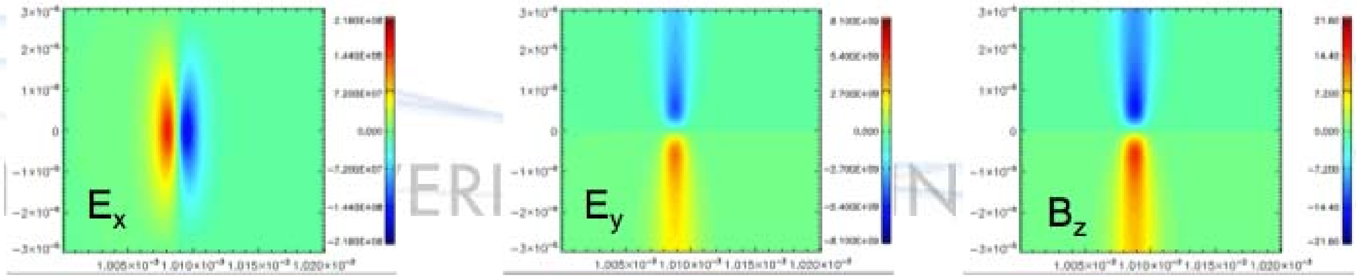
Self-fields of the e- bunch can be found from a Poisson solve in the beam frame

- Very similar to what is done in tracking codes
- The beam self-fields are calculated at each time step using a Poisson solver in the frame of the moving beam
- Works for low emittance, low divergence bunches
  - relative motion must be non-relativistic in the beam frame
  - we refer to this as the “beam frame Poisson solve” – **BFPS** – algorithm
- After 1 mm of propagation, fields are consistent with self-consistent PIC fields

BFPS fields at 1mm:



Self consistent electro-magnetic fields at 1 mm:



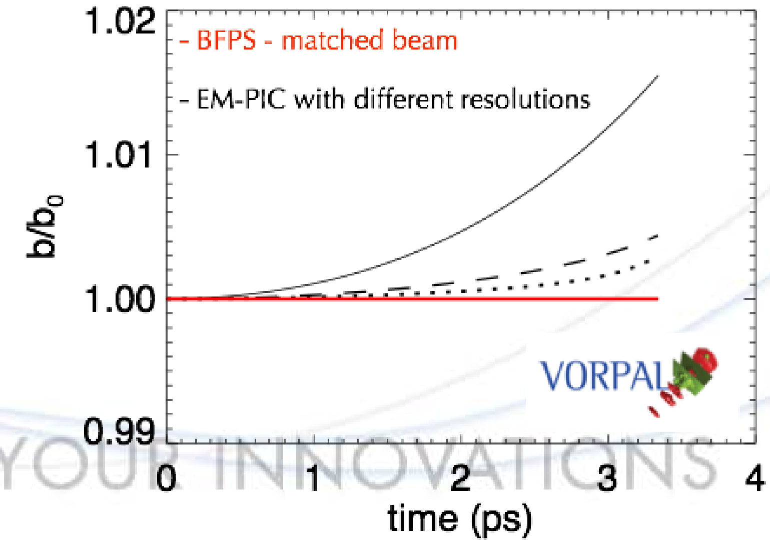
BFPS treatment of the e- beam self-fields enables correct modeling of transverse forces

- The uniformly-filled beam envelope equation has been modified in 2D slab geometry: here *a* is the beam half-length, *b* the radius, *y* the transverse coordinate, k_y the focusing wave number, ε_y the transverse geometric emittance

$$y'' + k_y^2 y - \frac{q^2 N/L}{m\beta^2 c^2 \gamma \pi \varepsilon_0 b(\gamma a + b)} y - \frac{\varepsilon_y^2}{y^3} = 0$$

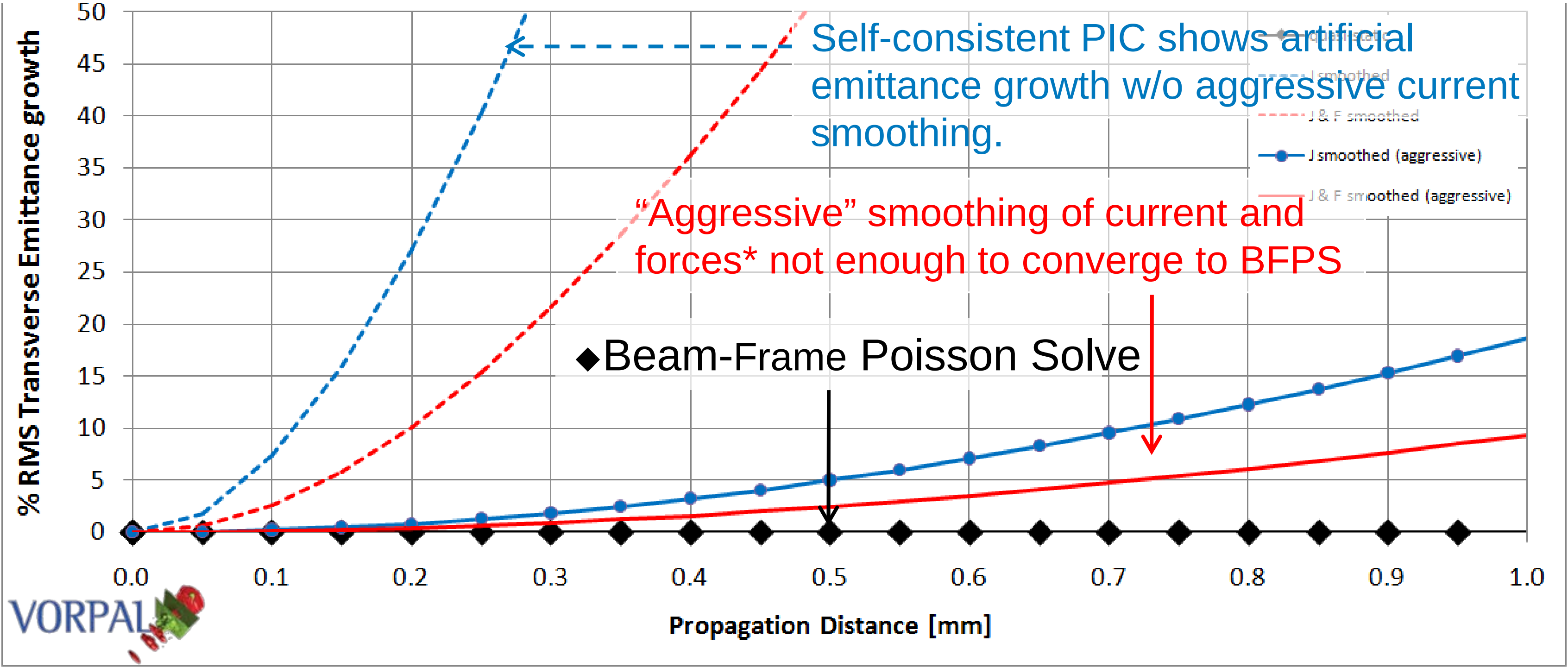
- The equation assumes correct cancellation of the transverse forces $\gamma >> 1$

- Evolution of theoretically matched beam in a linear focusing field
    - BFPS shows constant radius over 1 mm
    - EM PIC suffers from interpolation errors, higher resolution reduces artificial radius growth (2nd order convergence)
    - Shown: *dx = a/60, a/120, a/180 ; dy = 4dx ; a = b = 2* μm



BFPS shows no emittance growth for matched e- beam

- Theoretically matched beam in linear focusing field
- Beam parameters characteristic of a m-scale LPA stage:
    - 300 pC, 1 GeV Gaussian e- beam, ε_{ny} = 0.01 mm mrad, $\delta\gamma/\gamma$ = 1%
- EM PIC shows artificial emittance growth even with aggressive smoothing and higher resolution



Self-consistent PIC shows artificial emittance growth w/o aggressive current smoothing.

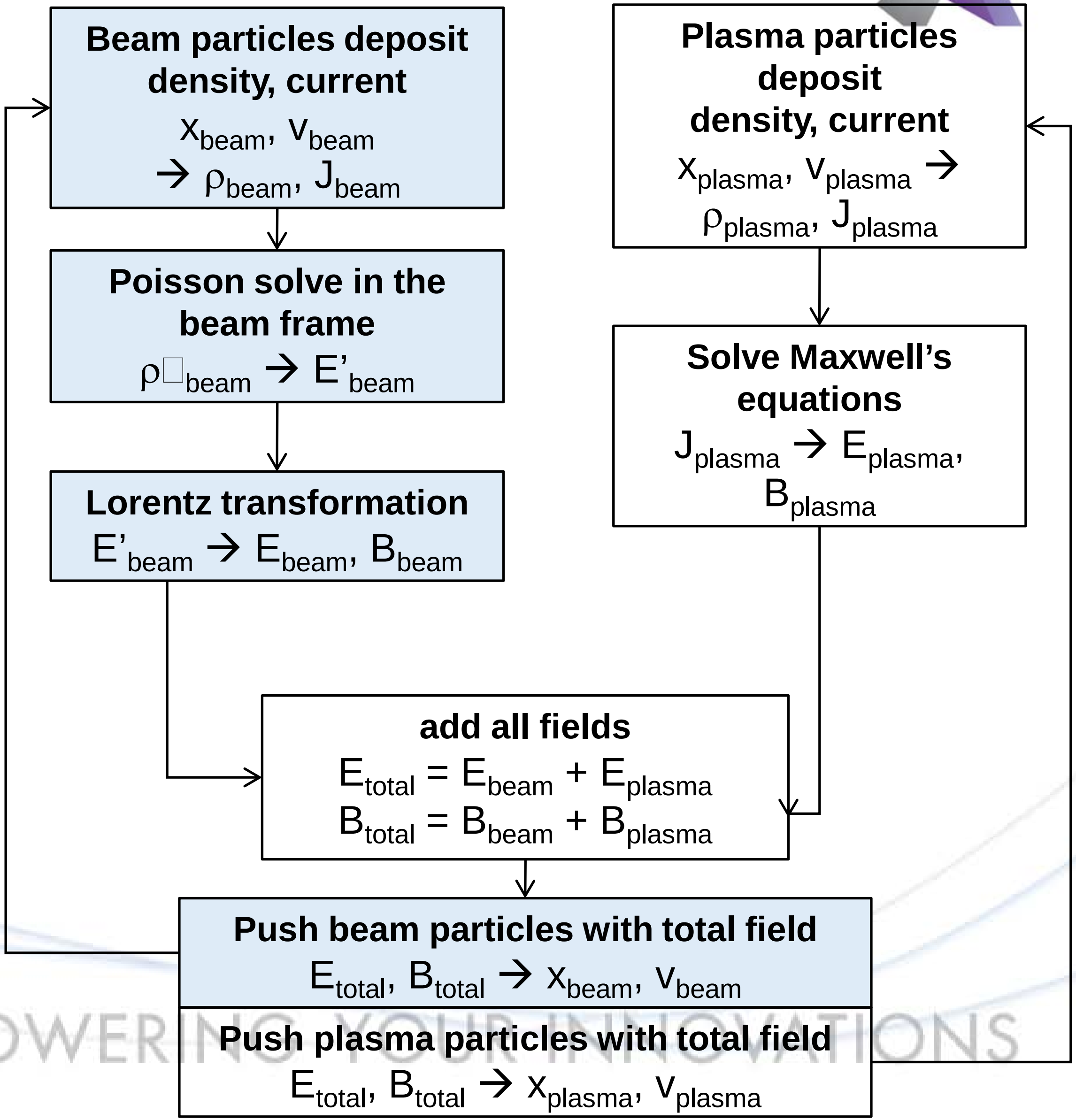
"Aggressive" smoothing of current and forces* not enough to converge to BFPS

