Laser-Plasma Simulations with the Computational Framework VORPAL

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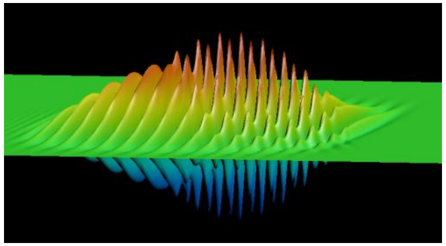
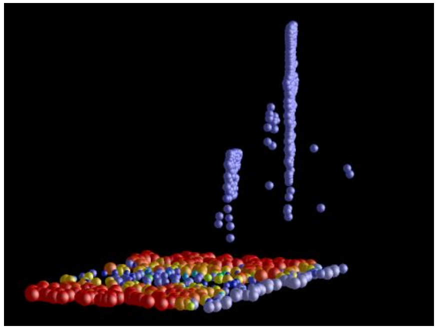
PIC and related algorithms in VORPAL for laser-plasma simulations

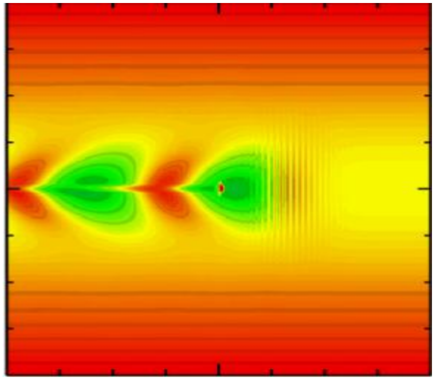
- Successfully applied to various LWFA problems
  - Geddes et al, PRL 100, 215004 (2008).
  - Nemeth et al., PRL 100, 095002 (2008)
  - Cary *et al*., Phys. Plasmas (2005), invited.
  - Geddes *et al.,* Nature 431, 538 (2004).
- Implements:
  - relativistic, electromagnetic time-explicit PIC and fluid
  - Lorentz-boosted simulations in 1-2D
  - Ponderomotive guiding center (PGC) PIC or “envelope” model
- Features include:
  - High-order spline-based particle shapes (up through 5^{th})
  - PML (perfectly matched layer) absorbing boundaries
  - Fluid methods; hybrid PIC/fluid
  - Cut cells (embedded boundaries) for rf cavity simulations
  - Impact & field ionization; secondary e- emission
  - Electrostatic PIC, binary collision models
- Framework for FDTD with particles and Cartesian meshes
  - Parallel (general domain decomposition) or serial
  - Cross-platform (Linux, AIX, OS X, Windows)
  - 1D, 2D, 3D; combine algorithms at run-time
- VORPAL development team
  - about 30 developers; >10 active at any time
  - software version control; branching; nightly regression tests
- Leveraged via SBIR funds: DOE, AFOSR, NASA, OSD



Colliding laser pulses

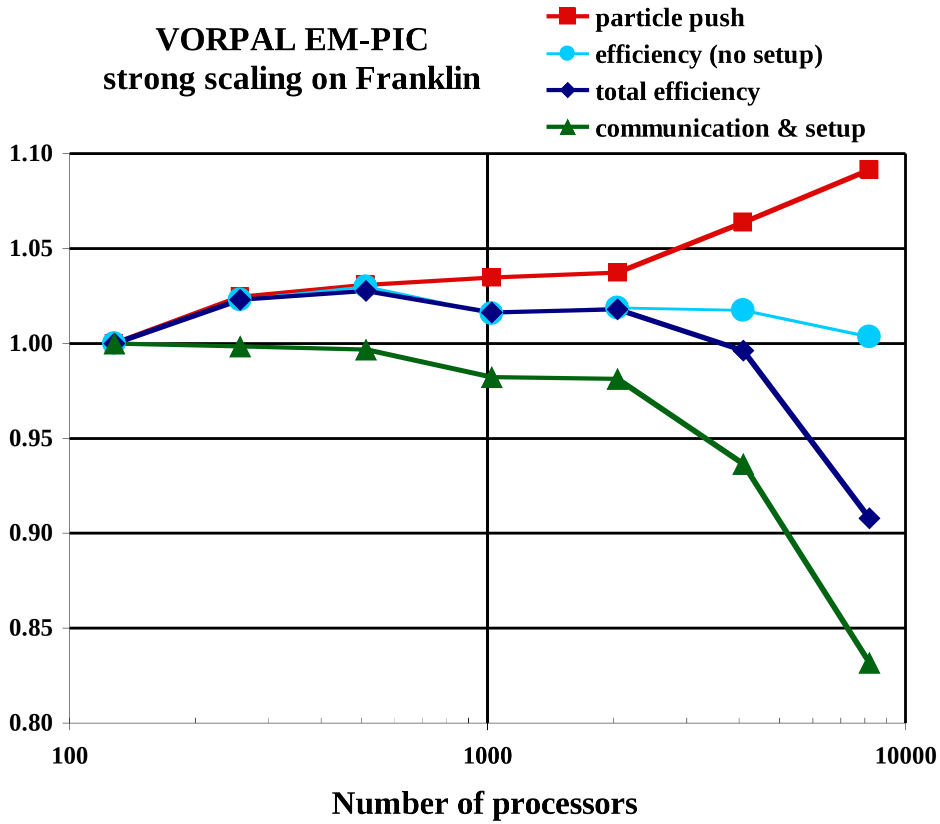


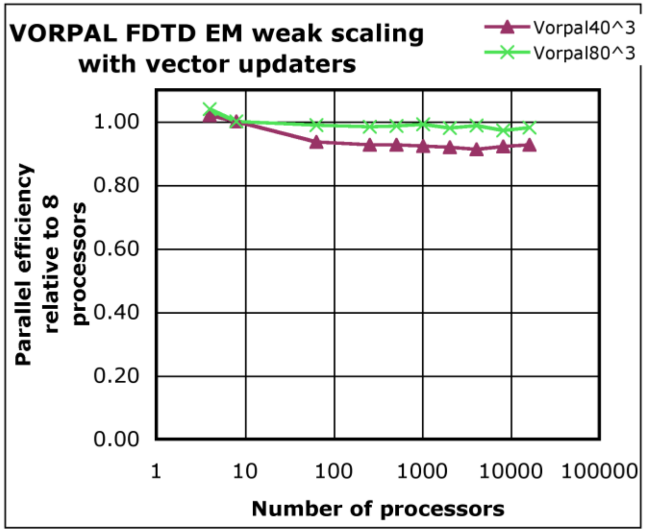
Particle beams



Hybrid Fluid-PIC

VORPAL shows excellent scaling on ~10^4 processors for both weak & strong cases





* pure EM scales well also
* efficient field I/O via parallel HDF5 requires equal domain sizes
* I/O not included in these plots

* thermal plasma plus relativistic beam; electromagnetic PIC
  – 512 x 256 x 512 = 67 x 10^6 cells; ~1x10^9 particles
* efficiency ~100% out to 8,192 proc's, for long simulations
  – particle push (dominates run time) speeds up by 10%
  – approx. balanced by communication overhead
  – for >4,096 proc's, set up time becomes significant

