Computational Techniques for Plasma Based Particle Acceleration*

T. Antonsen Jr,

Institute for Plasma Research

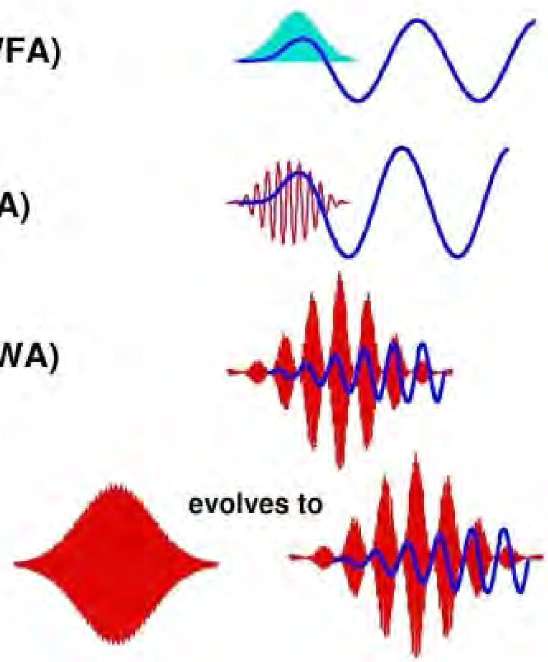
University of Maryland, College Park MD

Help: W. Mori, J. Palastro, S. Morshed, D. Gordon, S. Kalmykov, J-L Vay, B. Cowan, C. Geddes

*Supported by USDOE and NSF

Scope of Problem

- **Plasma Wake Field Accelerator(PWFA)**
  A high energy electron bunch
- **Laser Wake Field Accelerator(LWFA)**
  A single short-pulse of photons
- **Plasma Beat Wave Accelerator(PBWA)**
  Two-frequencies, i.e., a train of pulses
- **Self Modulated Laser Wake Field Accelerator(SMLWFA)**
  Raman forward scattering instability



- **Direct Acceleration in Modulated Channels**

Physical Processes

Important

- Relativistic Motion
- Plasma Wave Generation / Cavitation
- Laser Self Focusing / Scattering
- Ionization

Not Important

- Turbulence - most plasma particles interact for a short time, several plasma periods, then leave

  Our job is "relatively" easy.

Simulation has played an important role in the development of the field.

Guiding our understanding
Designing new experiments

Relevant Time Scales (LWFA)

- Laser Period λ =800 nm **T_L = 2.7 fs**
- Driver Duration ~ Plasma Period **T_D = 50 fs**
- Propagation Time (driver evolution, L= 1 cm) **$T_P = 3.3 \times 10^4$ fs**
  (driver evolution, L= 1 m) **$T_P = 3.3 \times 10^6$ fs**

> Propagation Time >> Driver Duration >> Laser Period
>
> **$T_P \gg T_D \gg T_L$**

- Disparity in time scales leads to both complications and simplifications

MODELS
APPROACHES / APPROXIMATIONS

• Laser		
	Full EM	- Laser Envelope
• Plasma		
	Particles	- Fluid
	Full Lorenz force	- Ponderomotive
	Dynamic response	- Quasi-static

Hierarchy of Descriptions

1. **Full Format Particle in Cell (PIC)**

    - Relativistic equations of motion for macro-particles
    - Maxwell's Equations on a grid
    - Most accurate but most computationally intensive

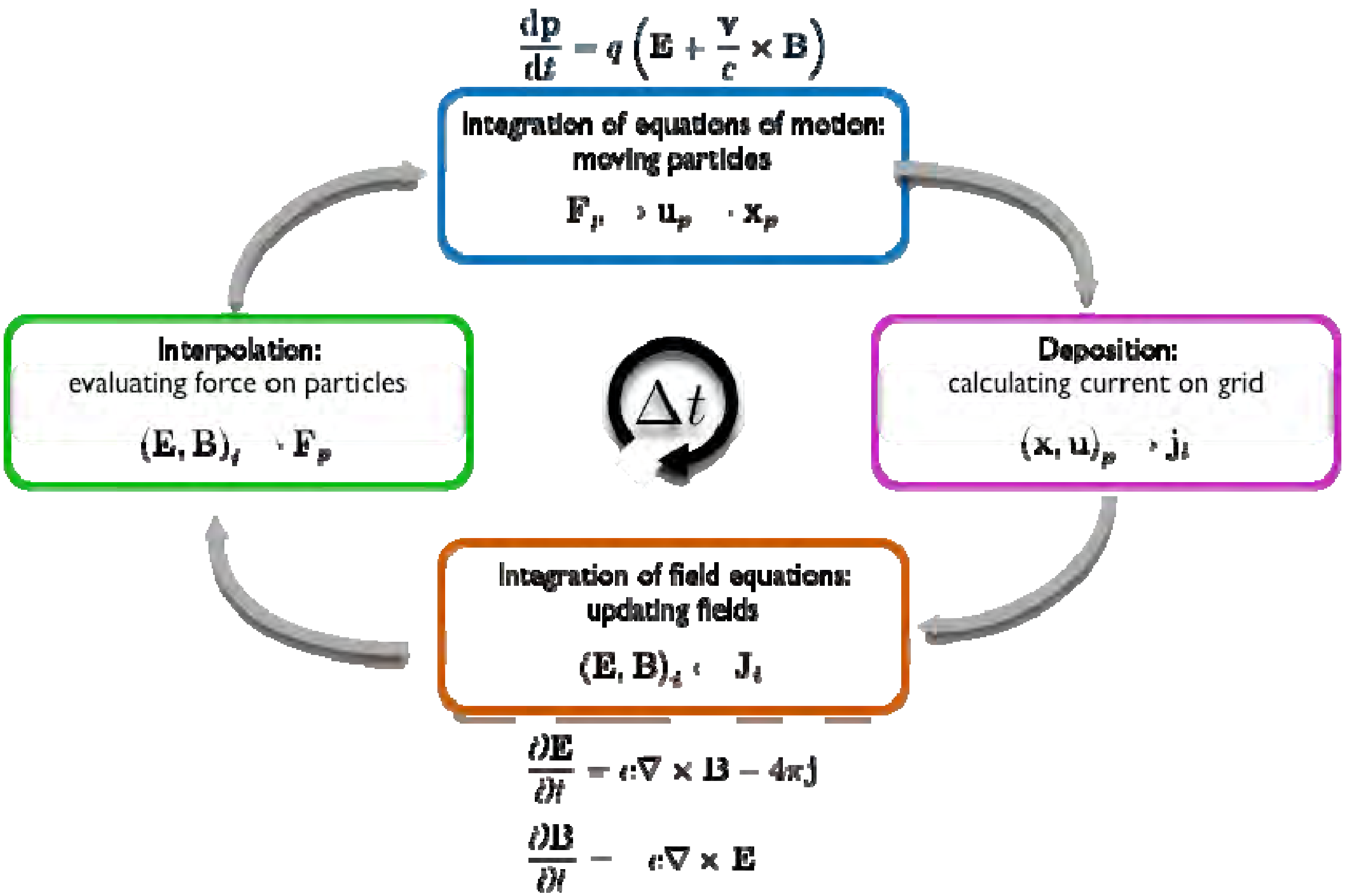
• **Laser**

Full EM	- Laser Envelope

• **Plasma**

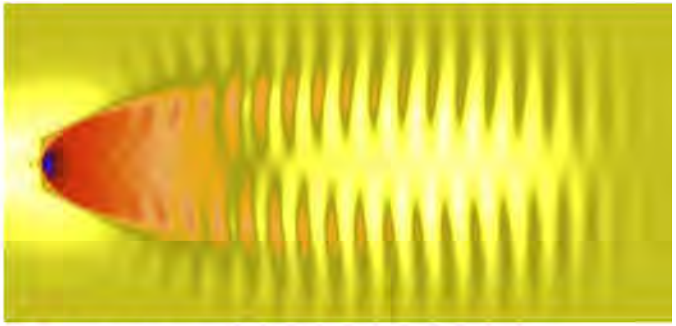
Particles	- Fluid
Full Lorenz force	- Ponderomotive
Dynamic response	- Quasi-static