◆Beam-Frame Poisson Solve

* *J.-L. Vay et al., Phys. Plasmas* ***18*** *(2011)*

BFPS is also valid inside the plasma

- Linearity of Maxwell's equations allows separate treatment of the beam in the plasma
    - beam and plasma must be separate at time 0
    - all particles respond to the combined fields
- Algorithm made possible by generality of Vorpal's structure, controlled from the input file



Beam particles deposit density, current
$x_{\text{beam}}, v_{\text{beam}} \rightarrow \rho_{\text{beam}}, J_{\text{beam}}$

Poisson solve in the beam frame
$\rho\square_{\text{beam}} \rightarrow E'_{\text{beam}}$

Lorentz transformation
$E'_{\text{beam}} \rightarrow E_{\text{beam}}, B_{\text{beam}}$

Plasma particles deposit density, current
$x_{\text{plasma}}, v_{\text{plasma}} \rightarrow \rho_{\text{plasma}}, J_{\text{plasma}}$

Solve Maxwell's equations
$J_{\text{plasma}} \rightarrow E_{\text{plasma}}, B_{\text{plasma}}$

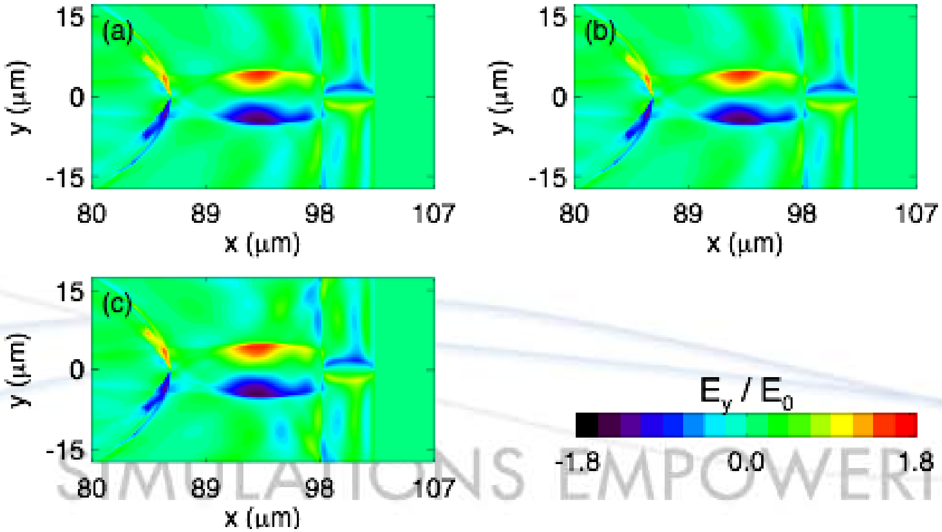
add all fields
$E_{\text{total}} = E_{\text{beam}} + E_{\text{plasma}}$
$B_{\text{total}} = B_{\text{beam}} + B_{\text{plasma}}$

Push beam particles with total field
$E_{\text{total}}, B_{\text{total}} \rightarrow x_{\text{beam}}, v_{\text{beam}}$

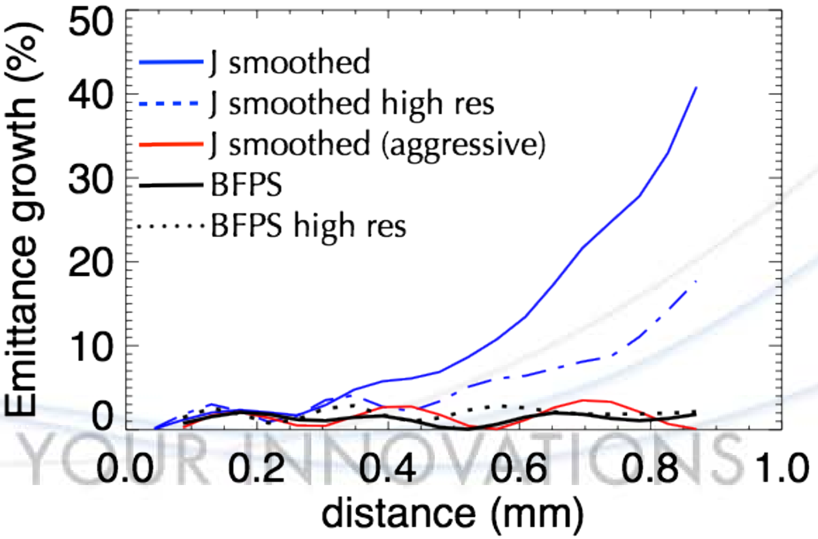
Push plasma particles with total field
$E_{\text{total}}, B_{\text{total}} \rightarrow x_{\text{plasma}}, v_{\text{plasma}}$

BFPS can be used inside the plasma wakefield to prevent artificial emittance growth

- Transverse fields when beam has propagated in the plasma
  - (a) self-consistent EM PIC
  - (b) self-consistent EM PIC with separate updates for the beam and the plasma
  - (c) beam fields calculated with the BFPS



- 100 MeV stage, $n_0 = 10^{19}$ cm^{-3}
- 10 pC, $\varepsilon_{ny} = 0.5$ mm mrad, Gaussian e- beam matched to the wakefield focusing field
- method can also be used in the boosted frame
- will enable m-scale LPA stage simulations with low particle noise
- will enable parameter scans to optimize BELLA-like 10 GeV stages

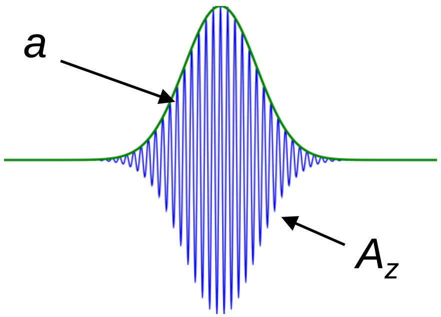


Talk highlights:

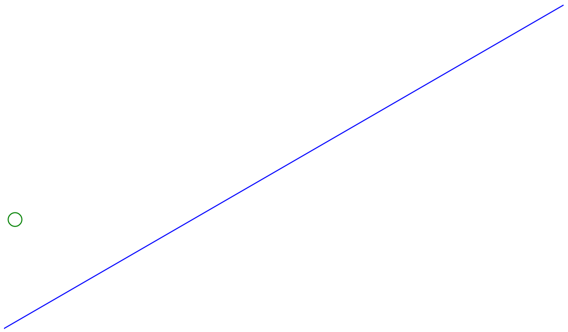
- Fundamentals of plasma acceleration and future experiments (5 mins)
- Learn about the basics of the FDTD technique and PiC simulation (10mins)
- Have an overview of the simulation software landscape (5 mins)
- Understand the source of common numerical instabilities. (10 mins)
- Find out about cutting edge techniques to improve accuracy (15 mins)
    - Quiet loading, enhanced loading
    - Vay push
    - Beam Frame Poisson Solve
    - Smoothing
    - Controlled (sometimes 'Perfect' Dispersion)
- Find out about cutting edge techniques to improve speed (10 mins)
    - Envelope models (with or without phase tracking) & QSA.
    - Boosted frame
- Learn about cutting edge dielectric acceleration algorithms
- If time allows… A few words on computational infrastructure requirements, visualisation and future direction.

Laser envelope model allows orders of magnitude speedup by averaging over laser fast oscillations

- Model the complex envelope *a* of the oscillating laser vector potential
- Ponderomotive force included in particle push



- Envelope model has correct dispersion

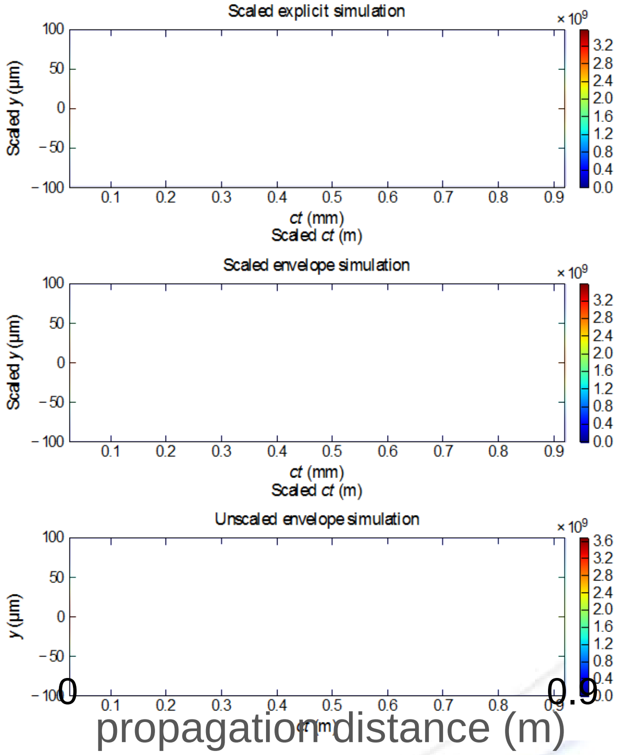


Explicit $\Delta y = \lambda/3$

- Good agreement with PIC for laser in channel
- 5 x10^4 speedup for full scale 10 GeV stage