Laser-plasma motivation for new algorithm development in VORPAL

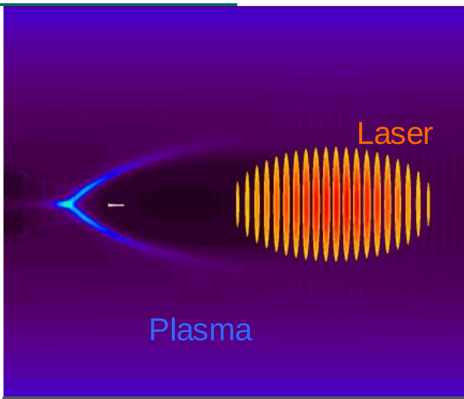
- Higher-energy beams require longer interaction lengths
- Time-explicit simulations must resolve the 0.8 μm laser wavelength
- for GeV scale simulations:

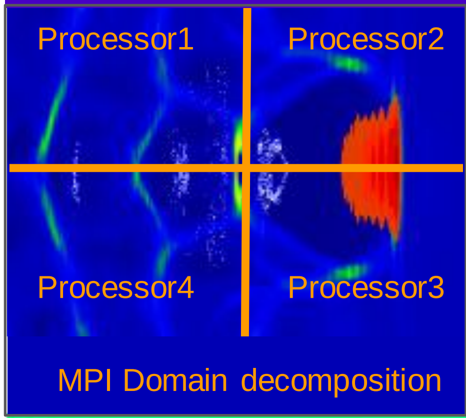
in space over 100 μm^3 requires	~ 200Mcell
interaction length ~3 cm	~ 1 Mstep
few particles / cell	~ Gparticle, TB

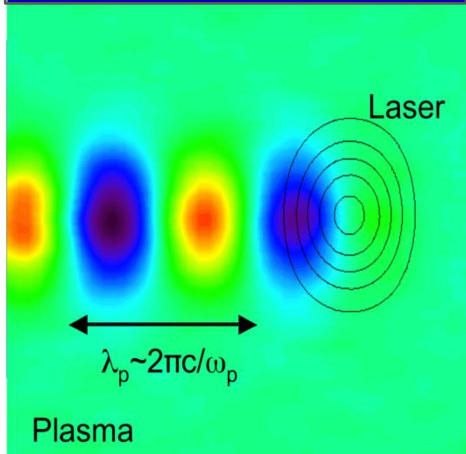
- Hundreds of simulations in 2D - exploration (khours)
- 3D simulations on 4000+ processors - quantitative (MHour)

- Need to simulate m-scale interaction lengths for ~10 GeV
- Accurate kinetics to resolve beam quality

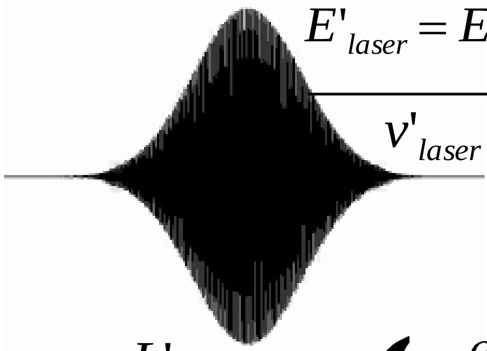
- Three approaches
  - scale all physical quantities to plasma wavelength
    - increase density, shorten interaction length
  - envelope model or PGC PIC (no laser wavelength)
    - saves >100x in cost; requires benchmarking
  - Lorentz boosted frame