Full Format: PIC Algorithm

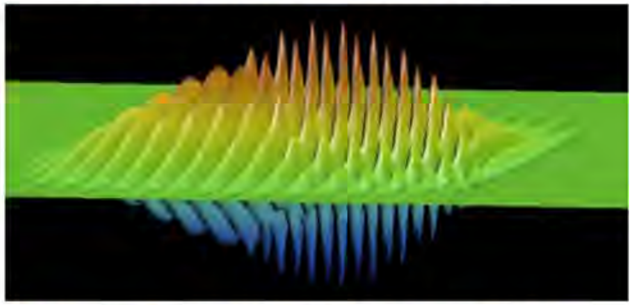


VORPAL provides state-of-the-art algorithms for laser-plasma simulations

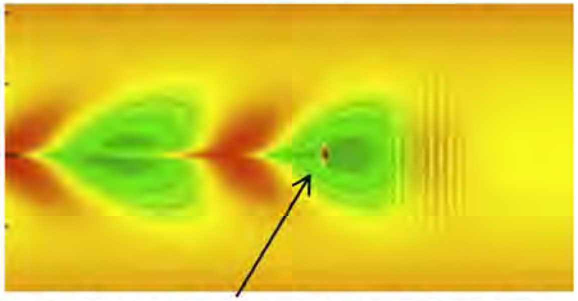
- Successfully applied to various LWFA problems:
  - C.G.R. Geddes *et al.*, in SciDAC Review (2009), to appear.
  - K.J. Wu *et al.*, in SciDAC Review (2009), to appear.
  - N. Hafz *et al.*, Nature Photonics **2**, 571 (2008).
  - C. Geddes *et al.*, Phys. Rev. Lett. **100**, 215004 (2008).
  - K. Nemeth *et al.*, Phys. Rev. Lett. **100**, 095002 (2008).
  - J.R. Cary *et al.*, Phys. Plasmas (2005), invited.
  - C. Geddes *et al.,* Nature **431**, 538 (2004).
  - C. Nieter & J.R. Cary, J. Comput. Phys. **196**, 448 (2004).
- Implemented algorithms include:
  - relativistic, electromagnetic time-explicit PIC and fluid
  - Lorentz-boosted simulations in 1D, 2D
  - Ponderomotive guiding center (PGC) PIC or “envelope” model
- Special features include:
  - High-order spline-based particle shapes (up through 5th)
  - PML (perfectly matched layer) absorbing boundaries
  - Tunneling-induced field ionization of H, He
- Parallel framework for particles and Cartesian meshes
  - Scales to >10,000 cores for production runs
  - 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



3D Laser wakefield accelerator



Obliquely colliding laser pulses



Fluid/PIC; e- bunch in channel

http://www.txcorp.com/products/VORPAL

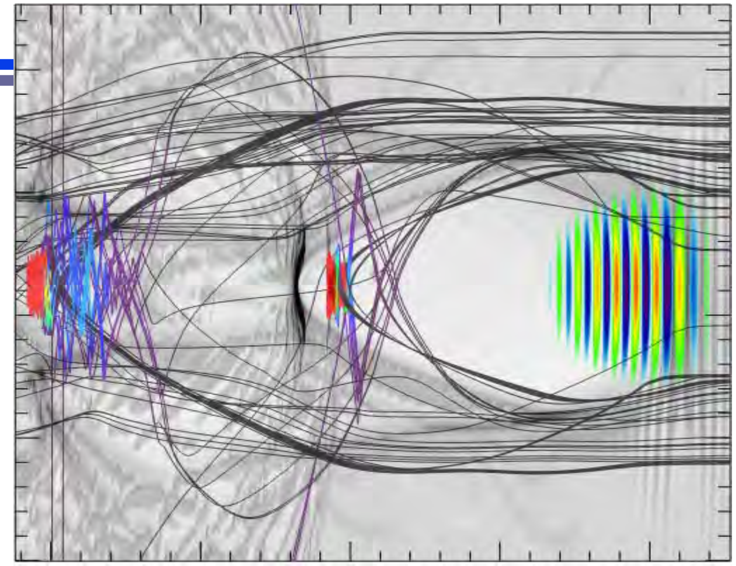
TECH-X CORPORATION

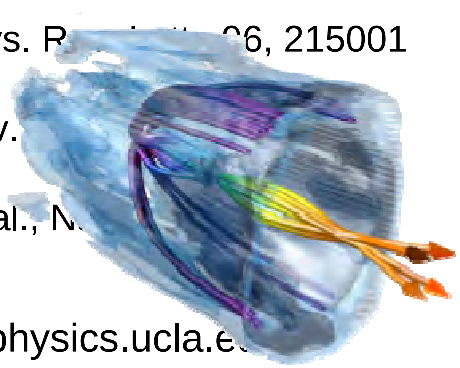
OSIRIS 2.0

osiris framework

- Massivelly Parallel, Fully Relativistic Particle-in-Cell (PIC) Code
- Visualization and Data Analysis Infrastructure
- Developed by the osiris.consortium: UCLA + IST
- Widely used: UCLA, SLAC, USC, Michigan, Rochester, IST, Imperial College, Max Planck Inst.

- Examples of applications
- Mangles et al., Nature 431 529 (2004).
- Tsung et al., Phys. Rev. Lett., 94 185002 (2004)
- Mangles et al., Phys. R[illegible]6, 215001 (2006)
- Lu et al., Phys. Rev. [illegible] (2007)
- I.A. Blumenfeld et al., N[illegible] (2007)





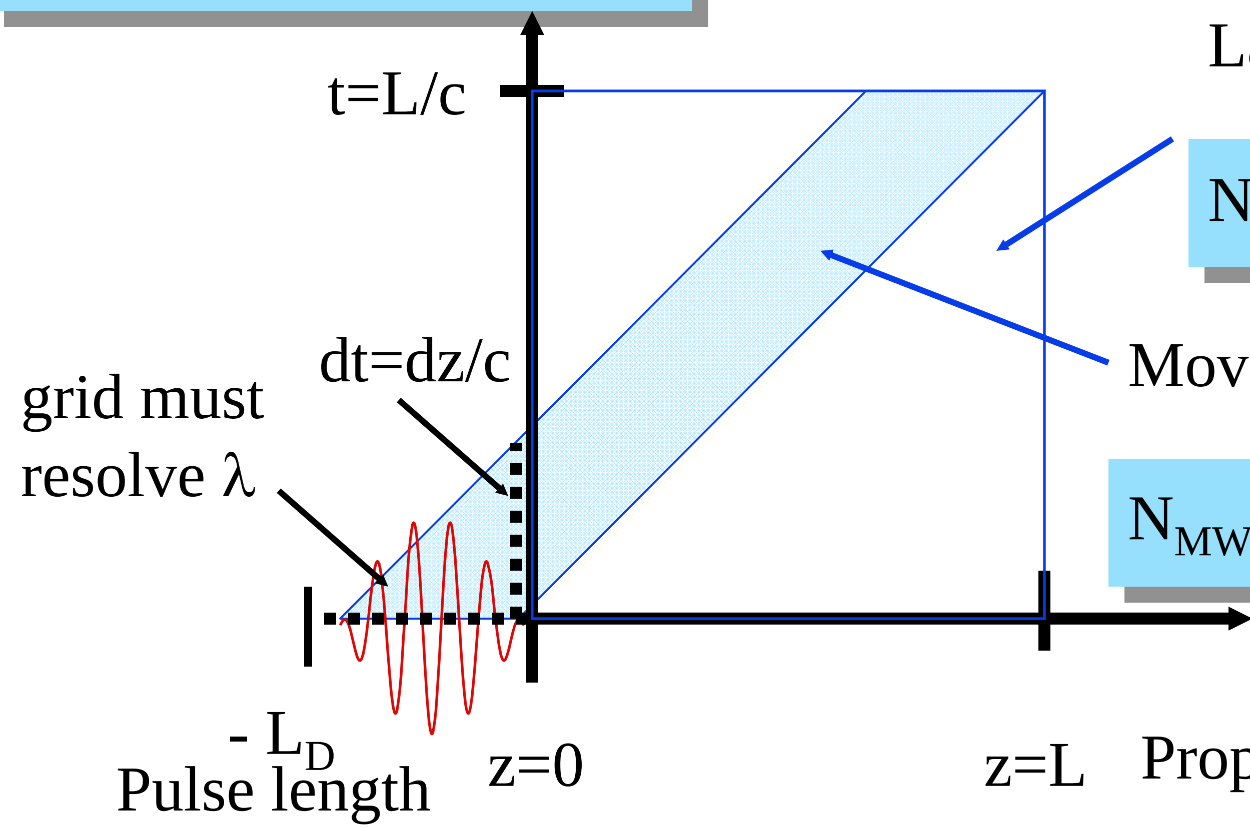
Frank Tsung: tsung@physics.ucla.e[illegible]
Ricardo Fonseca: ricardo.fonseca@ist.utl.pt
http://exodus.physics.ucla.edu
http://cfp.ist.utl.pt/golp/epp