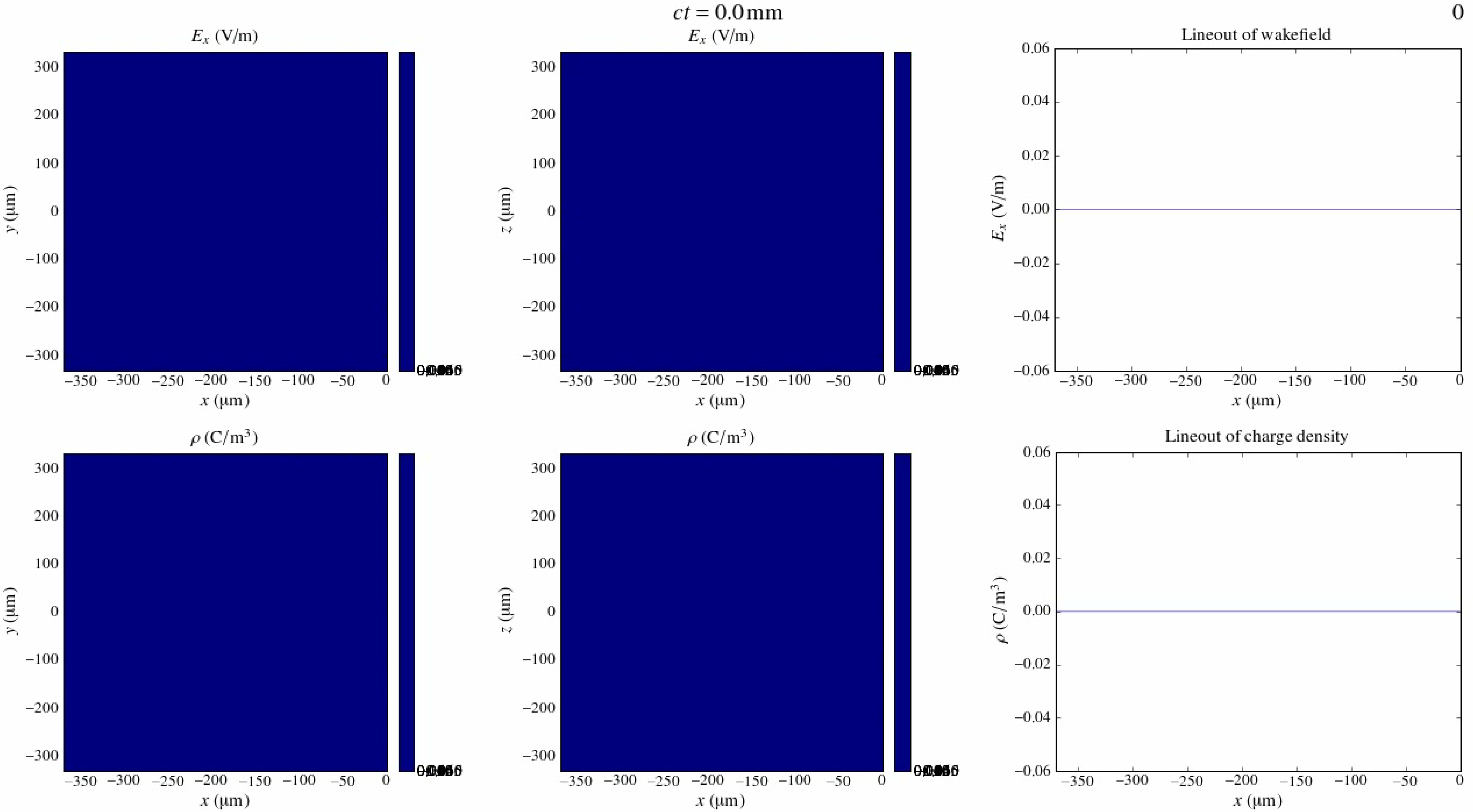
Laser evolution in plasma channel:

- scaled PIC $n_0 = 10^{19}$ cm^{-3}
- scaled envelope $n_0 = 10^{19}$ cm^{-3}
- unscaled envelope $n_0 = 10^{17}$ cm^{-3}

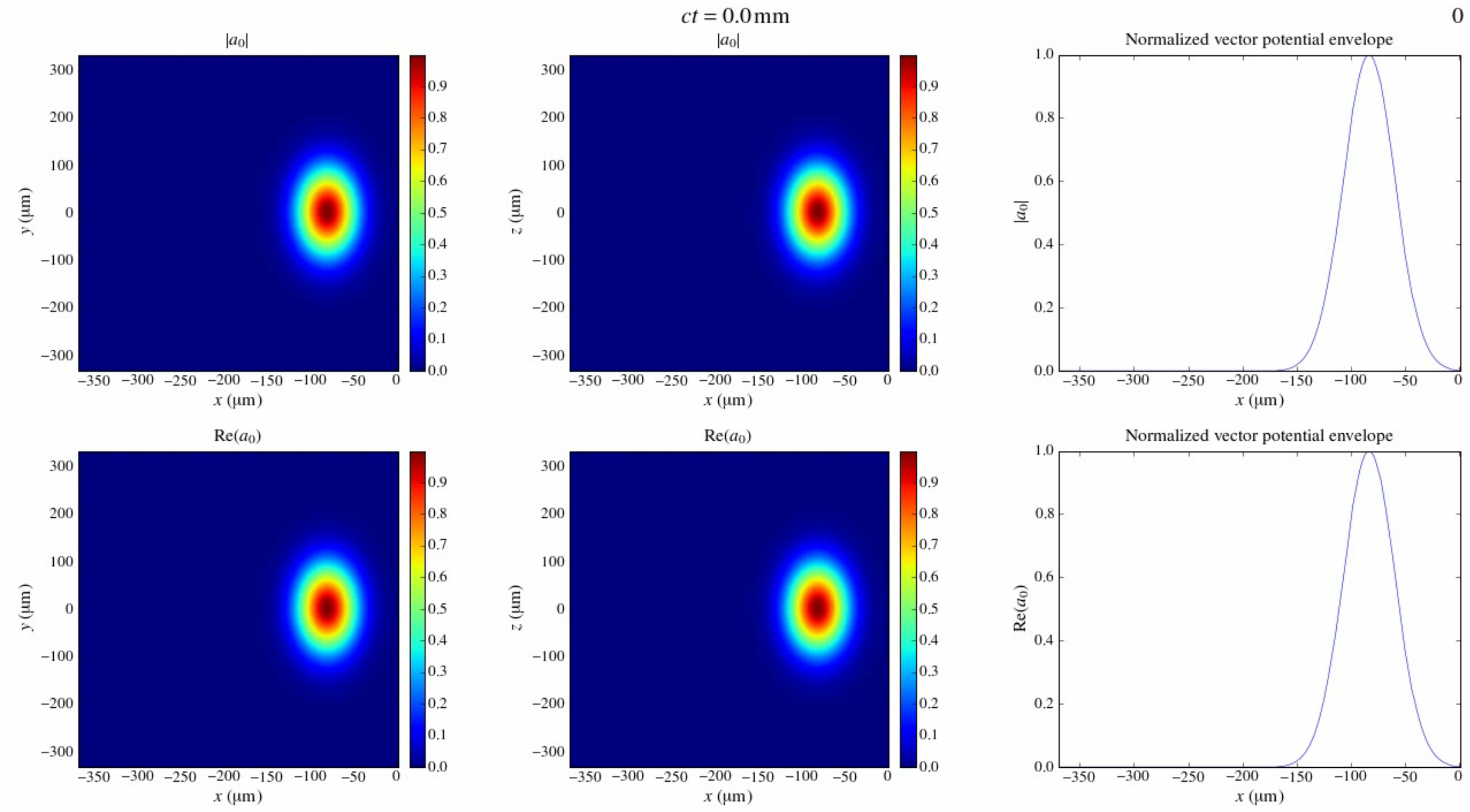


- B. Cowan *et al.*, J. Comput. Phys. **230**, 61 (2011)
- D. Gordon, IEEE Trans. Plasma Sci. (2007)
- P. Messmer *et al.*, Phys. Rev ST/AB (2006)
- P. Mora & T. Antonsen, Phys. Plasmas (1997)

3D run: Wake and charge density



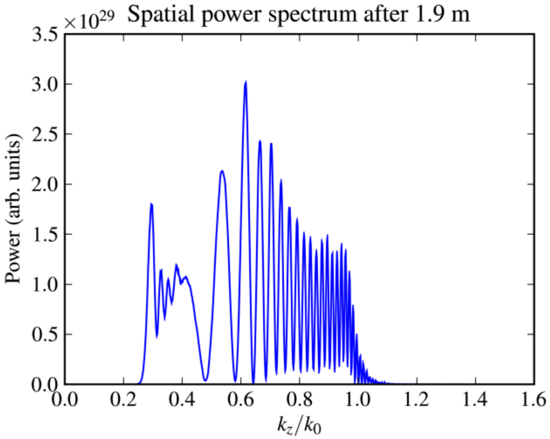
3D run: Envelope fields

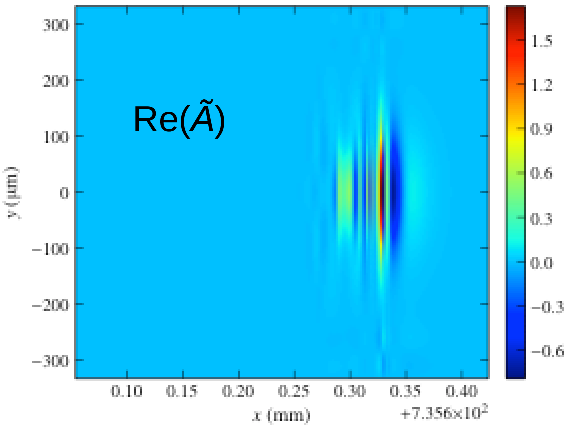


SIMULATIONS EMPOWERING YOUR INNOVATIONS

Envelope model limitations

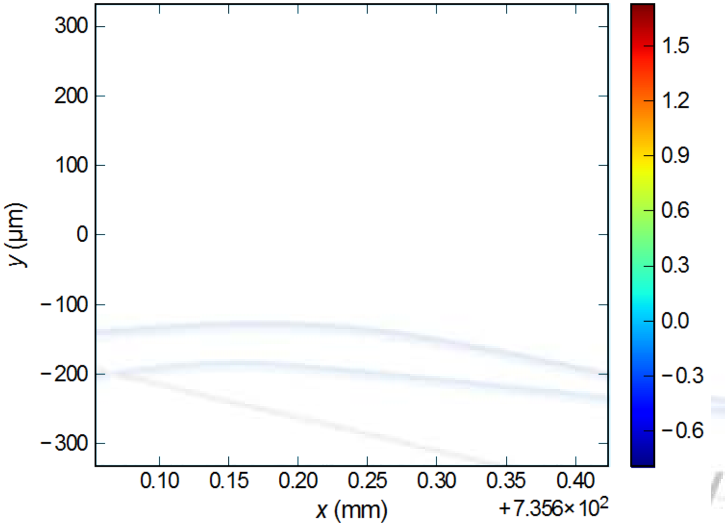
- Spectral limitation
  - Results become suspect close to depletion
  - Spectrum broadens during long propagation distances
  - Envelope becomes unresolved
- Coarse gridding
  - Speedup comes from coarser grid, but then beam becomes unresolved
  - Quasi-static models don’t capture trapping

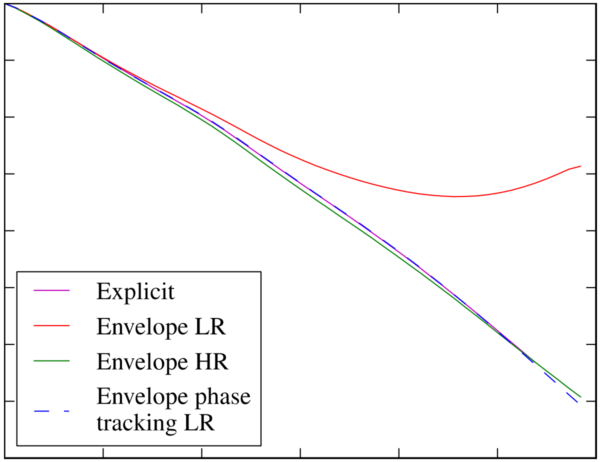




Laser envelope model pushed further in depletion by tracking envelope phase

- Envelope models typically become invalid as laser pulse depletes
  - spectral broadening makes carrier no longer sinusoidal
  - envelope field becomes unresolved
- Tracking evolution of phase oscillations in the envelope field allows laser envelope field to evolve more smoothly
- Envelope field valid further into laser depletion for reasonable resolution