Optimal Lorentz Frame offers Enormous Speed-up

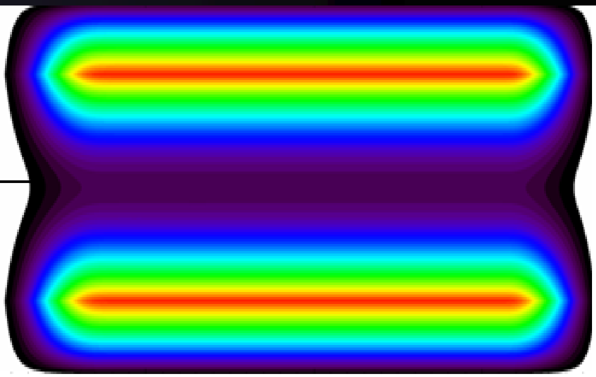


$$E'_{laser} = E_{laser}/\gamma_{boost}(1+\beta_{boost})$$

$$v'_{laser} = c$$

$$L'_{env} = \gamma_{boost}(1+\beta_{boost})L_{env}$$

$$\lambda' = \gamma_{boost}(1+\beta_{boost})\lambda$$



$$v'_{plasma} = -\beta_{boost}c$$

$$L'_{plasma} = L_{plasma}/\gamma_{boost} \qquad n_e' = \gamma_{boost} n_e$$

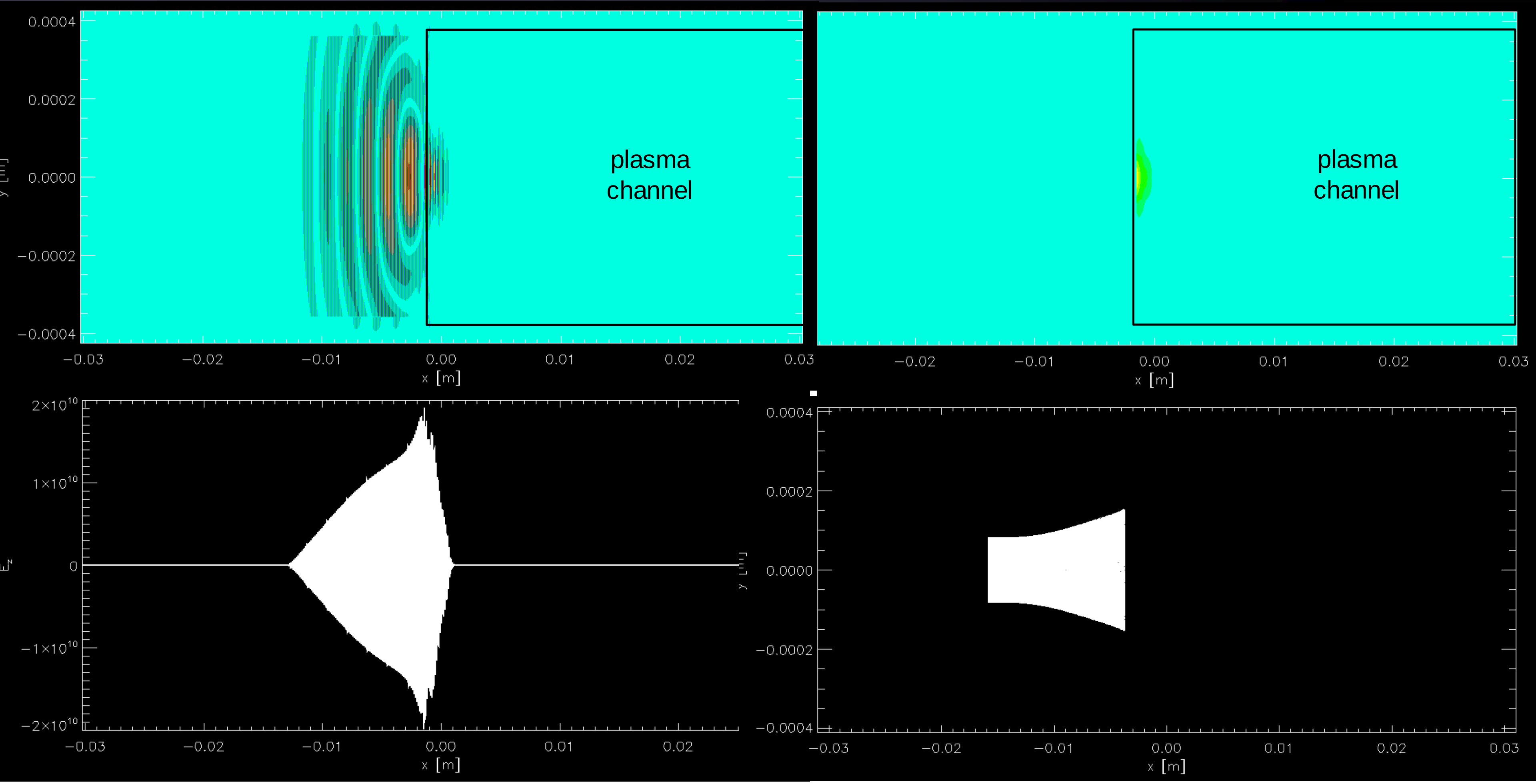
- **Lorentz transform laser pulse into right-moving frame**
  - vacuum velocity is still *c*; # of wavelengths is invariant
- **In boosted frame, plasma is Lorentz contracted**
  - n_e increases; integrated density is constant
- **N_{cells} is invariant**
- **$N'_{steps} \sim N_{steps}/2\gamma^2_{boost}$**
  - this is the idealized speedup

e^- 

$$v'_{beam} = \beta'_{beam}c$$

$$\gamma_{beam} \approx \gamma_{boost}(1+\beta_{boost})\gamma'_{beam}$$

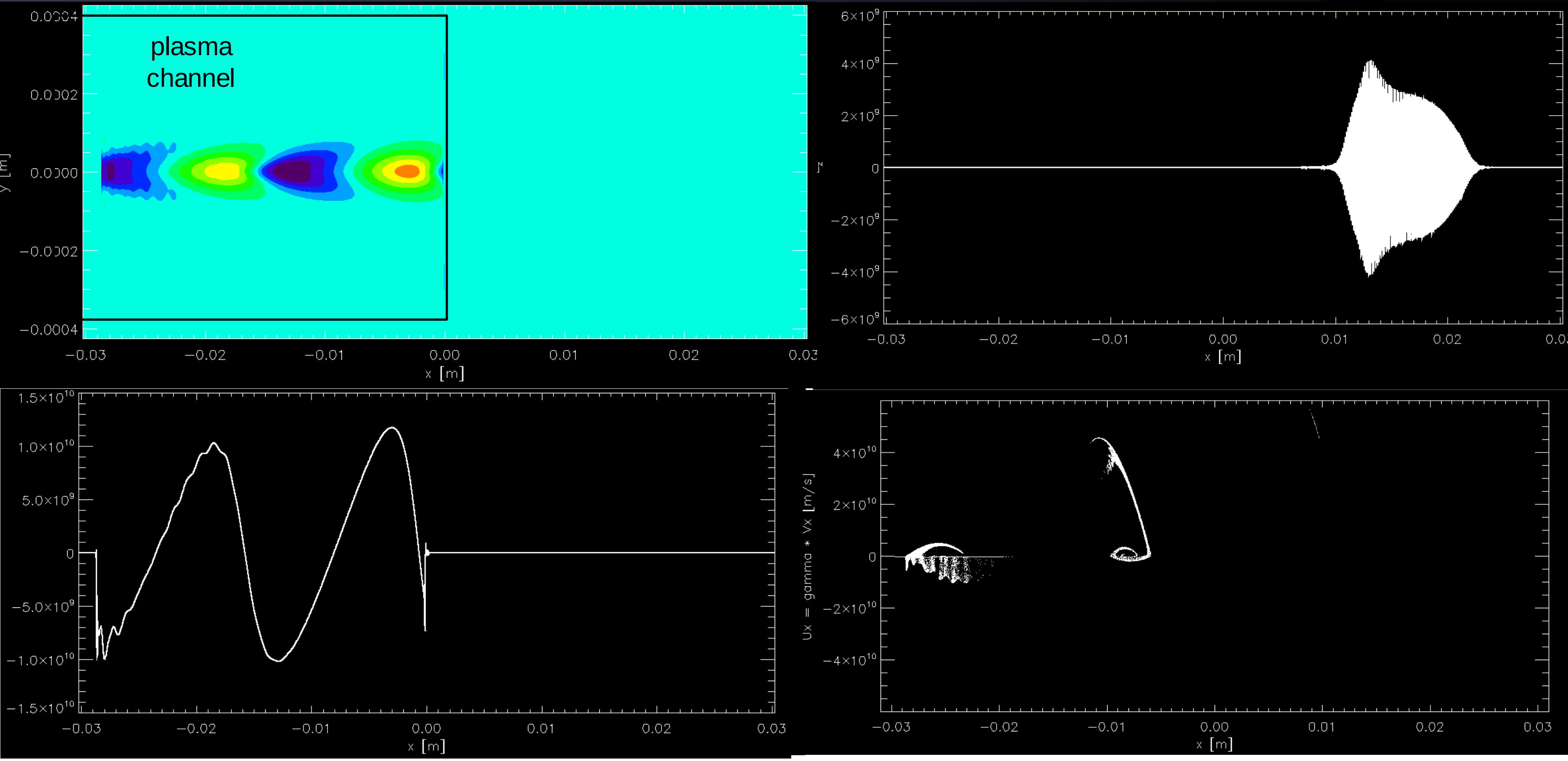
Start of a 2.4 m boosted-frame simulation



n_e=6 x 10^{16} cm^{-3}; L_{deph}~2.4 m; a_0=1; E_{final}~11 GeV

Higher transverse resolution required to suppress noise

End of a 2.4 m boosted-frame simulation



No moving window; laser & plasma cross paths;
More testing required to understand limits of the method

Initial boosted-frame results show ~10,000x speed-up is possible

- **very promising approach**
  - enables previously impossible simulations
  - can dramatically speed-up present simulations
  - we hope to pursue this further
- **implementation is not ready for practical use**
  - need to better understand the noise
  - must be careful to resolve physics in the
  - need to implement more infrastructure
    - transforming fields & particles between frames
    - generalize boosted-frame pulse launcher to 3D
  - benchmark with density-scaled simulations