New Features in v2.0

- Bessel Beams
- Binary Collision Module
- Tunnel (ADK) and Impact Ionization
- Dynamic Load Balancing
- PML absorbing BC
- Optimized Higher Order Splines
- Parallel I/O (HDF5)
- Boosted Frame in 1/2/3D

Windows and Frames

Three versions:
- Lab Frame
- Moving Window
- Boosted Frame



Propagation distance

Lab Frame - # Grids

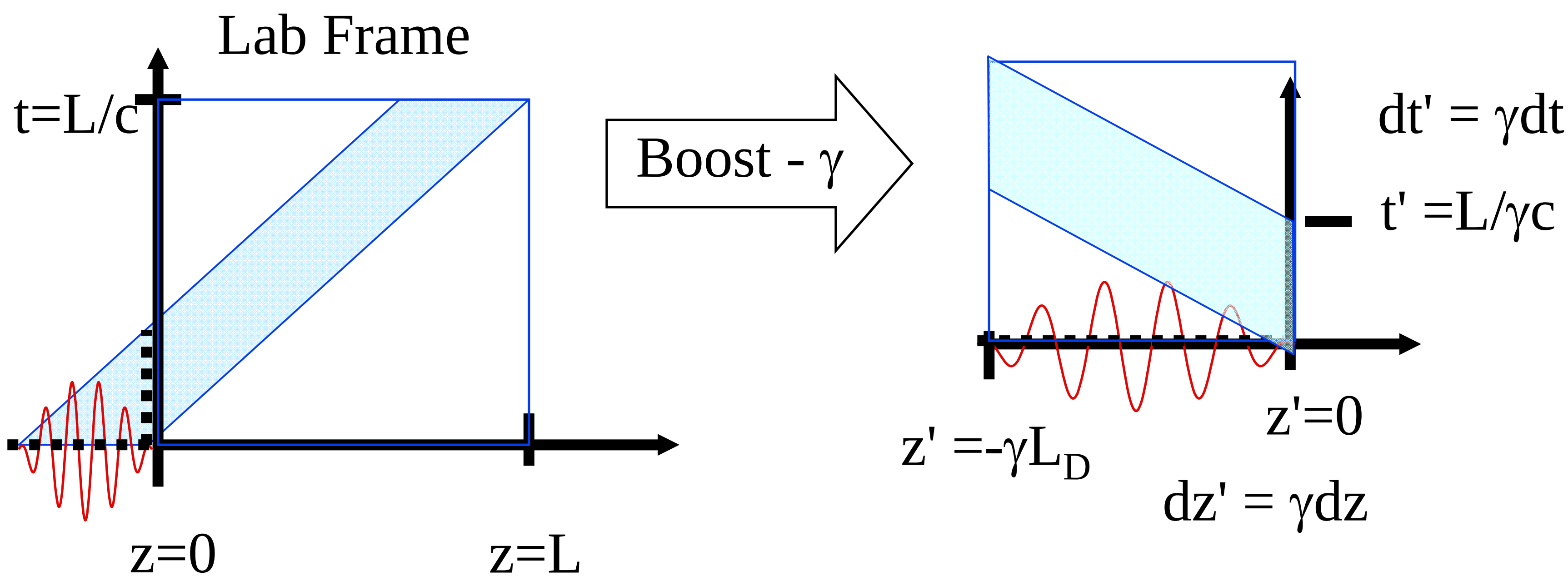
$$N_{LF} = (L/dz)^2 \sim (L/\lambda)^2$$

Moving Window - # Grids

$$N_{MW} = (L_D/L)\, N_{LF}$$

Boosted Frame

J-L Vay, PRL98, 130405 (2007)



Qualifications:

-no backscatter. In boosted frame gives upshift. Requires smaller dz'

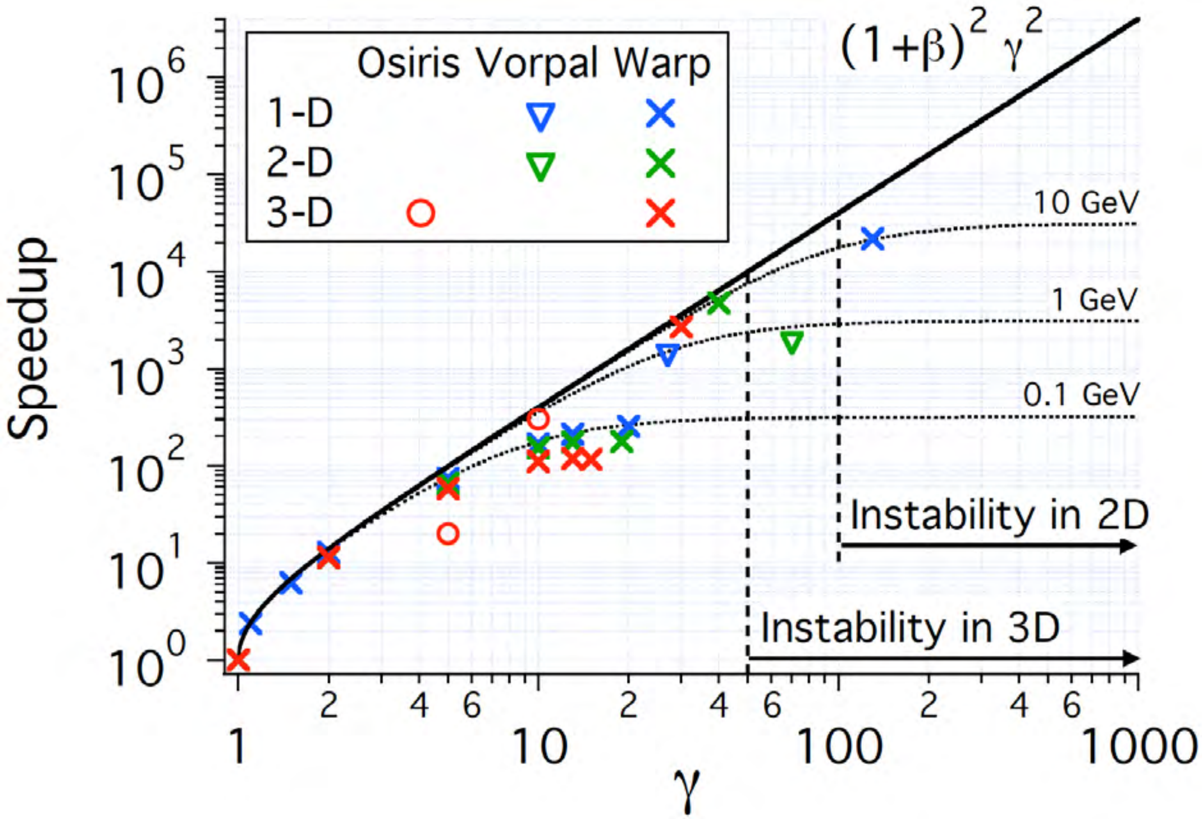
-transverse grid size sets limit on $dt' < dx'_{\perp} /c = dx_{\perp} /c$

Boosted frame - # grids

$N_{BF} = \gamma^{-2} N_{MW}$

Optimum based on 1D makes simulation “square”

Using conventional PIC techniques, 2-3 orders of magnitude speedup reported in 2D/3D by various groups