Special features implemented in Vorpal to enable simulation in a Lorentz boosted frame

- Simulation in a Lorentz boosted frame allows significant speedup
  - laser wavelength is increased by a factor ~$(1+\beta_{boost})\gamma_{boost}$
  - plasma length contracted by factor γ_{boost}
  - theoretical speedup ~$(1+\beta_{boost})^2\gamma^2_{boost}$
- Shortening of Rayleigh length requires special laser injector:
  - Implemented in Vorpal laser launcher from a moving plane (enables launching the laser close to focus position) *
- Requires special diagnostics to compare data between different frames
  - Implemented in Vorpal diagnostics for field and particle data on a moving plane (data can be transformed back to a fixed plane in the lab frame through Lorentz transformation) *
- Numerical instabilities at the entrance of the plasma at large γ_{boost} mitigated by using current smoothing with wide stencil **

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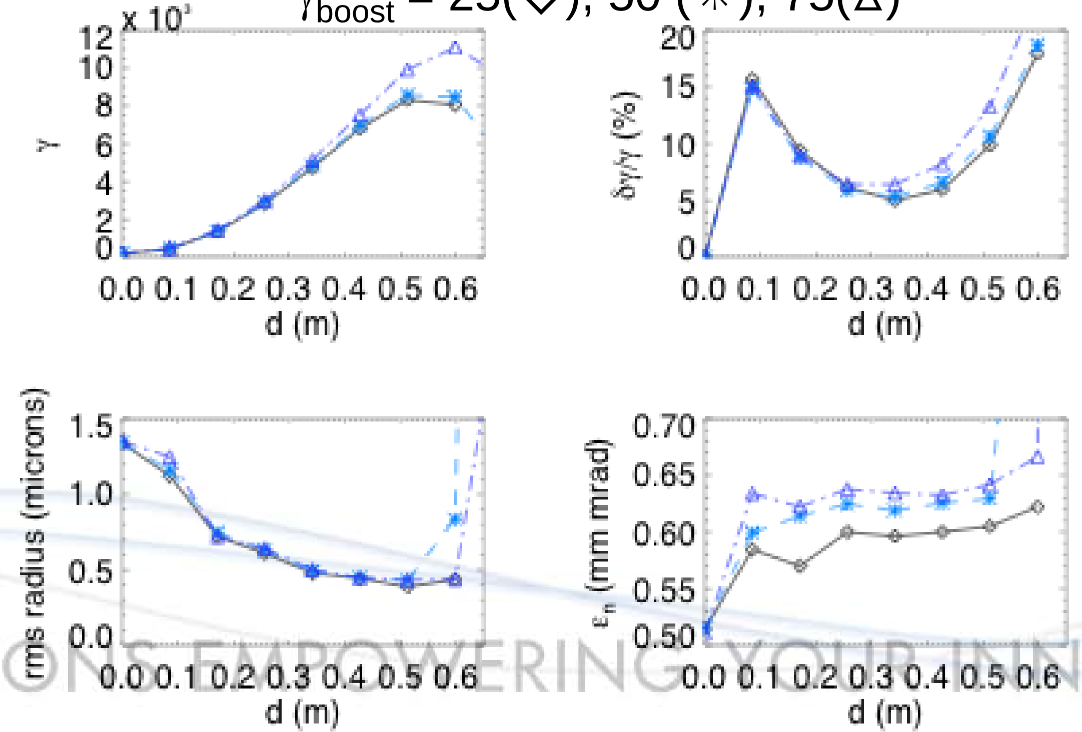
* J.-L. Vay *et al.* PoP **18** (2011)

** J.-L. Vay *et al.*, JCP **230** (2011)

Boosted frame technique enables full scale 10 GeV LPA stage simulation

- Successful benchmarking of accelerated electron beam properties for different boosted frame velocities at nominal density $n_0 = 10^{17}$ cm^{-3}
- Achieved up to 3,500x speedup:
  - normal PIC: 2.5×10^6 proc.h
  - boosted frame at $\gamma_{boost} = 75$: 706 proc.h

γ_{boost} = 25(◇), 50 (✳), 75(△)



Boosted frame references

- J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)
- S. F. Martins *et al.*, in *Thirteenth Advanced Accelerator Concepts*, 285 (2009)
- S. F. Martins *et al*., "Exploring laser-wakefield-accelerator regimes for near-term lasers using particle-in-cell simulation in Lorentz-boosted frames," Nature Physics **6**, 311 (2010).
- S. F. Martins *et al*., "Numerical simulations of laser wakefield accelerators in optimal Lorentz frames," Comp. Phys. Comm. **181**, 869 (2010).
- S. F. Martins *et al*., "Modeling laser wakefield accelerator experiments with ultrafast particle- in-cell simulations in boosted frames," Phys. Plasmas **17**, 056705 (2010).

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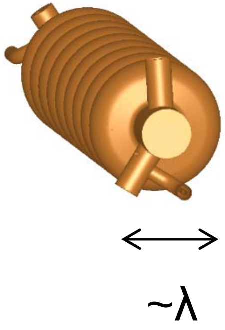
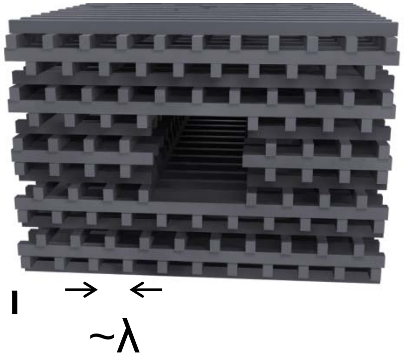
  - Boosted frame
- Learn about cutting edge dielectric acceleration algorithms
- If time allows… A few words on controlled injection, computational infrastructure requirements, visualisation and future direction.

Avenues for higher gradient

- Gradient fundamentally limited by material breakdown of the accelerator structure
- Dielectric laser acceleration (DLA)
  - Dielectric materials at optical and NIR wavelengths have breakdown threshold 1–2 orders of magnitude higher than metals at microwave frequencies
  - Many concepts from conventional acceleration carry over, but structures themselves are very different
- Laser-plasma acceleration (LPA)
  - Breakdown is not a problem if material is already broken down—a plasma!
  - Dynamics are nonlinear and highly complex

Computational challenges

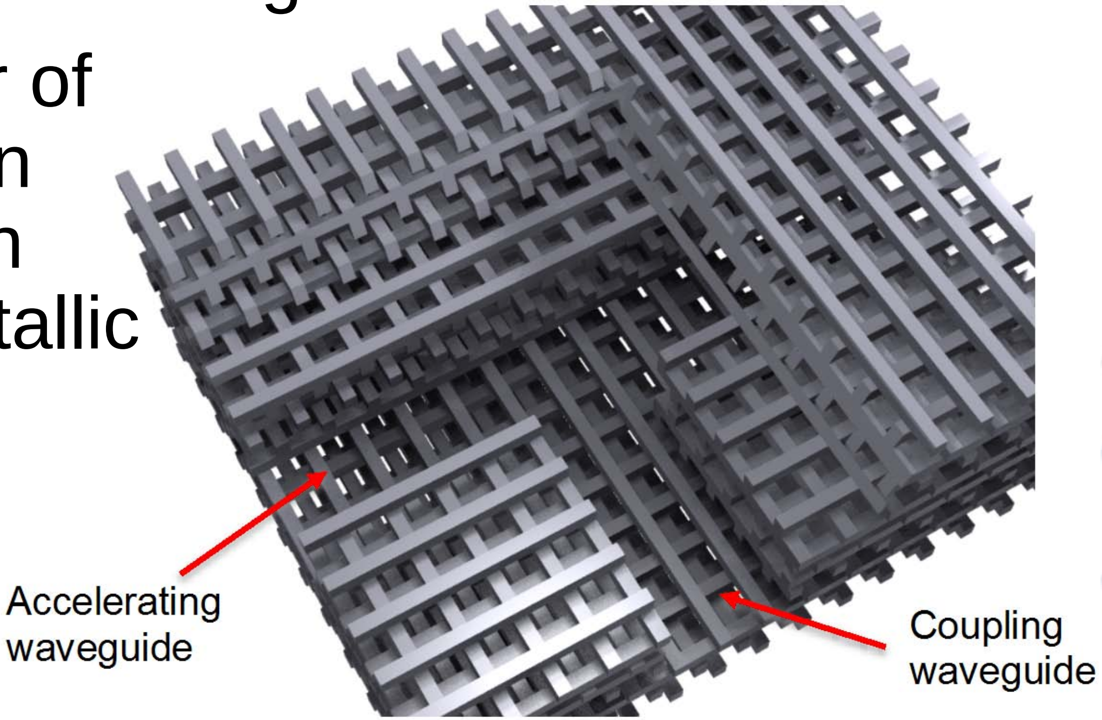




- Computations of laser-driven acceleration are hard
- DLA: Structures order of magnitude larger, more complex than conventional
- LPA:
  - Separation of length scales poses challenge
  - 10^7–10^8 grid points, 10^8–10^9 particles, 10^5–10^6 time steps in PIC simulation
  - 10^5–10^6 CPU hours typical
- Advanced simulation tools are critical for modeling laser accelerators

Coupling in photonic crystal structures

- A *photonic crystal* can confine fields in a waveguide using a periodic lattice
- Need to couple power into accelerating waveguide without blocking the beam
- Structure is ~order of magnitude larger in each direction than corresponding metallic structure