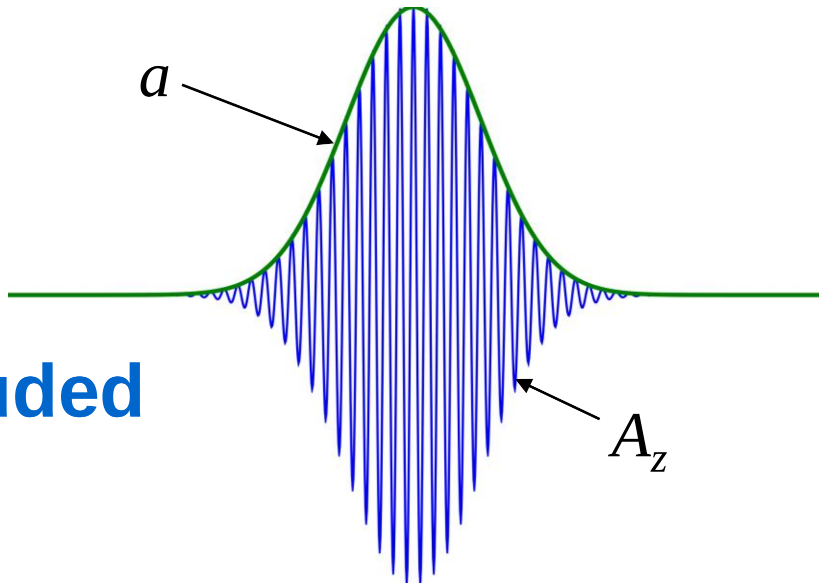
The ponderomotive guiding center (PGC) or "laser envelope" algorithm

- **Introduce the speed-of-light frame coordinate system (τ, ξ):** $\tau = t,\ \xi = x - ct$
- **We model the complex envelope *a* of the oscillating laser vector potential A, so that**

$$A_z = \mathrm{Re}\left[a e^{i(\omega t - k_0 x)}\right] = \mathrm{Re}\left[a e^{-ik_0\xi}\right]$$

- **Equation of motion:**

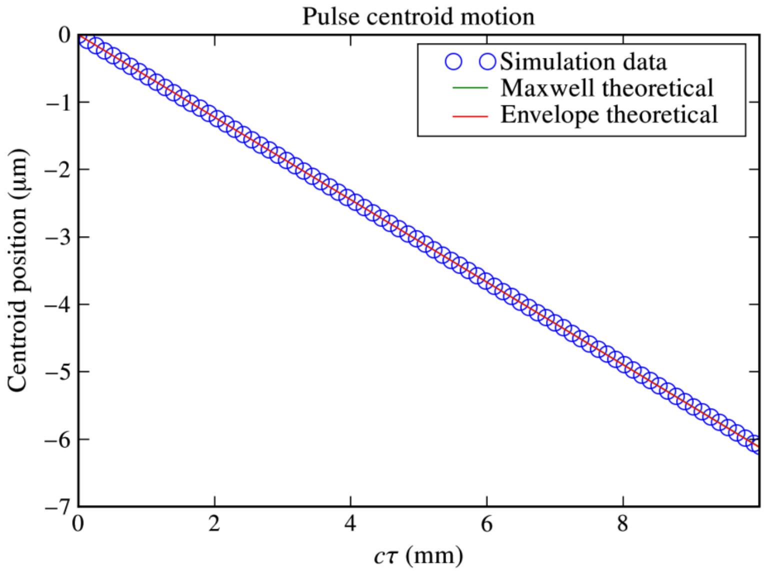
$$\left[\frac{2}{c}\frac{\partial}{\partial\tau}\left(\frac{\partial}{\partial\xi} - ik_0\right) + \nabla_\perp^2\right]a = -\mu_0 \chi a$$

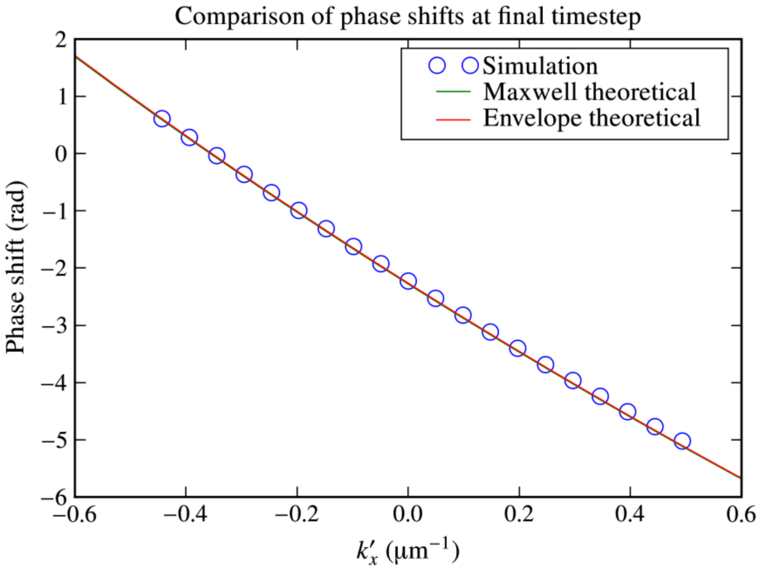


- **Ponderomotive force included in particle push**

Group velocity and dispersion check

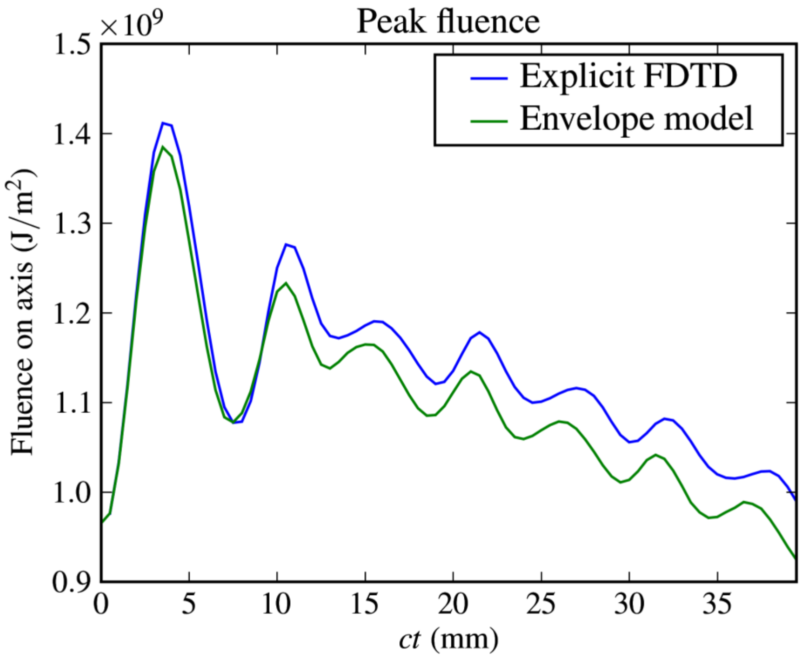
- Very good agreement among envelope simulation and envelope & explicit theory
- No group velocity error due to grid dispersion