Osiris: trapped injection

Vorpal: external injection w/ beam loading

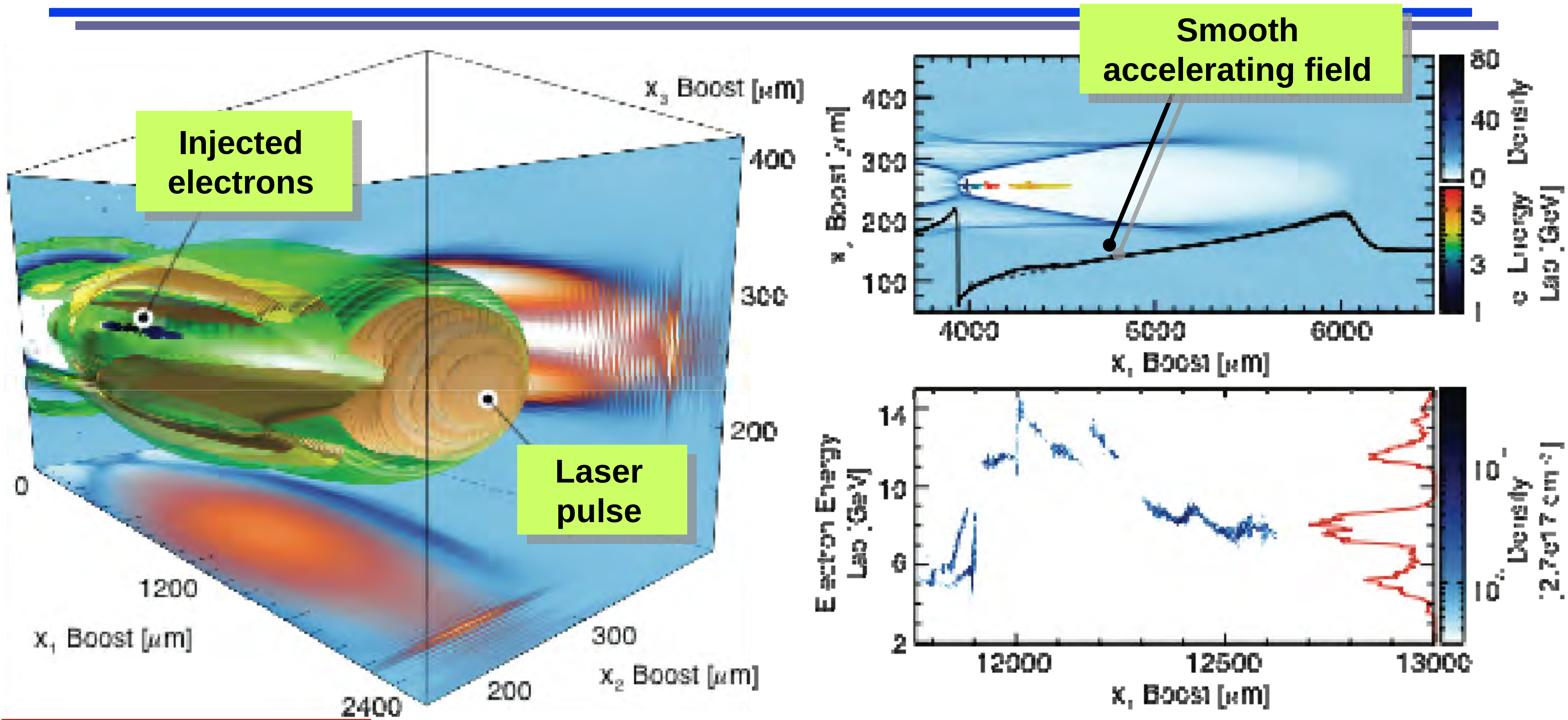
Warp: external injection wo/ beam loading

Reported speedups limited by various factors:

- laser transverse size at injection,
- statistics (trapped injection),
- short wavelength instability (most severe).

J-L Vay

+10GeV self-injection in nonlinear regime
Controlled self-guided a_0=5.8



Boosted frame
7000x256x256 cells
~10^9 particles
$3x10^4$ timesteps
Y=10

~300x faster
than lab

Samuel F. Martins et al.
Nature Physics V6, April 2010

7-12 GeV
1-2 nC

2. Full EM vs. Laser Envelope

Driver Duration >> Laser Period

$T_D >> T_L$

- Required Approximation for Laser envelope:

  $\omega_{laser}\, \tau_{pulse} >> 1, \qquad r_{spot} >> \lambda$

  $\omega_p / \omega_{laser} << 1$

- Advantages of envelope model:

  -Larger time steps

  Full EM stability: $\Delta t < \Delta x/c$

  Envelope accuracy: $\Delta t < 2\pi\, \Delta x^2/\lambda c$

  - No unphysical Cherenkov radiation

  - Further approximations

- Advantages of full EM: Includes Stimulated Raman back-scattering

  Also direct acceleration

  Can handle complete pump depletion

Laser Envelope Approximation

- Laser + Wake field: $E = \tilde{E}_{laser} + \bar{E}_{wake}$
- Vector Potential: $\tilde{\boldsymbol{A}}_{\boldsymbol{laser}} = \hat{A}_0(\xi, x_\perp, t)\exp(ik_0\xi) + c.c.$
- Laser Frame Coordinate: $\xi = ct - z$
- Envelope equation:

$$\frac{2}{c}\frac{\partial}{\partial t}\left(ik_0 - \frac{\partial}{\partial \xi}\right)\hat{A} - \frac{\partial^2}{c^2\partial t^2}\hat{A} + \nabla_\perp^2\hat{A} = -\frac{4\pi}{c}\hat{j}$$

Necessary for:
Raman Forward
Self phase modulation
$v_g < c$

Drop
(eliminates Raman back-scatter)

Validity of Envelope Equation

Extended Paraxial

$$v_g(\omega) = c \Big/ \left(1 + \frac{k_\perp^2 c^2 + \omega_p^2}{2\,\omega^2}\right)$$

True:

$$v_g(\omega) = c\left(1 - \frac{k_\perp^2 c^2 + \omega_p^2}{\omega^2}\right)^{1/2}$$

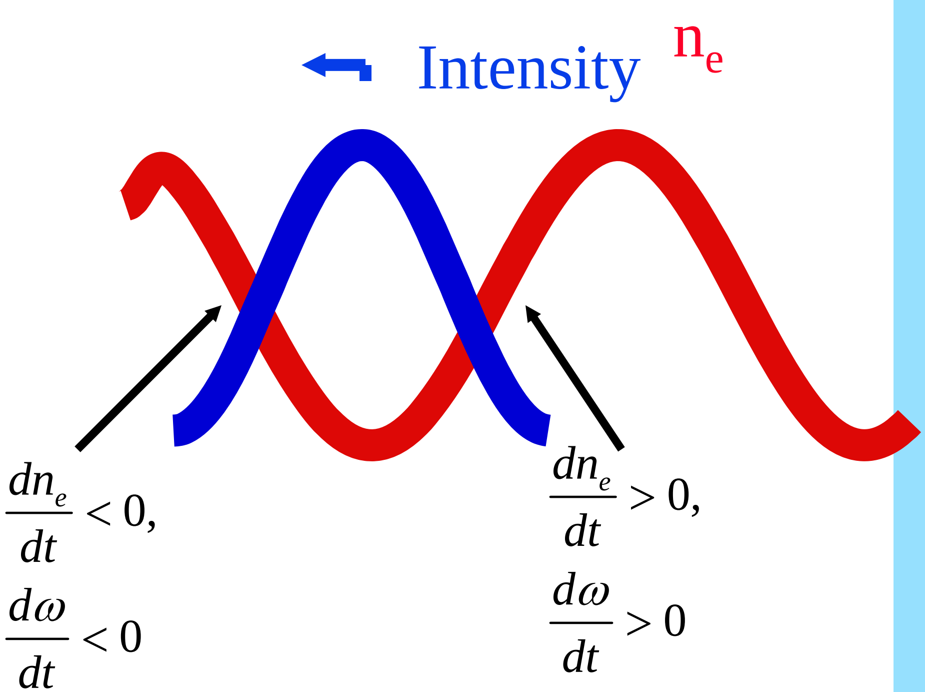
Requires :

$$k_\perp^2 c^2 ,\ \omega_p^2 \ll \omega^2$$

Extended Paraxial approximation

- **Correct treatment of forward and near forward scattered radiation**
- **Does not treat backscattered radiation**
- **If grid is dense enough can treat $\Delta\omega \sim \omega$**