VSim features and methods used

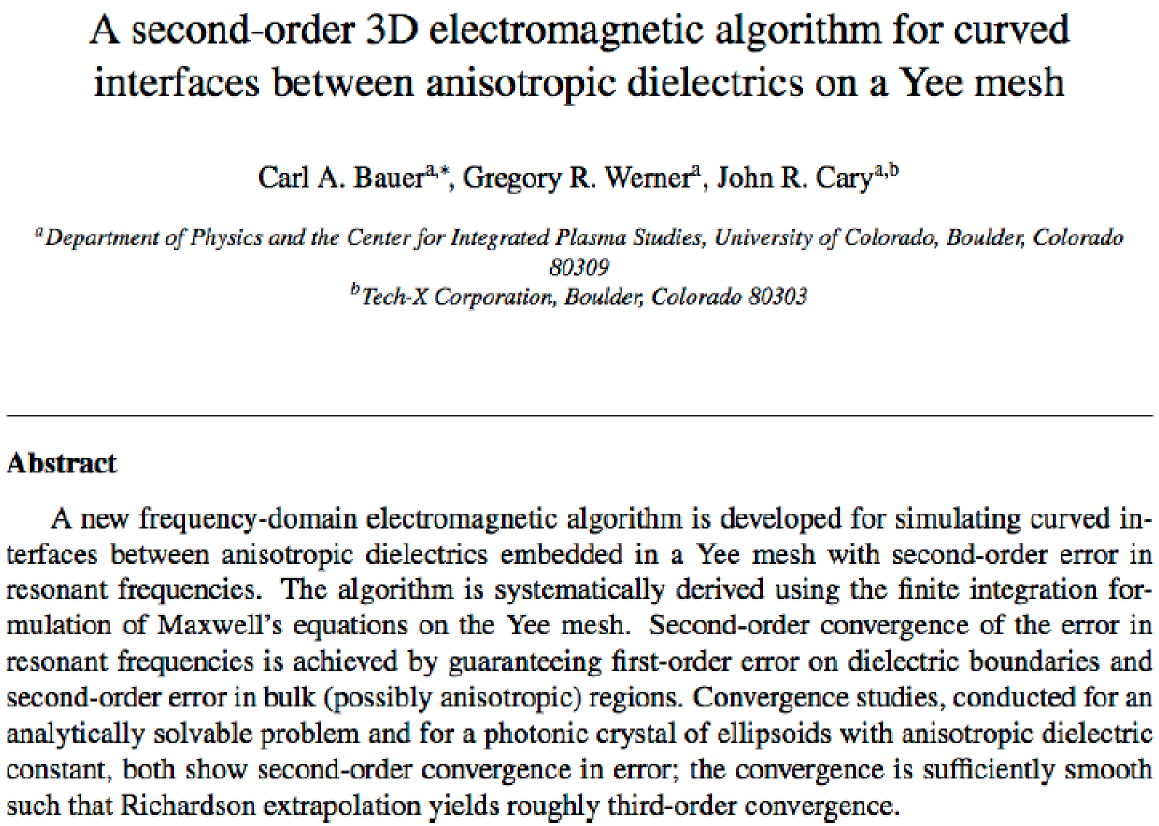
- Eigenmode solver
  - First solve for eigenmode in waveguide
  - Launch that mode in coupling structure
- MAL absorbing boundaries
  - Can overlap with dielectric structure while remaining stable
- Power flow history
  - Monitor power across planes to diagnose whether steady-state has been reached

We have made several algorithm advances

- First 2nd-order accurate embedded boundary algorithm for dielectrics
- First scalable frequency domain algorithm for embedded boundary metallics

What is the embedded boundary algorithm for dielectric conformal surfaces?

- J. Comput. Phys. **230**, 2060-2075 (2011)



A second-order 3D electromagnetic algorithm for curved interfaces between anisotropic dielectrics on a Yee mesh

Carl A. Bauer[a,*], Gregory R. Werner[a], John R. Cary[a,b]

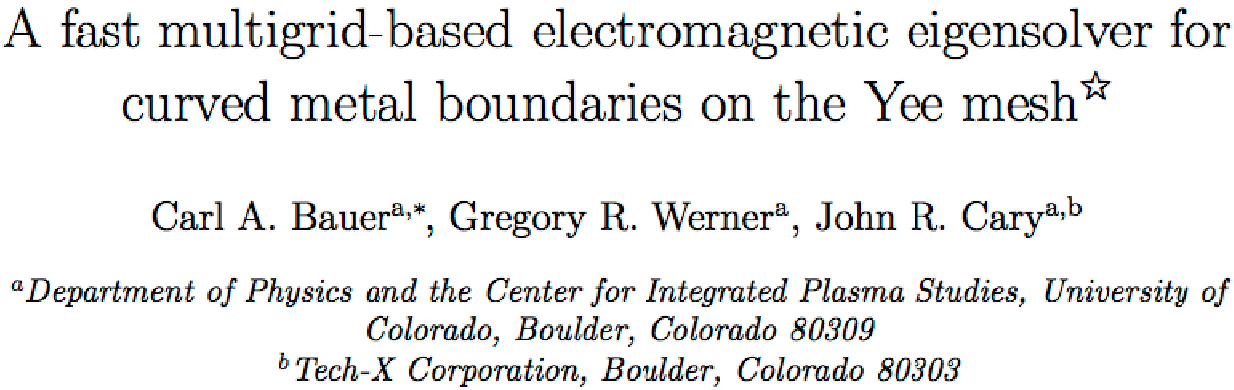
[a] *Department of Physics and the Center for Integrated Plasma Studies, University of Colorado, Boulder, Colorado 80309*
[b] *Tech-X Corporation, Boulder, Colorado 80303*

Abstract

A new frequency-domain electromagnetic algorithm is developed for simulating curved interfaces between anisotropic dielectrics embedded in a Yee mesh with second-order error in resonant frequencies. The algorithm is systematically derived using the finite integration formulation of Maxwell's equations on the Yee mesh. Second-order convergence of the error in resonant frequencies is achieved by guaranteeing first-order error on dielectric boundaries and second-order error in bulk (possibly anisotropic) regions. Convergence studies, conducted for an analytically solvable problem and for a photonic crystal of ellipsoids with anisotropic dielectric constant, both show second-order convergence in error; the convergence is sufficiently smooth such that Richardson extrapolation yields roughly third-order convergence.

One can have a frequency domain algorithm that scales to very high concurrency

- J. Comput. Phys.: http://arxiv.org/pdf/1301.3794



A fast multigrid-based electromagnetic eigensolver for curved metal boundaries on the Yee mesh[☆]

Carl A. Bauer[a,*], Gregory R. Werner[a], John R. Cary[a,b]

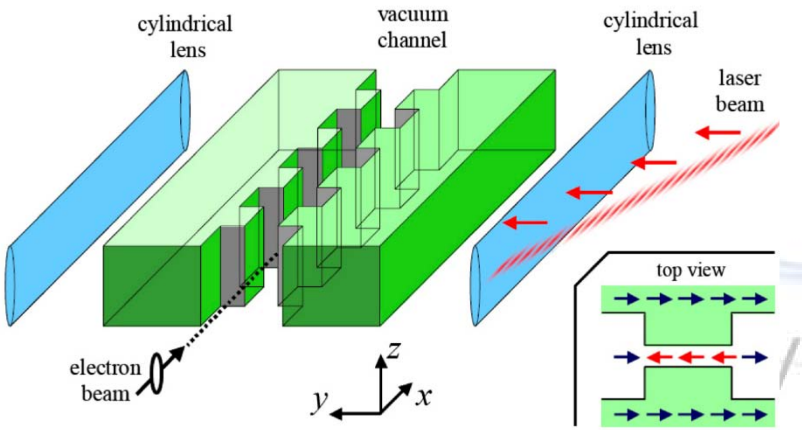
[a] *Department of Physics and the Center for Integrated Plasma Studies, University of Colorado, Boulder, Colorado 80309*
[b] *Tech-X Corporation, Boulder, Colorado 80303*

Parameter scans to optimize coupling

- Manipulated individual rods to improve coupling efficiency
- Found one that increases efficiency from 65% to 94%
- Supercomputers can run multiple jobs simultaneously

Grating structures

- Transform free-space mode from laser directly into accelerating field
- Recent results demonstrated high-gradient acceleration
- Dynamics are complex, especially in current experiments
  - Developed realistic model with current experimental parameters



From T. Plettner et al., PRST-AB **9**, 111301 (2006)

Peralta et al., Nature **503**, 91 (2013)

Material interactions

- Challenge: Many particles traverse the structure as they propagate
  - Their energy loss is superimposed on measured spectrum
  - Need to model material energy loss with full EM, particle dynamics
- Bremsstrahlung: e^{-}-nucleus collisions
- Ionization e^{-} collisions with electrons in the medium
  - High energy transfer interactions (relative to ionization energy) can be described by Møller scattering — e^{-} collisions with **free** electrons
  - Mean ionization energy of SiO_2 is $I = 139.2$ eV (according to pdg.lbl.gov)
- Warning: Not all codes/data tables/papers agree

Ionization model

- First, apply a deterministic energy loss using the stopping power in the NIST ESTAR database
- Then, apply a random energy loss using a Landau distribution, with parameters from known formulas
- Implemented in VSim, fast performance
- Uses exact Landau distribution for accuracy over many time steps

Bremsstrahlung cross sections

- We get the relevant cross-sections from the data tabulated by Seltzer and Berger (1986)
- Same data used in Geant4
- Data provides values of

  $$k\frac{d\sigma}{dk}$$

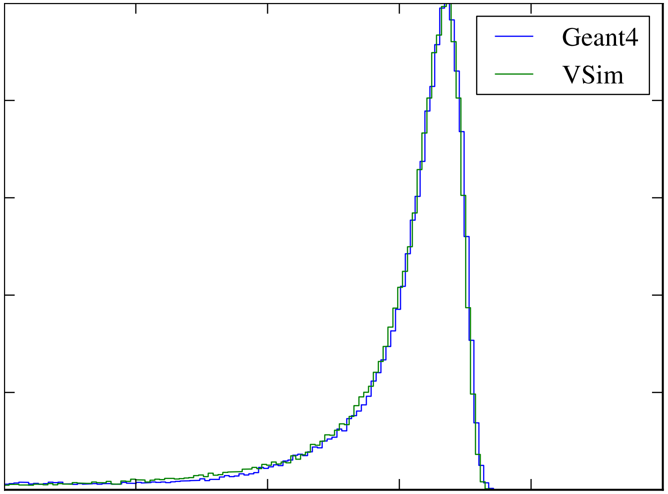
  for photon energy *k*
- As *k* → 0, the differential cross section *dσ/dk* diverges — the “infrared divergence” — so we treat soft photons separately

Hard photon model

- Above y_c, σ is finite, so we can integrate to get the total hard-photon cross section
- From this, compute the mean free path
- For a step of length L:
  - Generate a random segment length s based on the mean free path
  - If $s > L$, no hard photon event occurs
  - If $s \leq L$, choose a y based on the differential cross section, then repeat process for a step of length $L - s$

Complete energy loss results

- Propagate 100,000 particles through SiO_2 for 1 mm, in 10 µm steps, in VSim
- Spectrum has excellent agreement with Geant4
- Adjust stopping power function by a constant factor to make peak of spectrum agree with Geant4—this results in an overall shift of the spectrum



Design controlled injection for high quality electron beams
(if time)

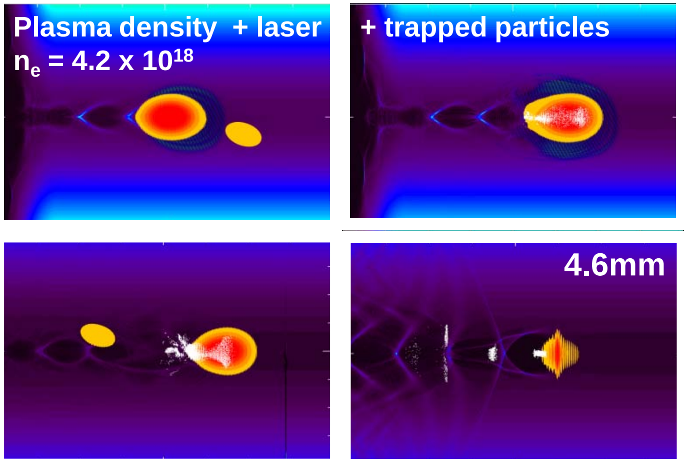
Vorpal is used to design injection of high quality beams in LPA

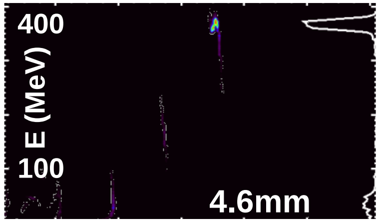
- Simulations allow design and optimization of production of high quality beam through controlled injection
  - 2-pulse colliding pulse injection:
    - simulations results agree with experimental data
    - parameter scans determine best conditions for production of highest quality electron beams – guide experimental parameters
  - Ionization injection:
    - modeling of current and future experiments possible in Vorpal through implementation of general ionization formula
    - successful benchmark with VLPL

- Post processing routine allow calculation of X-Ray spectra produced by the beam betatron oscillations

- Will are looking at further developments to integrate non linear optimization software to improve our simulations.