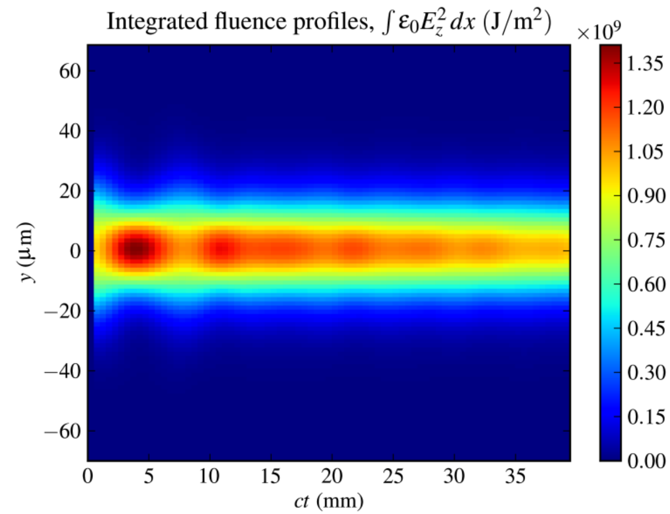
Good comparison with time-explicit PIC for experimental parameters

- **2D, scaled 10 GeV parameters**
  - $n_0 = 10^{24}\ \mathrm{m}^{-3}$; $a_0 = 1$

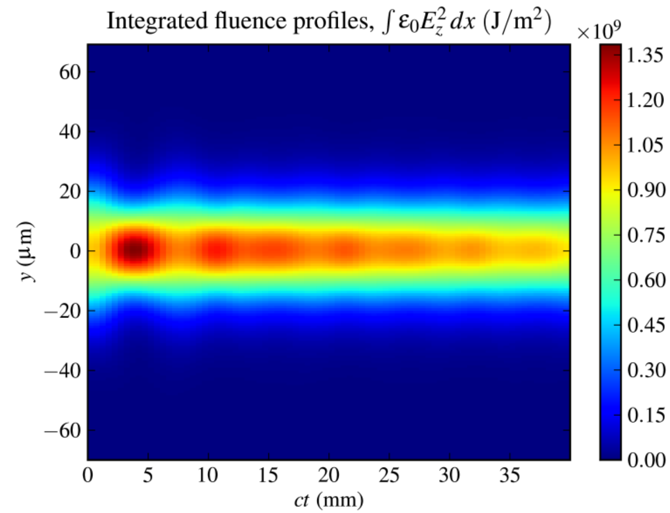


Envelope model captures main features of self-focusing oscillations; slight mismatch in amplitude; 18x speedup