LOCAL FREQUENCY MODIFICATION
M. Tsoufras, PhD Thesis, UCLA



Frequency shift is proportional to propagation distance

$$\frac{\Delta\omega}{\omega} = -\frac{z}{2c\omega^2}\frac{d\omega_p^2}{dt}$$

Assume complete cavitation

Relative frequency shift is unity at the dephasing distance

$$z_D = T_D \frac{c\omega^2}{\omega_p^2}$$

3. Full Lorenz Force vs. Ponderomotive Description

- Full Lorenz: $\frac{d\boldsymbol{p}_i}{dt} = q\left(\boldsymbol{E} + \frac{\boldsymbol{v}_i \times \boldsymbol{B}}{c}\right)$ $\quad \frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$ $\quad \gamma = \sqrt{1 + \frac{p^2}{m^2c^2}}$

- Separation of time scales

$$\boldsymbol{E} = \tilde{\boldsymbol{E}}_{laser} + \bar{\boldsymbol{E}}_{wake}$$

$$\boldsymbol{x}(t) = \tilde{\boldsymbol{x}}(t) + \bar{\boldsymbol{x}}(t)$$

- Requires small excursion

$$|\tilde{\boldsymbol{x}}(t) \cdot \nabla \tilde{\boldsymbol{E}}_{laser}| << |\tilde{\boldsymbol{E}}_{laser}|$$

- Ponderomotive Equations

$$\frac{d\bar{\boldsymbol{p}}}{dt} = q\left(\bar{\boldsymbol{E}}_{wake} + \frac{\bar{\boldsymbol{v}} \times \bar{\boldsymbol{B}}_{wake}}{c}\right) + \bar{\boldsymbol{F}}_p$$

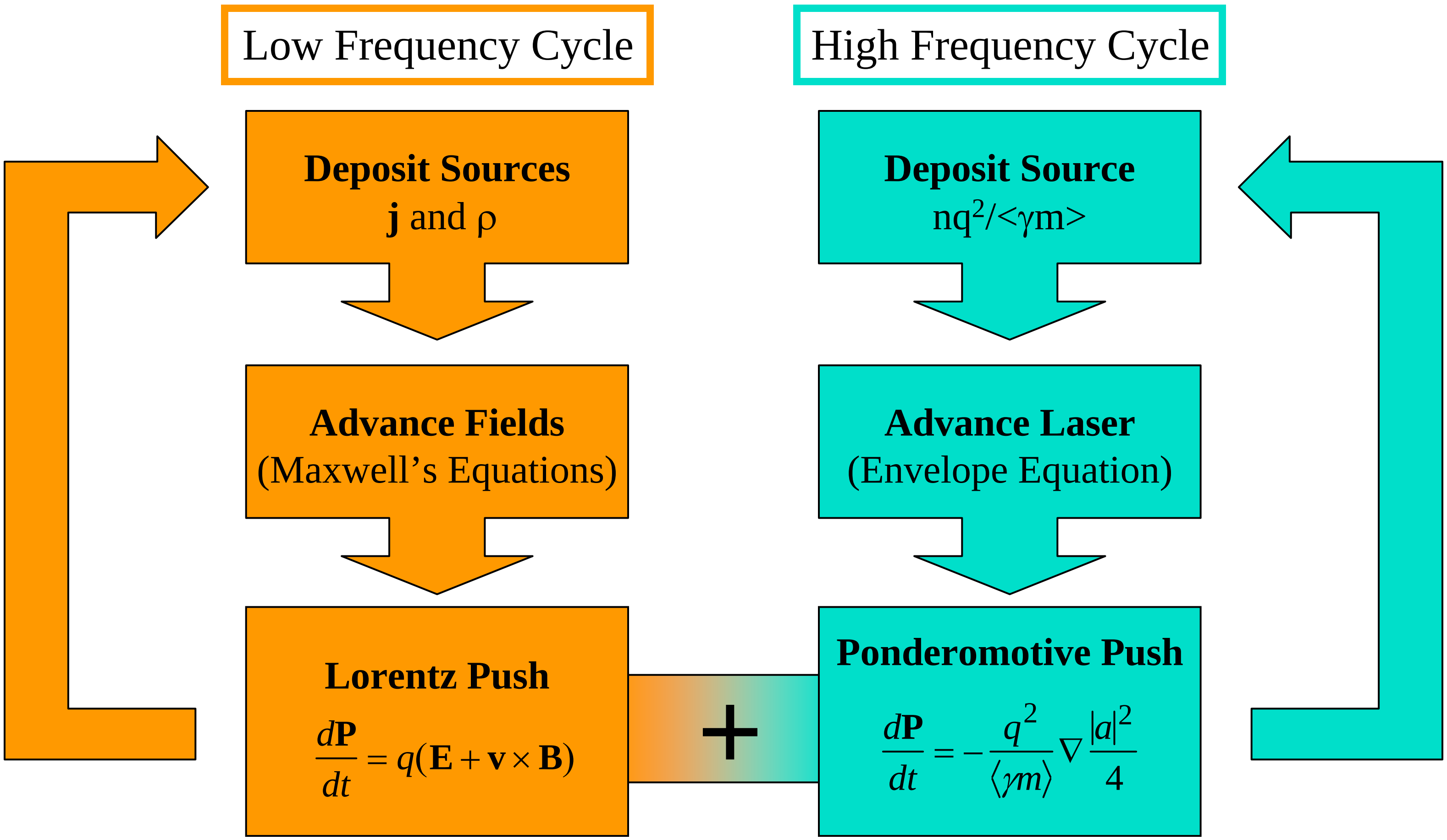
$$\bar{\boldsymbol{F}}_p = -\frac{mc^2}{2\bar{\gamma}} \nabla \left|\frac{q\hat{A}_{laser}}{mc^2}\right|^2$$

$$\bar{\gamma} = \sqrt{1 + \frac{\bar{p}^2}{m^2c^2} + \left|\frac{q\hat{A}_{laser}}{mc^2}\right|^2}$$

Ponderomotive Guiding Center PIC Code: TurboWAVE

D.F. Gordon, et al. , **IEEE TRANSACTIONS ON PLASMA SCIENCE** , V **28** , **1224-1232** (**2000**)

Fields are separated into high and low frequency components. The low frequency component is treated as in an ordinary PIC code. The high frequency component is treated using a reduced description which averages over optical cycles.



TurboWAVE Framework

PIC
EM pusher, ponderomotive pusher, gather/scatter

Nonlinear Optics
Anharmonic Lorentz model,

“SPARC”
Multi-species hydrodynamics

Field Solver Modules
Explicit, envelope, direct fields, coulomb gauge, electrostatic.
Lindman boundaries, simple conducting regions, PML media.

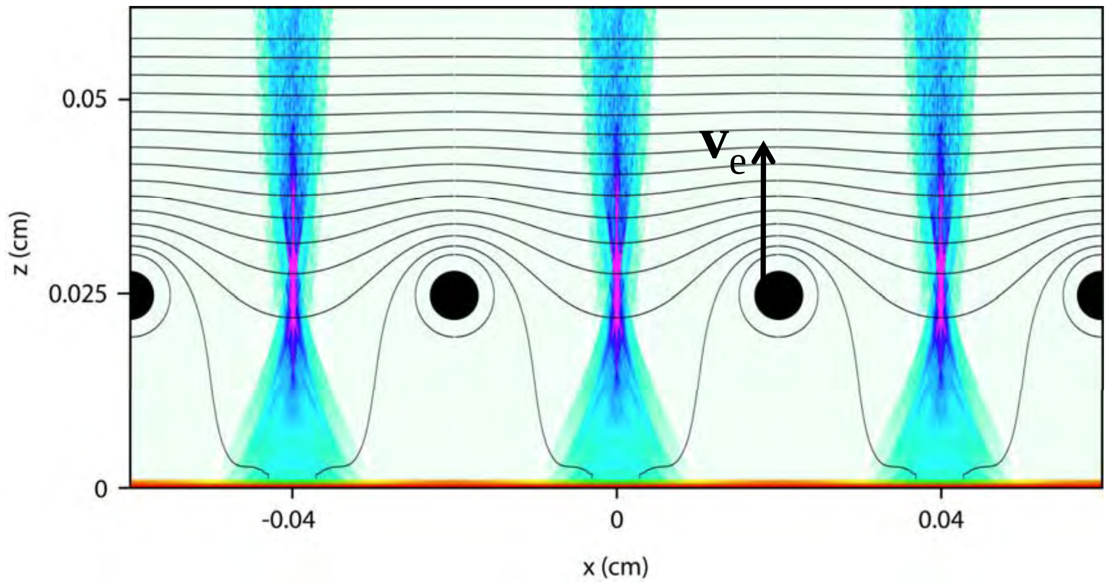
Chemistry
Arbitrary species, reactions

Numerical Framework
Linear algebra, elliptical solvers, fluid advection…

TurboWAVE Base
Grid geometry, regions, domain decomposition, diagnostics, input/output…