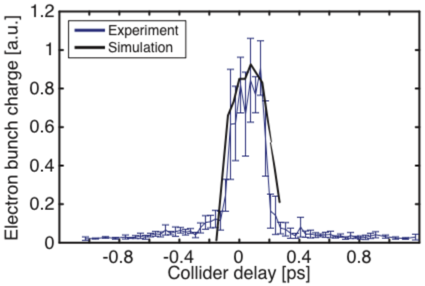
Simulations help design colliding pulse injection experiments



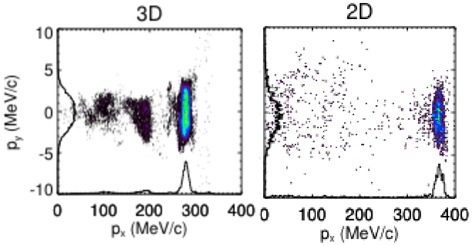


- Colliding pulse injection produce high quality electron beams
- Simulations allow parameter scan to predict best experimental setup

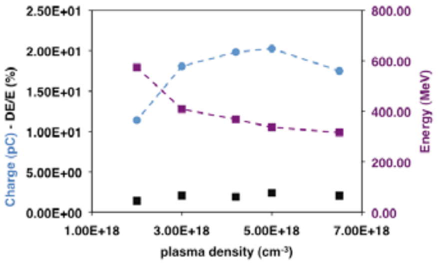
- Simulation results agree with experimental data



- 3D and 2D simulations show similar results

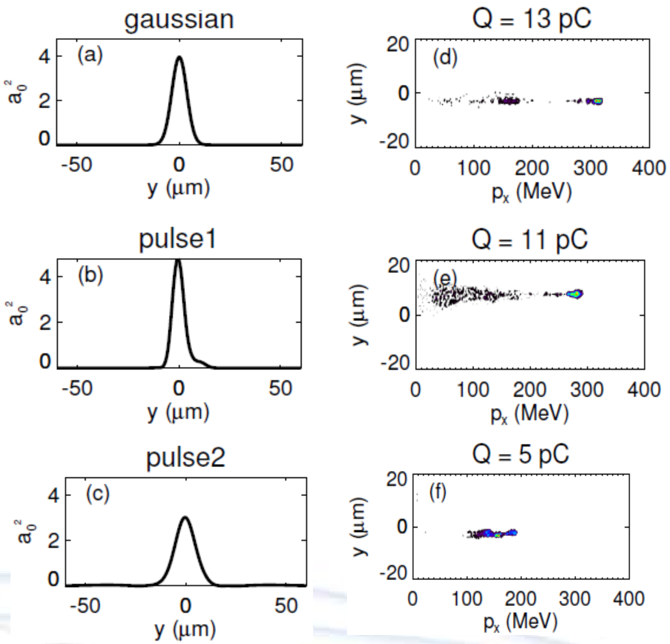


- Beam energy can be tuned by changing the plasma density

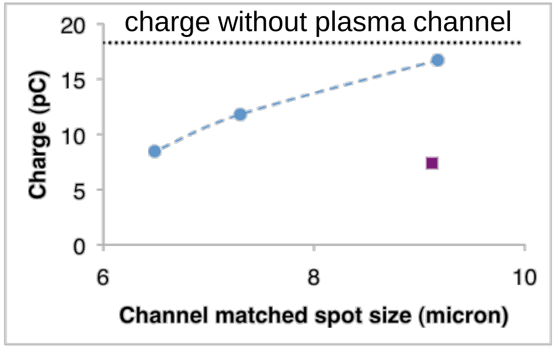


Simulations help study non-ideal effects in experiments

- Small deviation from Gaussian pulse modifies the beam position, charge and energy significantly.
- Deformable mirror is installed in experiments to control laser modes.

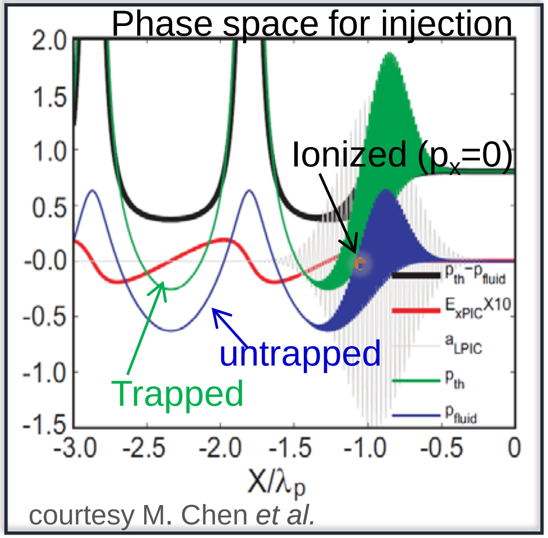


- Control of laser focusing with plasma channel is important to conserve charge in the beam
- When the laser focuses, the bubble length decreases, which truncates the back of the electron beam, resulting in loss of charge
- Optimal channel depth maximize charge in the beam while guiding laser at high intensity for electron beam larger energy gain



General tunneling ionization formula implemented in Vorpal allows simulation of ionization injection

- Injection by ionization at phase where stationary particle is on trapped orbit *
- Achieved through high Z gas with state near $I_{\text{laser,peak}}$
- General AC and DC ionization rates implemented in Vorpal **
  - DC model for explicit PIC
  - AC model when averaging over laser oscillations (envelope model)



courtesy M. Chen *et al.*

$$W_{\text{AC}} = \omega_a \sqrt{3}\left(\frac{e}{\pi}\right)^{3/2} \frac{Z^2}{n^{*9/2}} \left(4e\frac{E_a}{E_L}\frac{Z^3}{n^{*4}}\right)^{2n^*-3/2} \exp\left[-\frac{2}{3}\frac{E_a}{E_L}\left(\frac{Z}{n^*}\right)^3\right]$$

$$W_{\text{AC}} = \left[\frac{3}{\pi}\frac{E_L}{E_a}\left(\frac{U_H}{U_{ion}}\right)^{3/2}\right]^{1/2} W_{\text{DC}}$$

$$eE_a/m_e c^2 = \alpha^4/r_e \sim 5.1\text{GV/cm}$$

$$\omega_{\text{a}} = \alpha^3 c/r_e \sim 4.13\times 10^{16}\,\text{s}^{-1}$$

$$U_H = 13.6\text{eV}$$

$$n^* = Z/\sqrt{U_{\text{ion}}/U_H}$$

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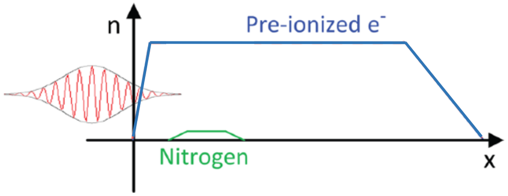
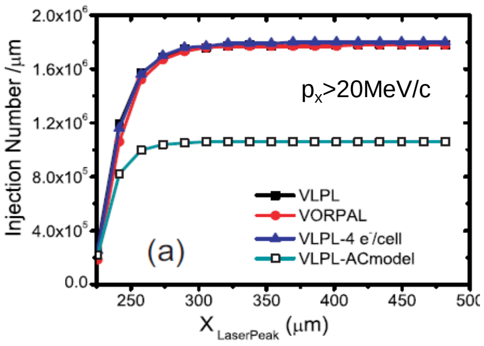
* M. Chen *et al.*, Phys. Plasmas 19 (2012), M. Chen *et al.*, J. Appl. Phys. 99 (2006)

**M. Chen *et al.*, AAC 2012, JCP 236 (2013)

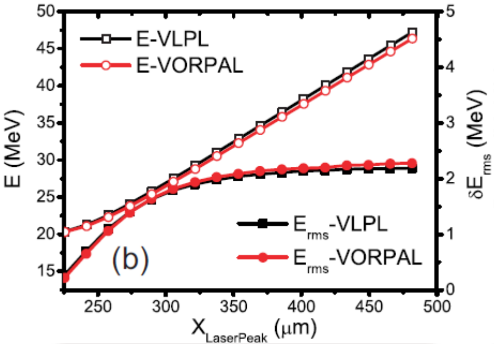
Benchmarking successful between Vorpal and VLPL on a case of ionization injection in LPA

- Nitrogen mixed to hydrogen gas is ionized by the laser field leading to trapping of electrons and acceleration by the plasma wakefield
- Successful benchmarking between Vorpal and VLPL*
- Benchmarked both trapping process and subsequent propagation and acceleration
- Optimization of LPA ionization injector now possible with Vorpal

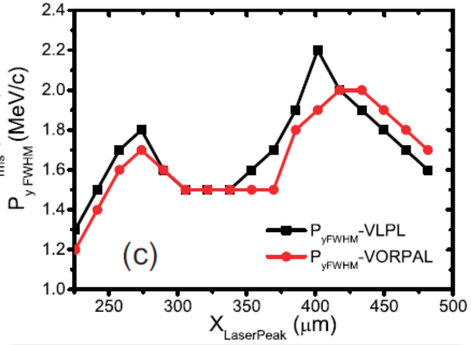




Injection number evolution



Energy and energy spread evolution



Transverse momentum spread evolution

🟥 VORPAL

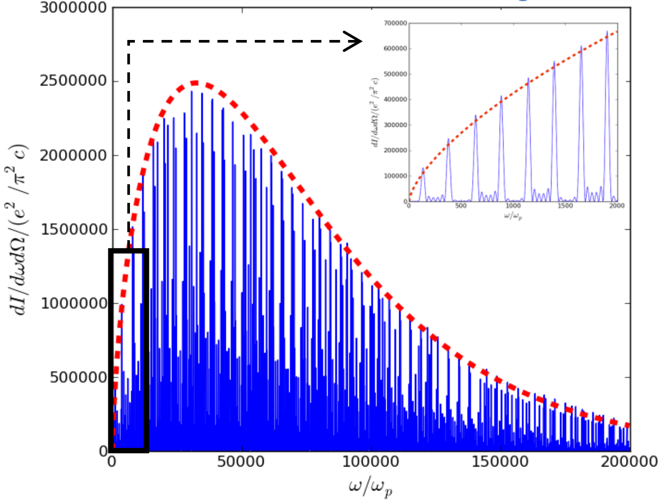
■ VLPL

* A. Pukhov, J. Pl. Phys. (1998)