explicit PIC

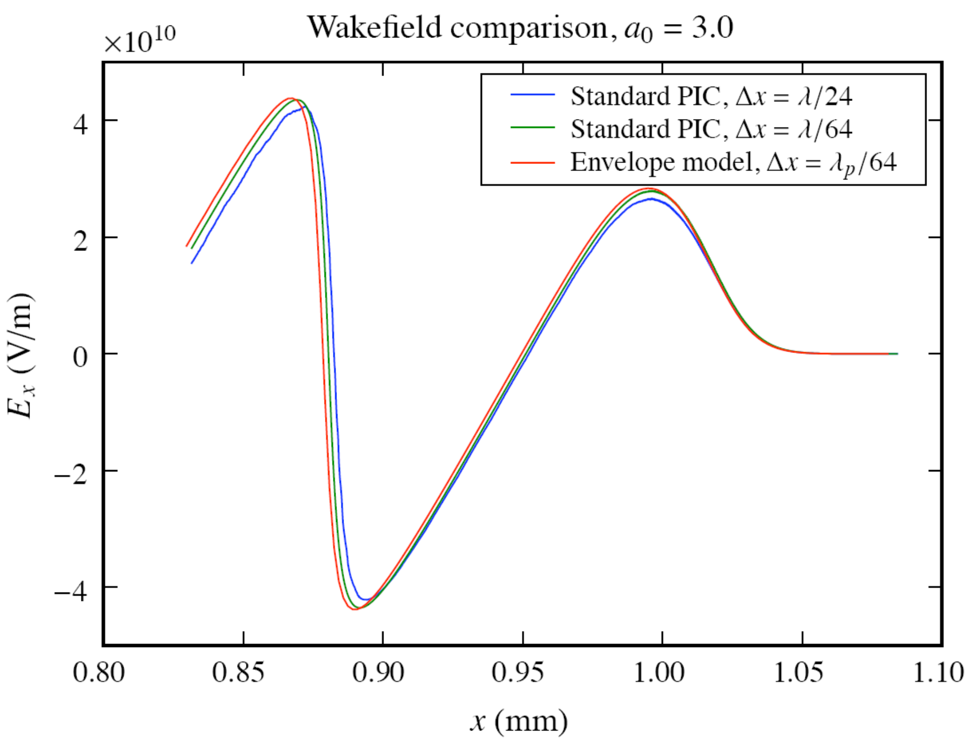


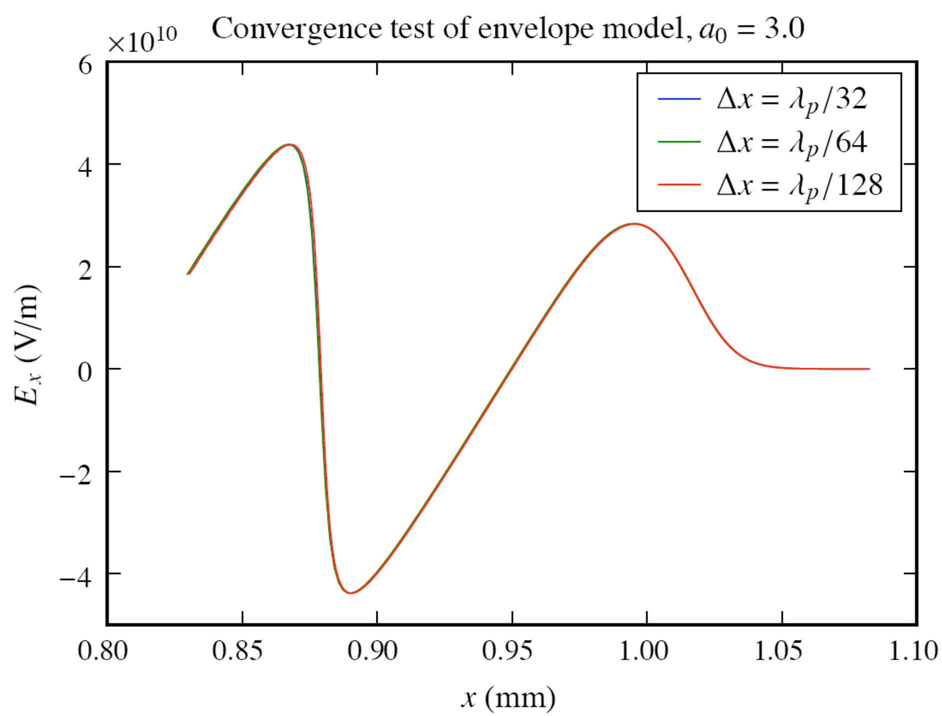
envelope



1D comparison of plasma wake for a_0=3

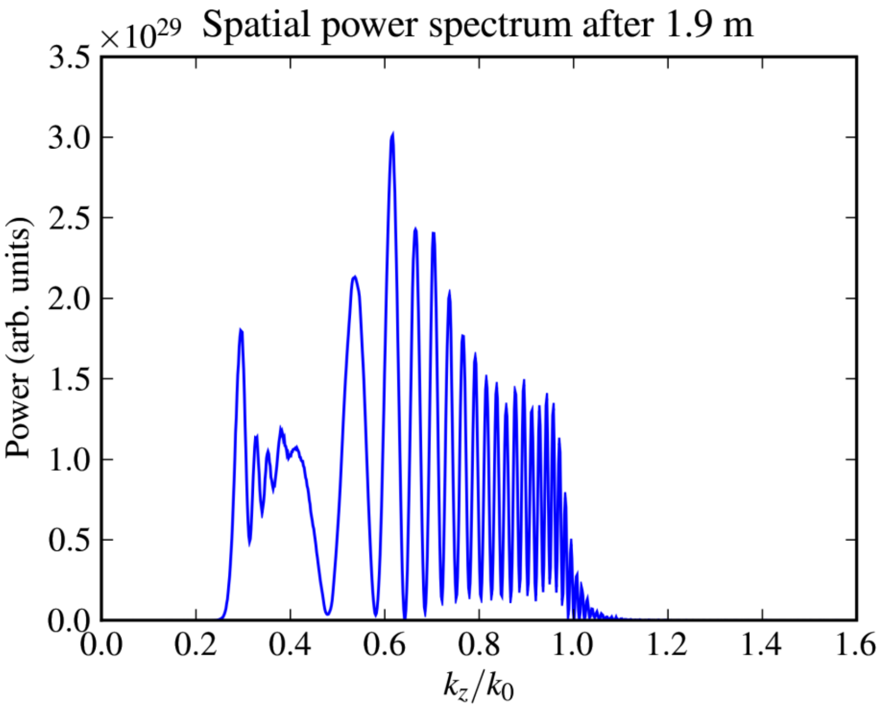
- **Envelope model is converged at $\Delta x=\lambda_p/32$**
- **Time-explicit PIC not converged until $\Delta x=\lambda_0/64$**





Pump depletion → spectral broadening (red shifting), and limits envelope model

- **We have ideas for improvements**
  - however, any envelope model breaks at some point before the laser pulse is fully depleted



Preserving low emittance → low noise

- **Higher-fidelity simulations & noise reduction**
  - High-order particle shapes
    - splines for current deposition & force interpolation
    - 1st-order is standard “area weighting”
  - Current smoothing
  - Higher resolution
  - Fluid representation of the plasma is quiet
- **Cold, relativistic charged fluid model in VORPAL**
  - eliminates particle noise → no kinetic effects
  - Cartesian FDTD implementation is uniquely powerful
    - handles vacuum interfaces, large aspect-ratio cells
    - serial or parallel; 1D, 2D, 3D; other VORPAL features
    - hybrid mode with PIC, to include injected beams

Cold, relativistic fluid model in VORPAL

- **Eulerian, FDTD, Cartesian mesh**

$$\frac{\partial \mathbf{p}}{\partial t} + \nabla \cdot (\mathbf{p}\mathbf{v}) = qn\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right)$$
$$\frac{\partial n}{\partial t} + \nabla \cdot n\mathbf{v} = 0$$
$$\mathbf{p} = \gamma m n \mathbf{v}$$

$\longrightarrow$

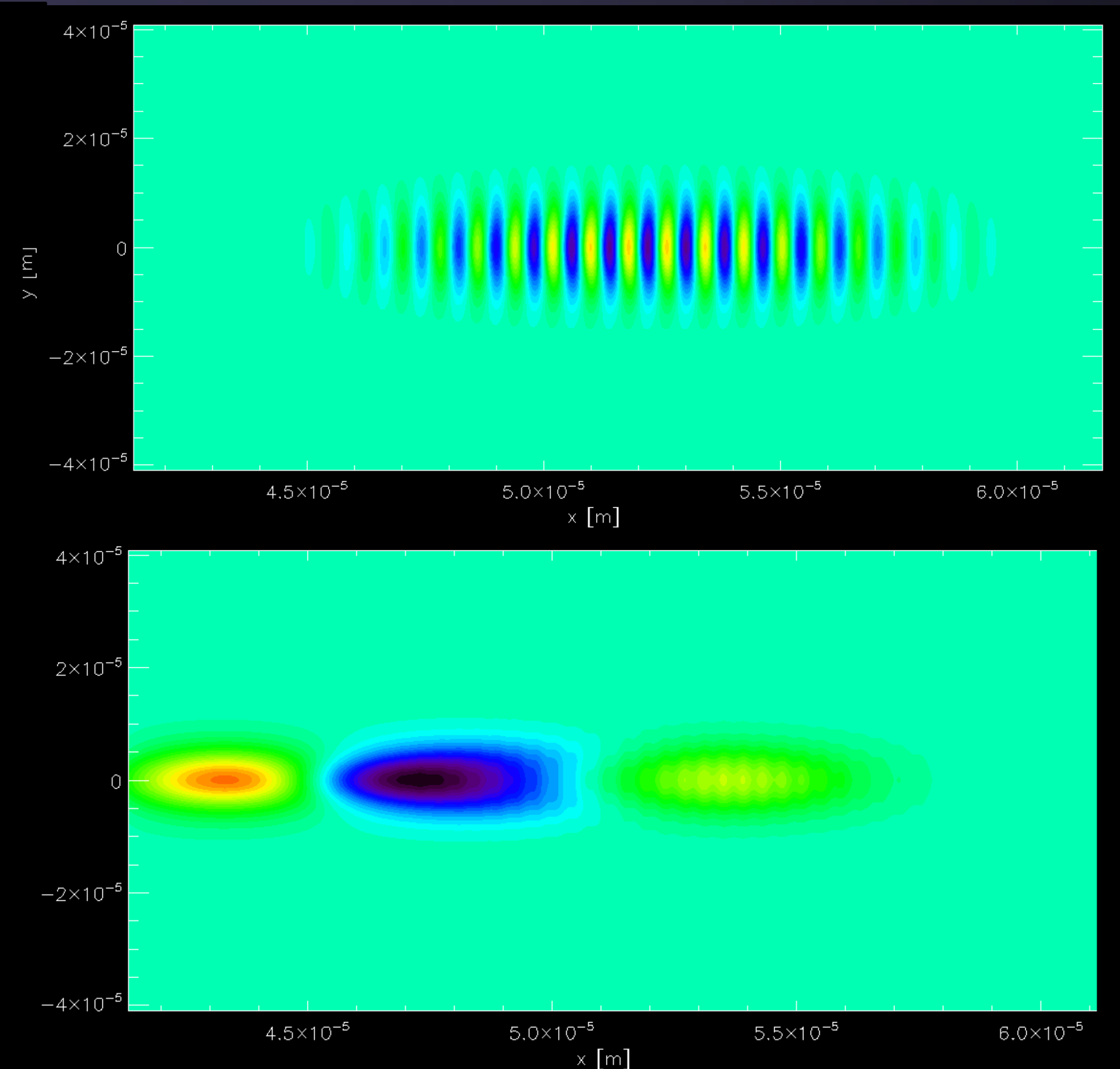
$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} = \frac{q}{m}\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right)$$
$$\mathbf{u} = \gamma \mathbf{v}$$