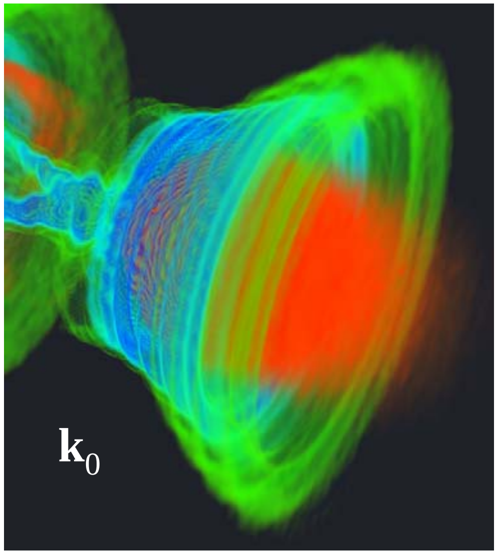
Images from TurboWAVE

Gridded Gun Modeling
Contours are equipotential lines.
Colors represent current density.
Black circles represent grid wires.



Utilizes 2D electrostatic PIC (slab or cylindrical) with conducting regions

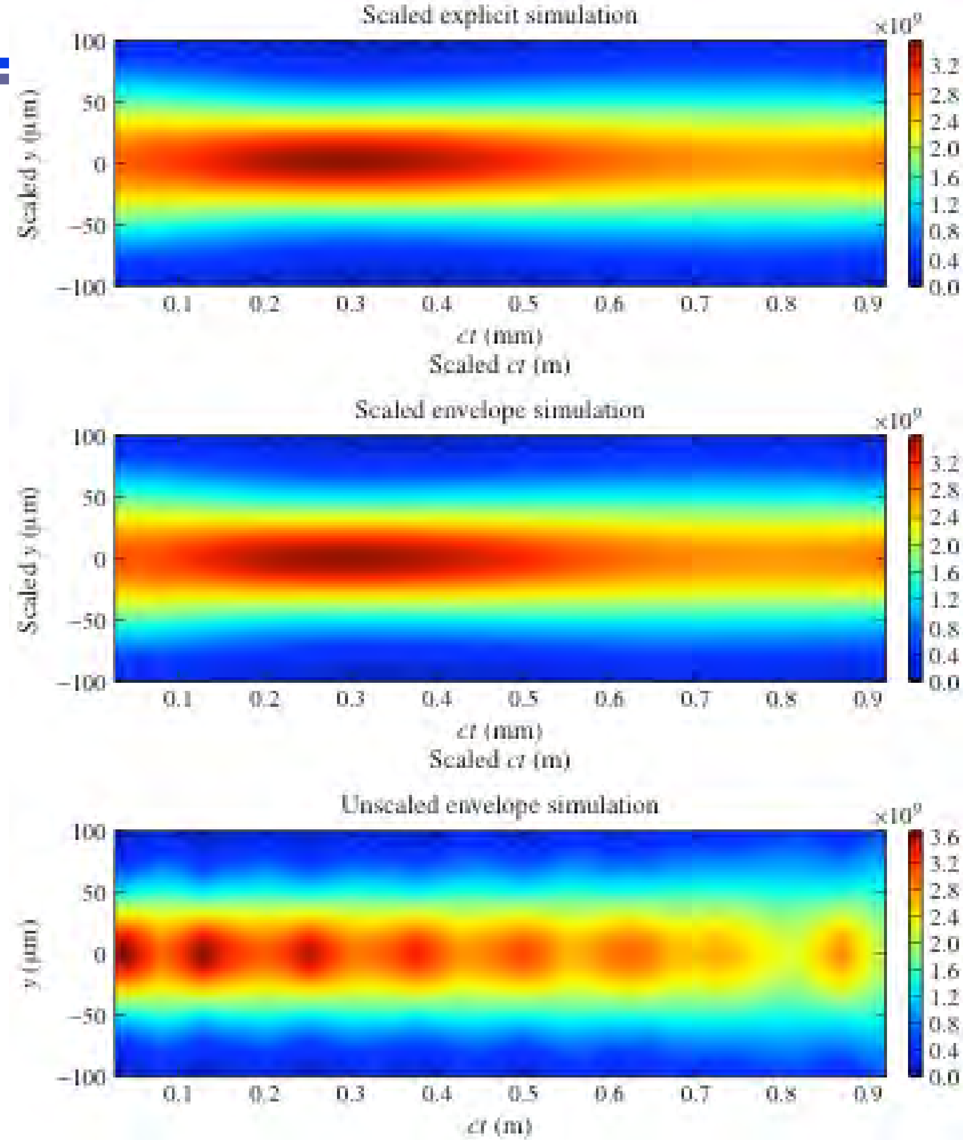
Blowout Wakefield
Red = ion rich
Blue = electron rich



Utilizes 3D electromagnetic PIC

Envelope model in VORPAL enables full 3D simulations of meter-scale LPA stages

- Speedup of 50,000 shown for meter-scale parameters
- Rigorously tested, showing second-order convergence and correct laser group velocity
- Benchmarks against scaled simulations show excellent agreement



Ben Cowan

[1] B. Cowan *et al.*, Proc. AAC 2008

[2] P. Messmer and D. Bruhwiler, PRST-AB **9**, 031302 (2006)

[3] D. Gordon, IEEE Trans. Plasma Sci. **35**, 1486 (2007)

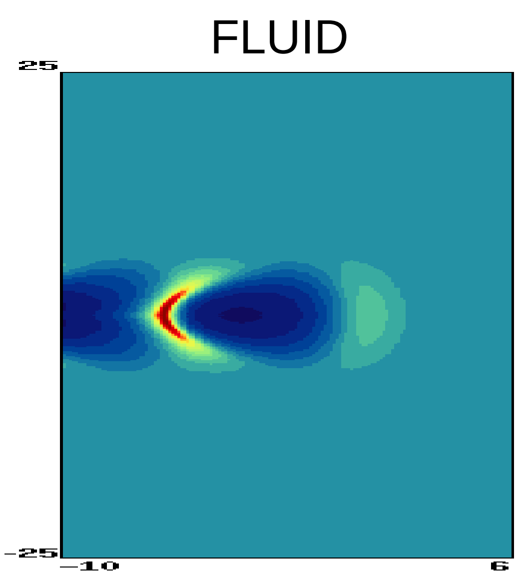
[4] P. Mora and T. M. Antonsen, Phys. Plasmas **4**, 217 (1997)

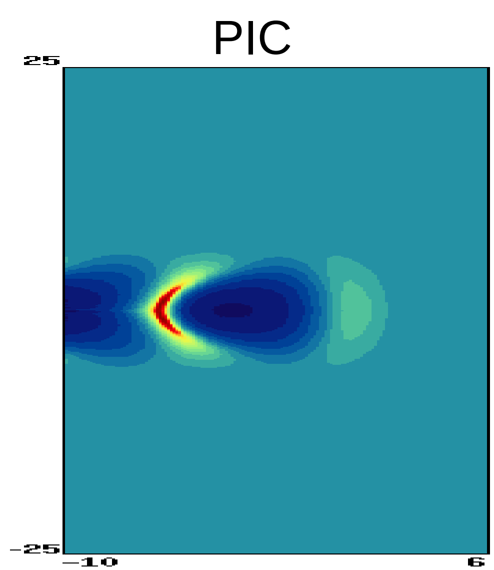
INF&RNO

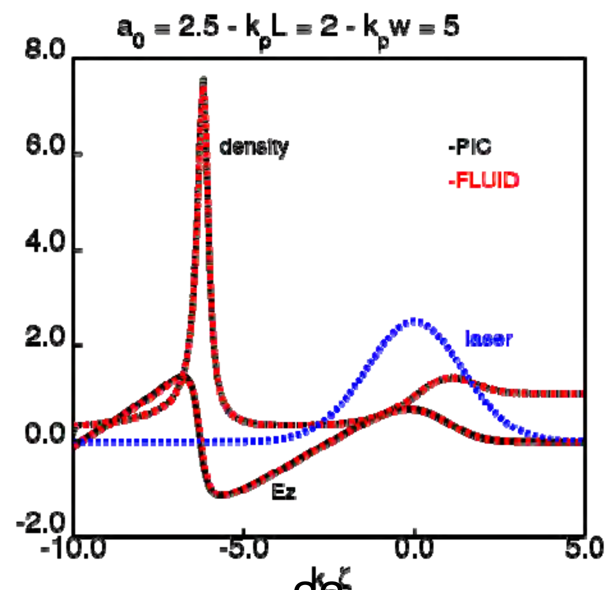
(INtegrated Fluid & paRticle simulatioN cOde)