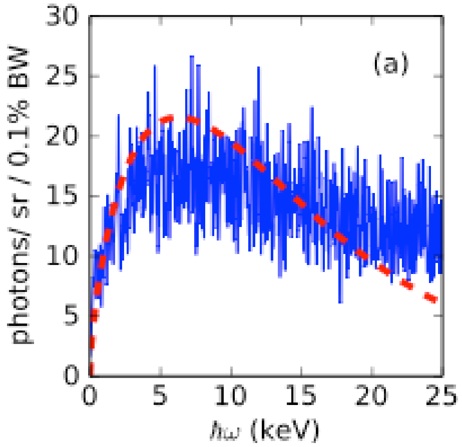
Post-processing allows calculation of X-ray spectrum due to e- betatron oscillation

- Post-processing analysis developed in Vorpal to calculate radiation spectrum from particles in betatron motion
- Benchmarked against theoretical spectrum (test particle in linear focusing field – Esarey *et al.* PRE 2002)
- Calculation of the spectrum from an accelerated electron beam in a focusing field
- Friction force due to emission of synchrotron radiation implemented in Vorpal

Spectrum on axis of an electron in betatron motion in linear focusing field



Spectrum from particle beam in linear focusing and accelerating fields



Talk highlights:

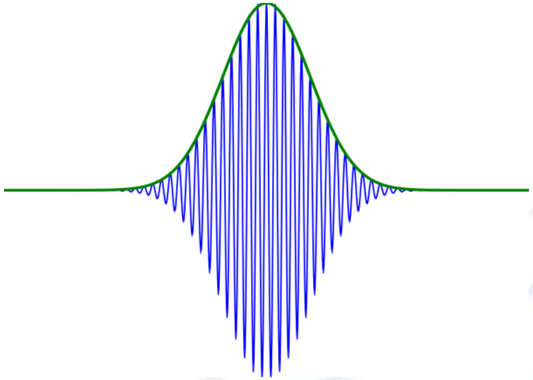
- Fundamentals of plasma acceleration and future experiments (5 mins)
- Learn about the basics of the FDTD technique and PIC simulation (10mins)
- Have an overview of the simulation software landscape (5 mins)
- Understand the source of common numerical instabilities. (10 mins)
- Find out about cutting edge techniques to improve accuracy (15 mins)
    - Quiet loading, enhanced loading
    - Vay push
    - Beam Frame Poisson Solve
    - Smoothing
    - Controlled (sometimes 'Perfect' Dispersion)
- Find out about cutting edge techniques to improve speed (10 mins)
    - Envelope models (with or without phase tracking) & QSA.
    - Boosted frame
- Learn about cutting edge dielectric acceleration algorithms
- If time allows… A few words on computational infrastructure requirements, visualisation and future direction. Benchmarking.
- THANK YOU FOR YOUR ATTENTION

SIMULATIONS EMPOWERING YOUR INNOVATIONS

Speedup trick: Envelope models

Theoretical details

- Major difficulty of explicit PIC simulations is the need to resolve laser wavelength
  - Makes Δ*x* very small ⇒ large grid size
  - Small Δ*x* dominates Courant limit on time step, making Δ*t* very small ⇒ many time steps required
  - Introduced $1/\lambda^2$ dependence of computation time from longitudinal resolution alone
- Trick: Model the envelope of the laser field instead of the fast oscillations



Relativistic ponderomotive force

- If the laser is modeled by its envelope, how do we advance particles?
  - Reducing envelope to electromagnetic fields requires moving particles through laser oscillations ⇒ oscillations must be resolved
  - So we need to average over fast oscillations
- First define the envelope $\tilde{\mathbf{A}}$ of the transverse vector potential:

$$\mathbf{A}_\perp = \mathrm{Re}\left[\tilde{\mathbf{A}} e^{i(\omega t - k_0 x)}\right]$$

where ω is the laser angular frequency and $k_0 = \omega/c$

Ponderomotive force:
Average Lorentz factor justification

- Motion is relativistic, so to average the motion we need average γ
- Look at the “quiver energy” of the particles from the fast oscillations:

$$\mathbf{p}_\perp = -q\mathbf{A}_\perp \Longrightarrow \langle \gamma^2 \rangle = \left\langle 1 + \frac{\left| -q\,\mathrm{Re}\left[\tilde{\mathbf{A}} e^{i(\omega t - k_0 x)} \right] \right|^2}{m^2c^2} \right\rangle = 1 + \frac{q^2 \left| \tilde{\mathbf{A}} \right|^2}{2m^2c^2}$$

$$\bar{\gamma} = \sqrt{1 + \frac{\left| \bar{\mathbf{p}} \right|^2}{m^2c^2} + \frac{q^2 \left| \tilde{\mathbf{A}} \right|^2}{2m^2c^2}}$$

- Add this to the averaged momentum $\bar{\mathbf{p}}$:

Ponderomotive force expression

- The laser field creates an effective “potential” for the plasma particles
- Adds ponderomotive force to Lorentz force:

$$\frac{d\bar{\mathbf{p}}}{dt} = q(\bar{\mathbf{E}} + \bar{\mathbf{v}} \times \bar{\mathbf{B}}) - \frac{q^2}{4\bar{\gamma}m} \nabla |\tilde{\mathbf{A}}|^2$$

(bars denote averaged quantities)

Envelope evolution

- To evolve the laser envelope, start with equation for vector potential in Coulomb or Lorenz gauge

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} = \mu_0 \mathbf{J}$$

$$\left.\begin{aligned} \tau &= t \\ \xi &= x - ct \end{aligned}\right\} \Longrightarrow \left\{\begin{aligned} \partial_t &= \partial_\tau - c\partial_\xi \\ \partial_x &= \partial_\xi \end{aligned}\right.$$

- Approximate: Envelope varies much slower than fast laser oscillation
- Transform to speed-of-light Galilean frame to apply approximation

Envelope evolution: Light frame

- Transformed equation for vector potential:

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial\tau^2} - \frac{2}{c}\frac{\partial}{\partial\tau}\frac{\partial}{\partial\xi} - \nabla_\perp^2\right)\mathbf{A} = \mu_0\mathbf{J}$$

- Next, apply envelope definition $\mathbf{A}_{\Re} = \mathrm{Re}(\tilde{\mathbf{A}} e^{-ik_0 x})$ to obtain

$$\frac{1}{c^2}\frac{\partial^2\tilde{\mathbf{A}}}{\partial\tau^2} - \frac{2}{c}\frac{\partial}{\partial\tau}\left(\frac{\partial\tilde{\mathbf{A}}}{\partial\xi} - ik_0\tilde{\mathbf{A}}\right) - \nabla_\perp^2\tilde{\mathbf{A}} = \mu_0\tilde{\mathbf{J}}$$

- Approximate: Envelope evolves slowly in light frame, so drop first term

$$\boxed{\frac{2}{c}\frac{\partial}{\partial\tau}\left(\frac{\partial\tilde{\mathbf{A}}}{\partial\xi} - ik_0\tilde{\mathbf{A}}\right) + \nabla_\perp^2\tilde{\mathbf{A}} = -\mu_0\tilde{\mathbf{J}}}$$

Envelope evolution: Oscillating current

- To determine the linear relationship between $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{J}}$, use the averaged Lorentz factor:

$$\tilde{\mathbf{p}} = -q\tilde{\mathbf{A}} \implies \tilde{\mathbf{v}} = -\frac{q\tilde{\mathbf{A}}}{\bar{\gamma} m}$$

- Sum up currents from ensemble of particles, with ρ_i the charge density of the ith particle:

$$\tilde{\mathbf{J}} = \left(-\sum_i \frac{q\rho_i}{\bar{\gamma}_i m} \right) \tilde{\mathbf{A}}$$

- We can then define the plasma susceptibility:

$$\chi = \mu_0 \sum_i \frac{q\rho_i}{\bar{\gamma}_i m}$$

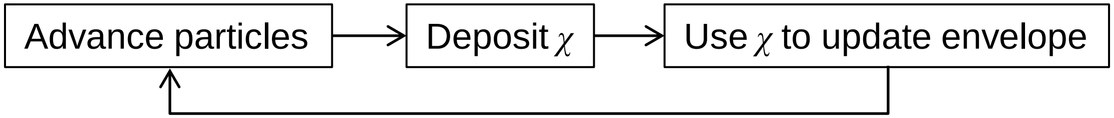
Note that this corresponds to the square of the local plasma wavenumber, $k_p{}^2$.

Envelope update

- Final envelope evolution equation:

$$\left[\frac{2}{c}\frac{\partial}{\partial\tau}\left(\frac{\partial}{\partial\xi}-ik_0\right)+\nabla_\perp^2\right]\tilde{\mathbf{A}}=\chi\tilde{\mathbf{A}}$$

- The envelope update cycle:



Advance particles

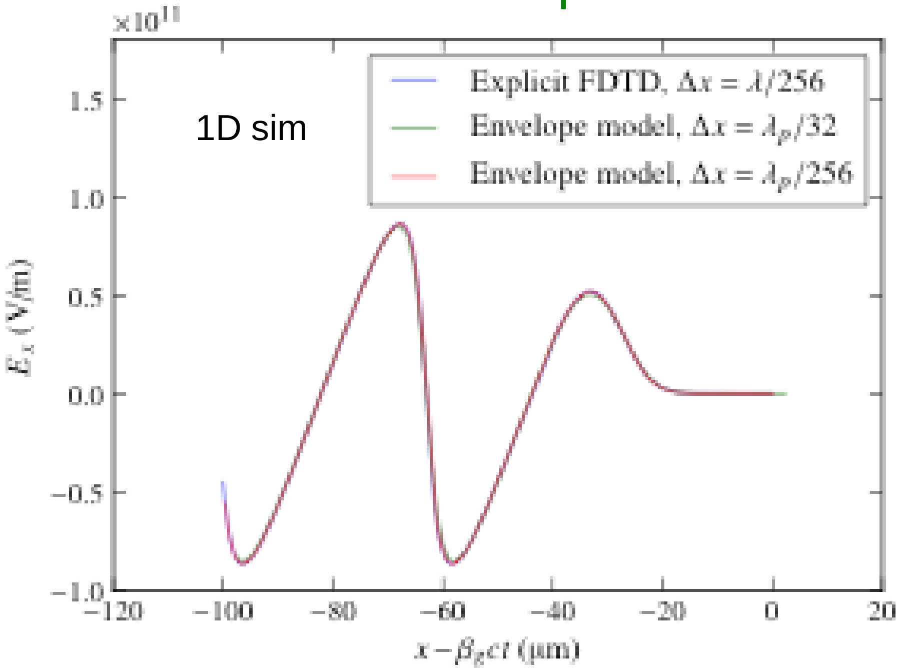
Deposit χ

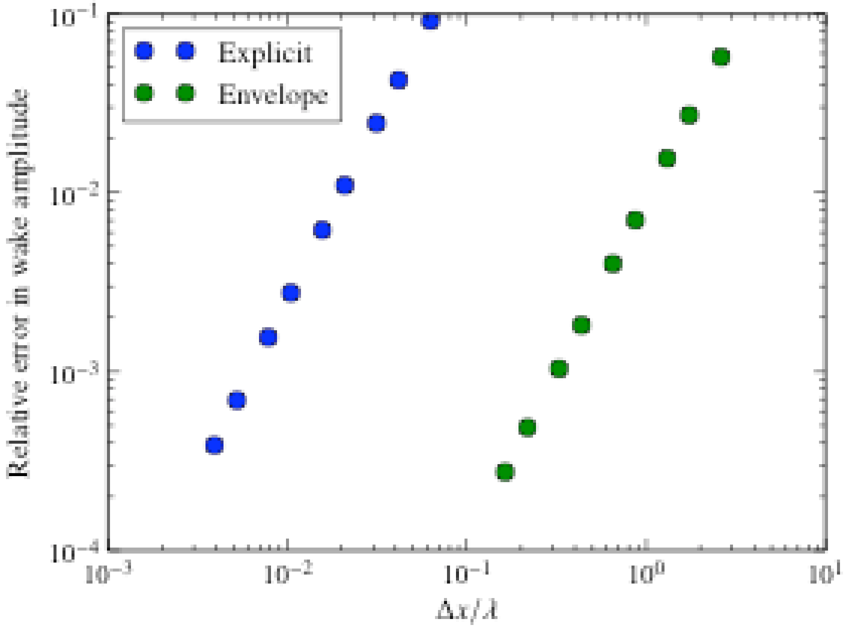
Use χ to update envelope

- Implicit solve required to update envelope
- Use of χ gives self-consistent behavior