- **What's the trick?**
  - Handling vacuum interfaces:

    C. Nieter & J.R. Cary, 'VORPAL: a versatile plasma simulation code,' JCP (2004).

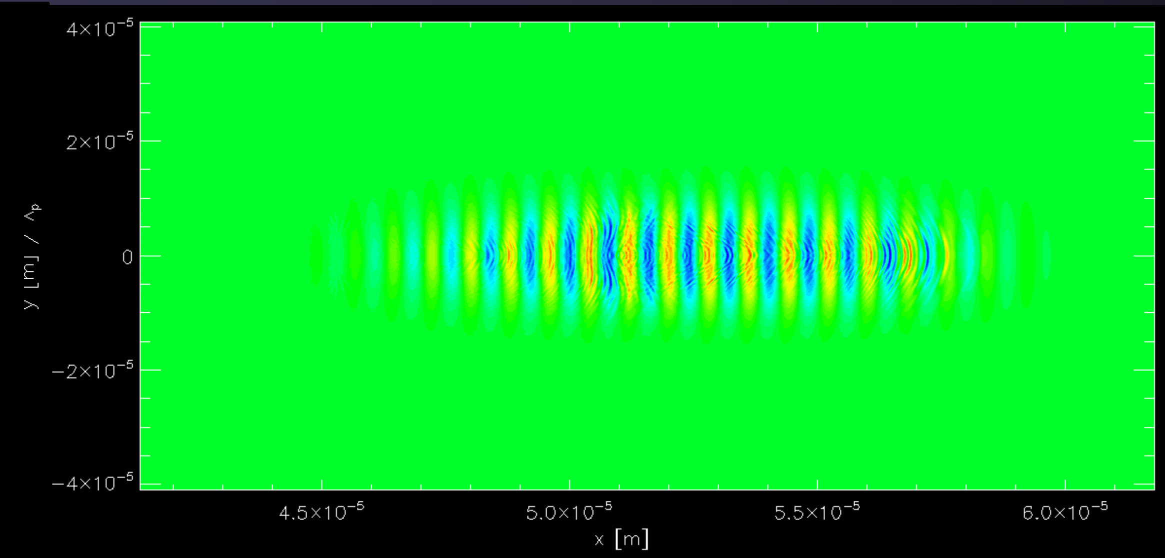
    - PIC-like treatment of momentum kick *a la* Boris
    - momentum is valid everywhere, even in vacuum
  - Recent modifications for 2nd-order accuracy
    - 2nd-order flux calculations (density is always 0th-order)
    - Stable 2nd-order momentum advection

2D VORPAL convergence & benchmarking; short laser pulse in uniform plasma, $a_0 = 1$

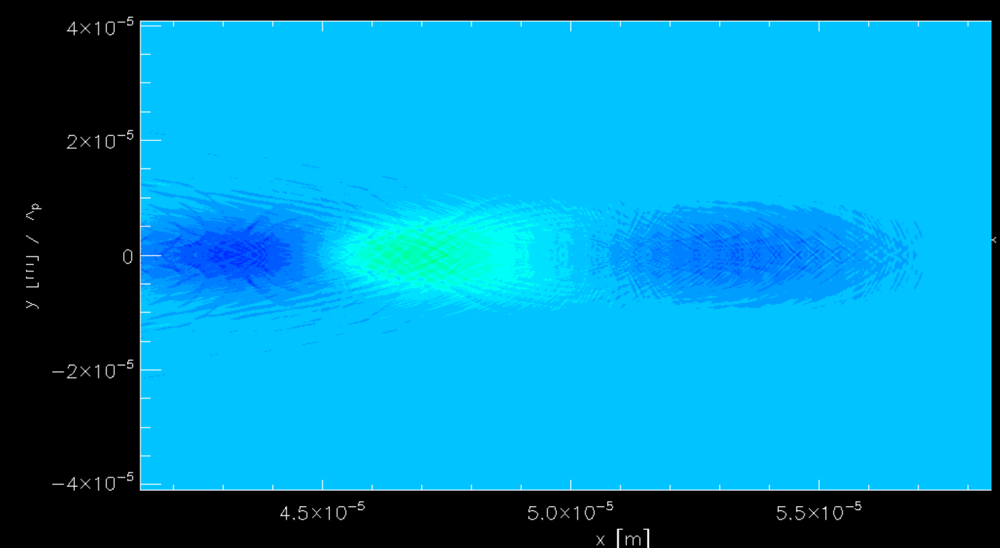


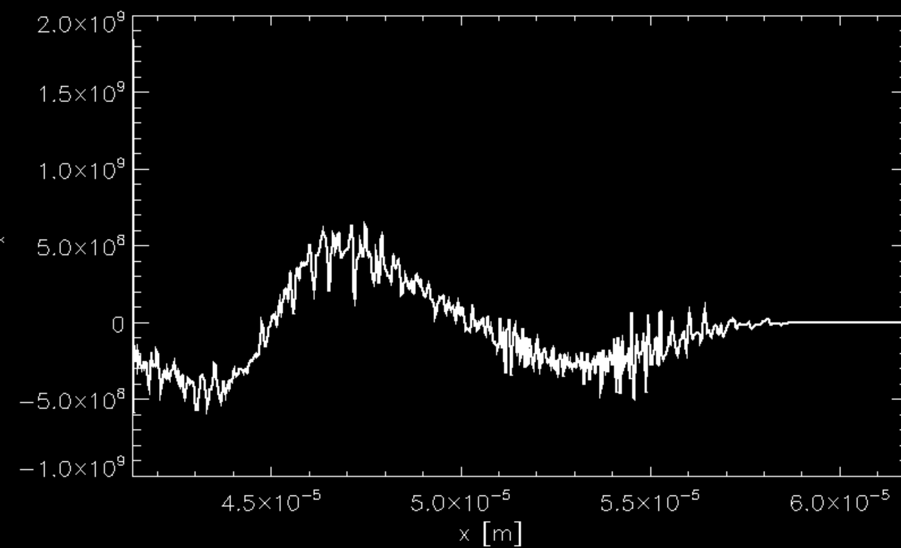
- **Laser E field along z out-of-plane (upper)**
- **Longitudinal plasma E field along x (lower)**
- n_e **= 1.4 x 10^19** cm^-3 ($n_e = 1.4 \times 10^{19}\ \mathrm{cm}^{-3}$)
- τ_{fwhm} **= 30** fs
- w_0 **= 8.2** μm
- λ_0 **= 0.8** μm
- λ_0/dx = 20,40,80,160
- dy/dx = 8
- 4 particles per cell
  - increased quadratically with res. for 1st-order