C. Benedetti at al. (LBNL)

- 2D cylindrical + envelope for the laser (ponderomotive approximation)
- **full PIC/fluid description** for plasma particle (quasi-static approx. is *also* available)
- switching between PIC/fluid modalities (hybrid PIC-fluid sim. are possible)
- dynamical particle resampling to reduce on-axis noise
- 2nd order upwind/centered FD schemes + RK2/RK4 (& Implicit) for time integration
- linear/quadratic shape functions for force interpolation/charge deposition
- high order low-pass compact filter for current/field smoothing
- "BELLA"-like runs (10GeV in ~ 1m) become **feasible in a few days on small machines**

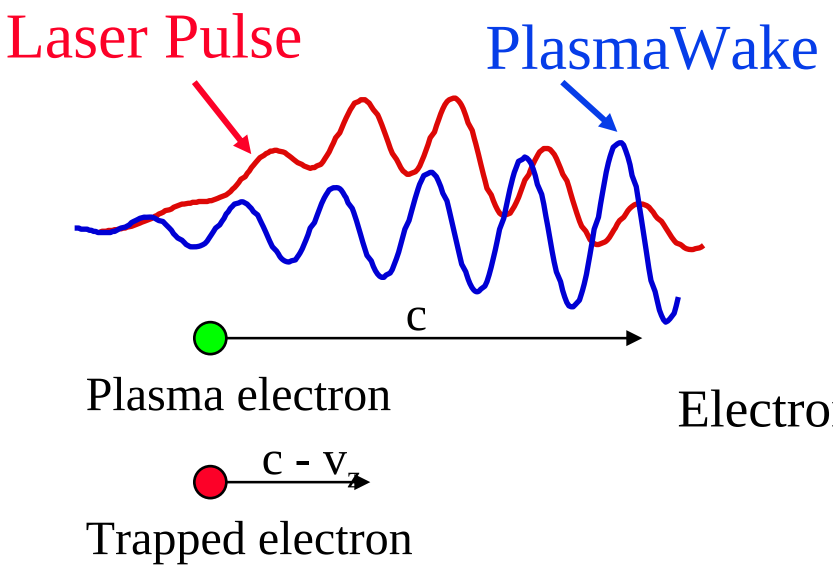






4. Quasi - Static vs. Dynamic Wake

P. Sprangle, E. Esarey and A. Ting, Phys. Rev. Lett. 64, 2011 (1990)



Electron transit time: $\tau_e = \dfrac{\tau_{pulse}}{1 - v_z / c}$

Electron transit time << Pulse modification time

$$\frac{d}{dt} = \cancel{\frac{\partial}{\partial t}} + (c - v_z)\frac{\partial}{\partial \xi} + \boldsymbol{v}_\perp \cdot \nabla_\perp$$

Advantages: fewer particles, less noise (particles marched in ct-z)

Disadvantages: particles are not trapped

Quasi Static Simulation Code WAKE

P. Mora and T. M. Antonsen Jr. - Phys Plasma 4, 217 (1997)

Two Time Scales

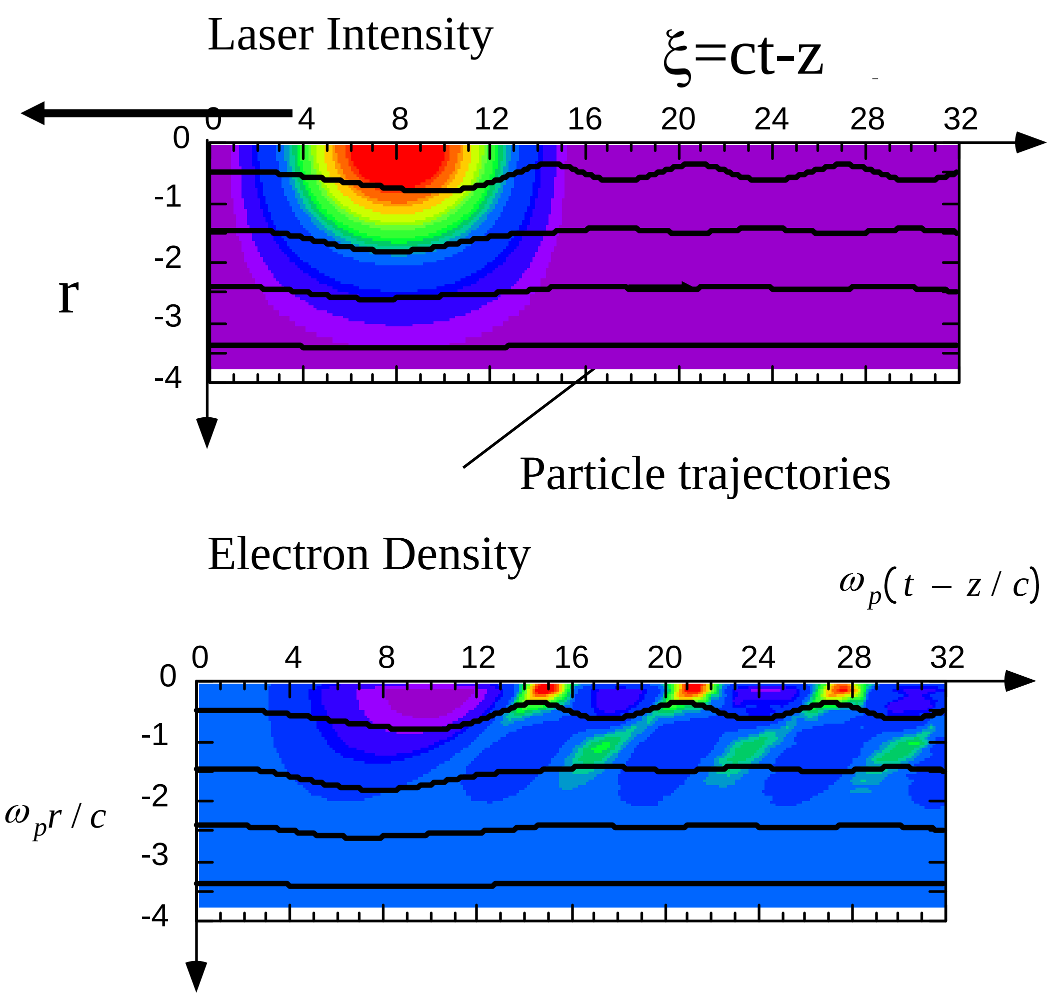
1. "fast time"

   $t \sim T_D \sim \omega_p^{-1}$

particle trajectories and wake fields determined

2. "slow time"

laser pulse evolves
diffraction
self-focusing
depletion



QUASI-STATIC CODE STRUCTURE

Laser

"slow time - t"

$$\frac{2}{c}\frac{\partial}{\partial t}\left(ik_0 - \frac{\partial}{\partial \xi}\right)\hat{A} + \nabla_\perp^2 \hat{A} = -\left\langle \frac{\omega_p^2}{c^2\gamma} \right\rangle \hat{A}$$

$$F_p$$

"fast time ξ=ct-z"

Particles and Wake

$$\frac{d\boldsymbol{p}_\perp}{d\xi} = \frac{1}{c - v_z}\left[q\left(\boldsymbol{E} + \frac{\boldsymbol{v}\times\boldsymbol{B}}{c} \right) + \boldsymbol{F}_p \right]_\perp$$

$$\frac{d\boldsymbol{r}_\perp}{d\xi} = \frac{\boldsymbol{v}_\perp}{c - v_z}$$

$$\nabla \times \boldsymbol{B} = \frac{4\pi q}{c}\left\langle \frac{n}{\gamma}\boldsymbol{p} \right\rangle_{particles} + \frac{\partial \boldsymbol{E}}{\partial \xi}$$

$$\left\langle \frac{\omega_p^2}{c^2\gamma} \right\rangle$$

PARTICLES CONTINUED
constant of motion

- Hamiltonian: $H = H(\xi = ct - z, \boldsymbol{r}_\perp, \boldsymbol{p}) = mc^2\gamma + q\phi$