Envelope sanity check: Convergence

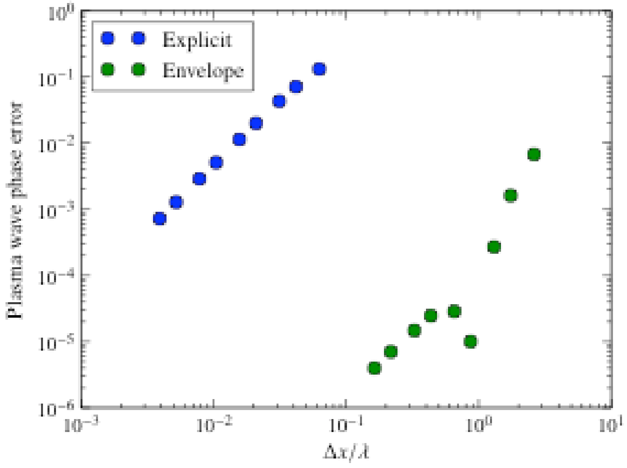
- Does the envelope model exhibit second-order error?
- Look at wake amplitude and phase in 1D
- $n = 10^{24}$, $a_0 = 2.0$, matched pulse length
- Obtained quadratic convergence in amplitude

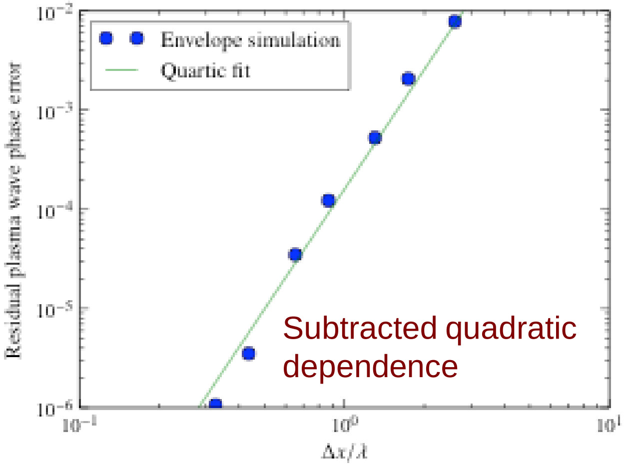




Phase convergence

- Used wakefield zero-crossing to determine phase, correcting for dump time
- Phase exhibits quadratic convergence at high resolution
- Quartic dependence dominates at low resolution





Subtracted quadratic dependence

Dispersion relation and group velocity

- Transform to speed-of-light frame phase-space coordinates (ω', k_x'): $\omega' = \omega - ck_x$, $k_x' = k_x - k_0$; let $k' = \omega'/c$
- Define parameter k_1 for matched spot in channel by

$$k_1^2 = k_p^{(0)2} + \frac{2}{w_y^2} + \frac{2}{w_z^2}$$

- Can then find dispersion relations and group velocities:

$$\text{Exact Maxwell:} \quad k' = \sqrt{(k_0 + k_x')^2 + k_1^2} - (k_0 + k_x'), \qquad \beta_g' = \left(1 + \frac{k_1^2}{k_0^2}\right)^{-1/2} - 1$$

$$\text{Envelope:} \quad k' = \frac{k_1^2}{2(k_0 + k_x')}, \qquad \beta_g' = -\frac{k_1^2}{2k_0}$$

- These expressions agree to 2nd order in k_1/k_0

Envelope models can improve group velocity

- Explicit FDTD has numerical dispersion: Look at wave propagating along *x* axis

$$\frac{1}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right)=\frac{1}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right)$$

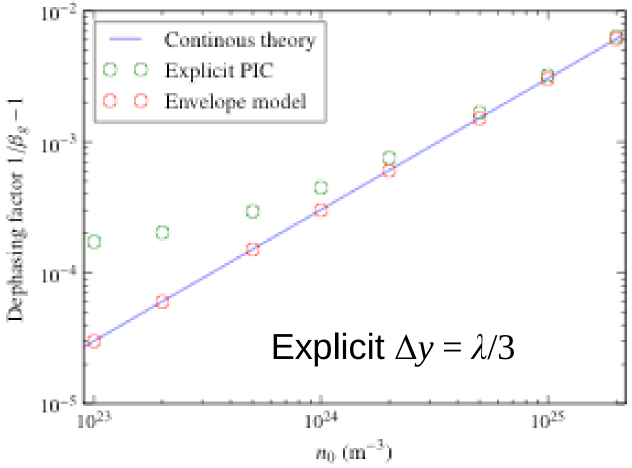
- Group velocity $< c$ unless $c\Delta t = \Delta x$, which is prohibited in > 1D
- Look at envelope equation in vacuum with no transverse variation:

$$\frac{2}{c}\frac{\partial}{\partial\tau}\left(\frac{\partial}{\partial\xi}-ik_0\right)\tilde{\mathbf{A}}=0$$

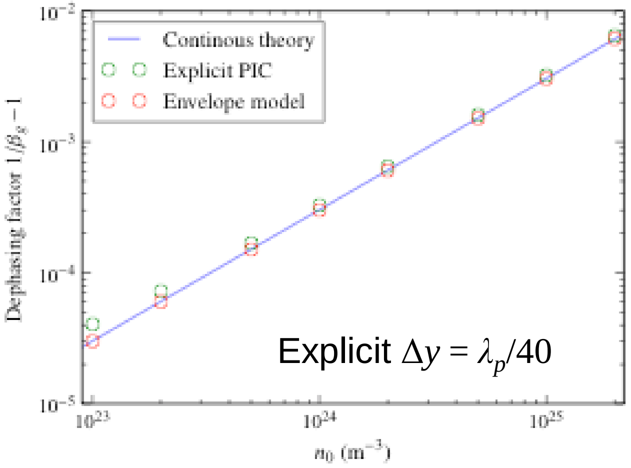
- $\partial/\partial\tau = 0 \Rightarrow$ pulse moves at speed of light

Group velocity test: Linear propagation in plasma channel

- 2D simulation: $k_pL = 1$, $w_0 = \lambda_p$, $a_0 \ll 1$ for linearity
- Observed numerical dephasing error for both FDTD and envelope, for range of densities
- Envelope: $\Delta x = \Delta y = \lambda_p/40$; explicit: $\Delta x = \lambda/24$



Explicit $\Delta y = \lambda/3$



Explicit $\Delta y = \lambda_p/40$

- Other techniques exist for numerical-dispersion-free propagation along an axis

Envelope model speedup

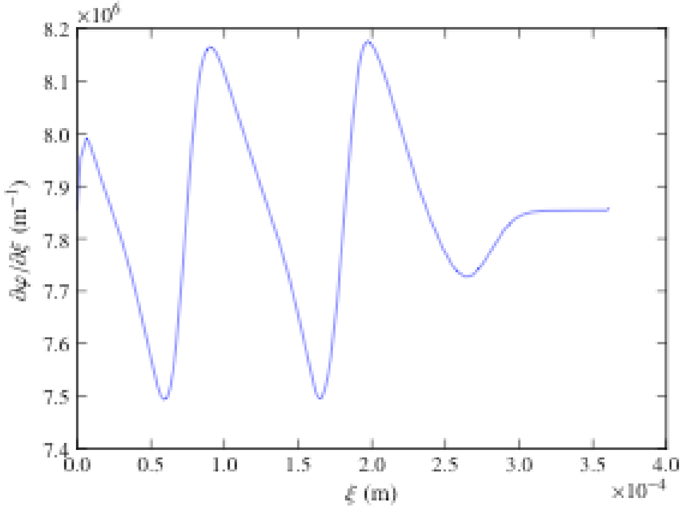
- Meter-scale 3D run required 35,000 CPU hours
- Grid spacing: $\Delta x = 2.1\ \mu\text{m}$, $\Delta y = \Delta z = 2.6\ \mu\text{m}$
- Grid size: 176 x 252 x 252
- Grid too small to massively parallelize ⇒ used 144 cores
- ~660,000 time steps required; run took ~10 days
- But it’s possible!
- 5 orders of magnitude speedup over explicit FDTD

Solution to spectral limitation: Track phase of laser field

- Model envelope with arbitrary longitudinal phase variation

$$A_z = \mathrm{Re}\left[ae^{i\varphi(\tau,\xi)}\right]$$

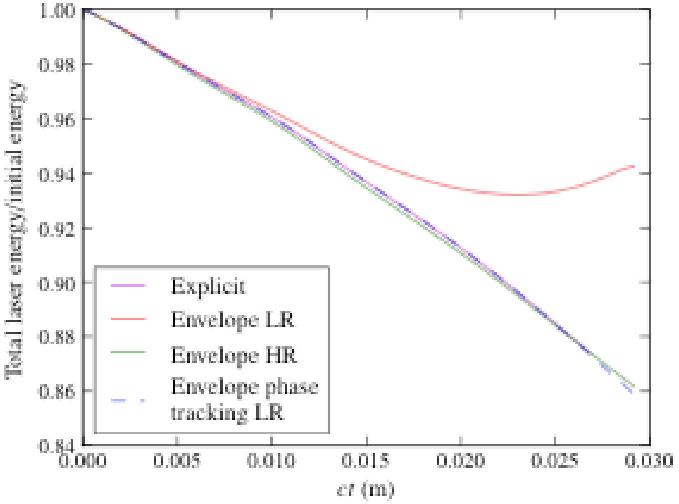
- Here φ is an arbitrary scalar function; does not vary transversely
- Phase remains smooth even when complex components oscillate



Phase tracking solves the problem

- Compared phase-tracked envelope at low resolution to explicit FDTD and original envelope at low and high resolution
  - Used total laser energy benchmark: known to indicate problem
  - Phase-tracked envelope matches known well-resolved cases

- We can now resolve the laser field over an entire meter-scale stage using the envelope model



Envelope models: References

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