Comparison of 1st-order & 3rd-order spline particles shows noise for "area weighting"

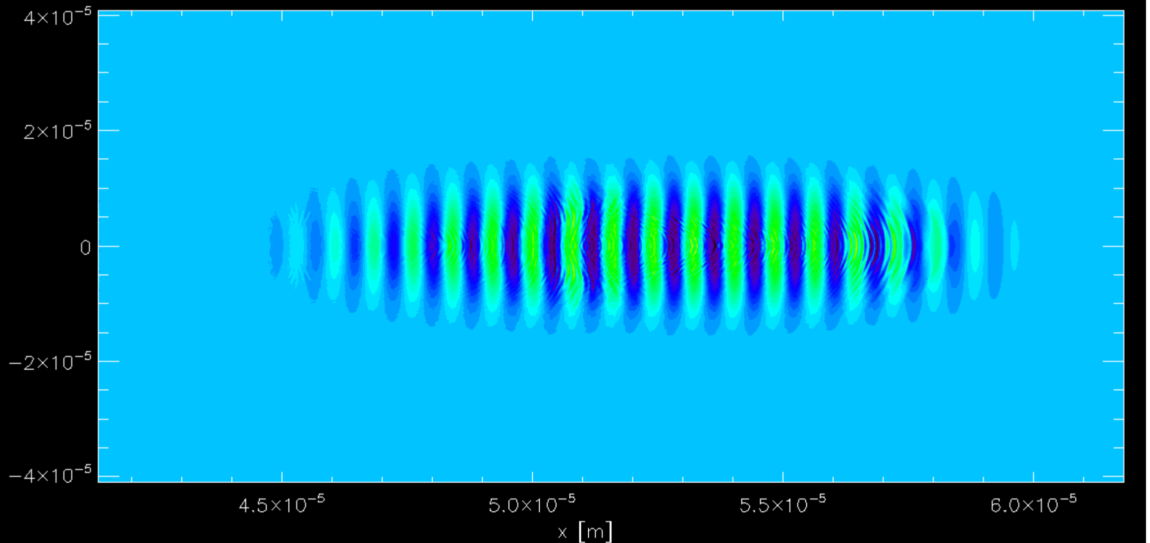


- **Laser E field differences** **(upper)**
- **Plasma wakefield differences** **(lower)**
- λ_0/dx=40

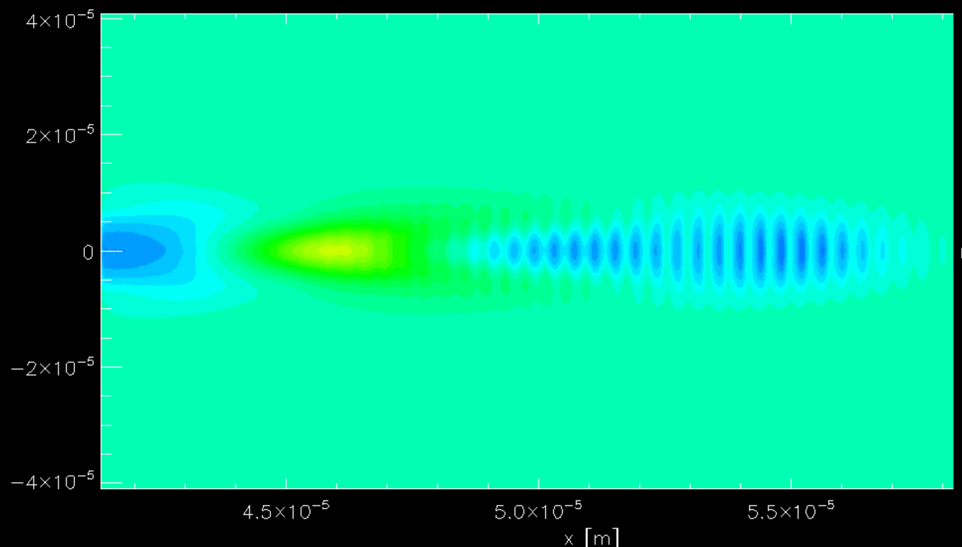


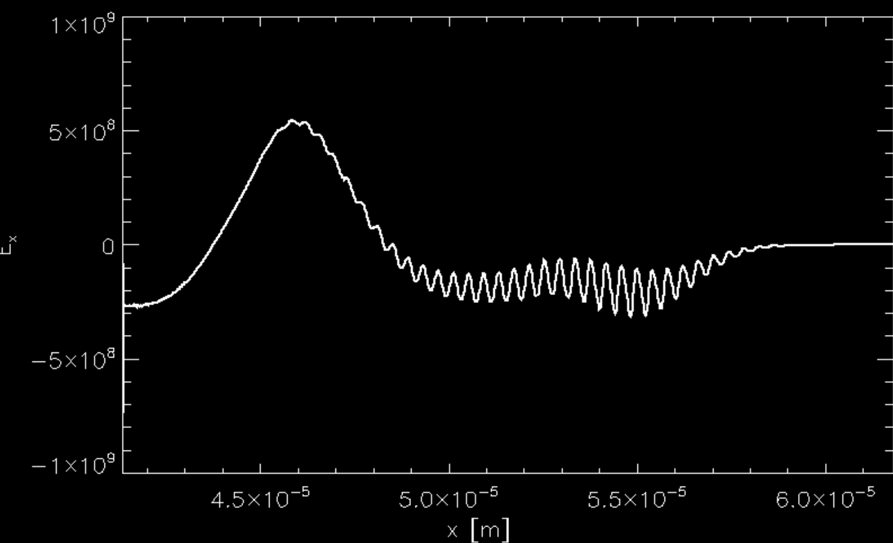


Comparison of fluid & 3rd-order PIC shows modest changes in the wake, low noise



- **Laser E field differences** (upper)
- **Plasma wakefield differences** (lower)
- $\lambda_0/dx=40$





All approaches converge with 2nd-order accuracy (quadratically with resolution)

- **Resolution is doubled along both axes (3 times)**
  – Run-time increases by 8x with each doubling

- 32x for area-weighting, because ptcls-per-cell must be quadrupled to prevent noise from dominating
- run-time scaling is 2x worse in 3D
- high cost in run-time buys 4x reduction in errors