- Weak dependence on "t" in the laser frame $H - cP_z = const.$

Transverse Dynamics

$$\frac{d\boldsymbol{p}_\perp}{d\xi} = \frac{1}{c - v_z}\left[q\left(\boldsymbol{E} + \frac{\boldsymbol{v} \times \boldsymbol{B}}{c} \right) + \boldsymbol{F}_p \right]_\perp$$

$$\frac{d\boldsymbol{r}_\perp}{d\xi} = \frac{\boldsymbol{v}_\perp}{c - v_z}$$

- Introduce potentials

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} \qquad \boldsymbol{E} = -\nabla\phi - \frac{\partial \boldsymbol{A}}{\partial \xi}$$

- Algebraic equation:

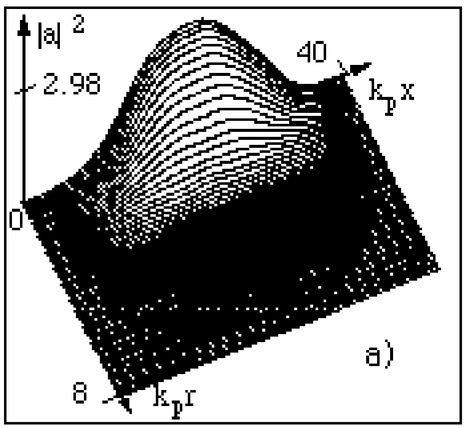
$$p_z = p_z(\boldsymbol{p}_\perp, \psi = \phi - A_z, |\boldsymbol{a}|^2)$$

$$\gamma = \gamma(\boldsymbol{p}_\perp, \psi = \phi - A_z, |\boldsymbol{a}|^2)$$

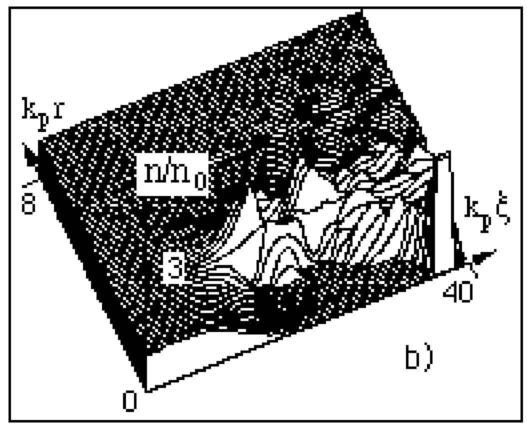
WAKE - Cavitation

P. Mora and T. Antonsen PHYSICAL REVIEW E, Volume: 53 R2068 (1996)

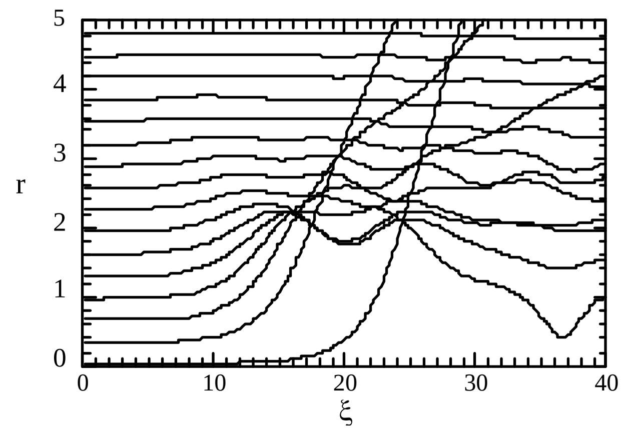
Intensity



Density



Trajectories



Complete cavitation

Suppression of Raman instability

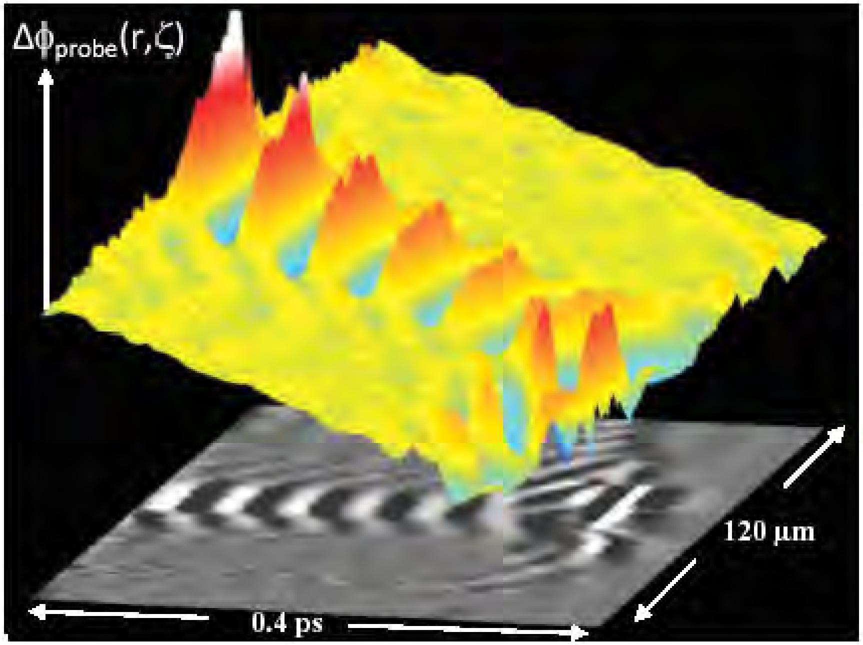
Stable propagation for 30 Rayleigh lengths

Wakefield snapshots see laser-plasma acceleration physics in unprecedented detail

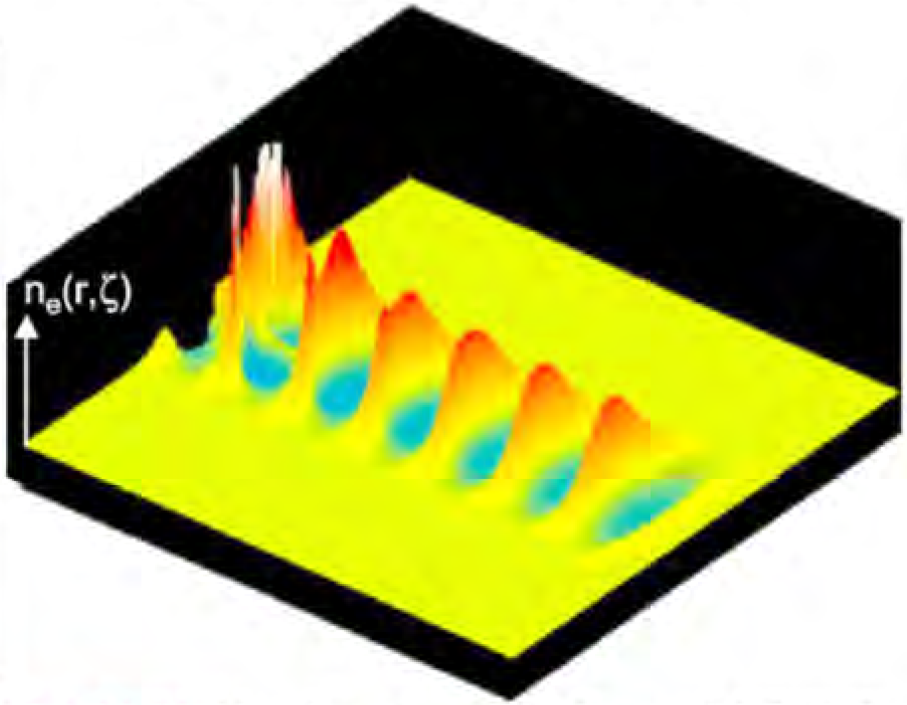
N. Matlis *et al.*, "Snapshots of laser wakefields," *Nature Physics* **2**, 749 (2006)

P. Dong *et al.*, "Holographic Visualization of Laser Wakefields," *New Journal of Physics* **12**, 045016 (2010).

Experiment



Simulation*



*Code WAKE: Mora & Antonsen, *Phys. Plasmas* **4**, 217 (1997)
Simulation by S. Y. Kalmykov

Wake simulation of pulse propagation in corrugated plasma channels

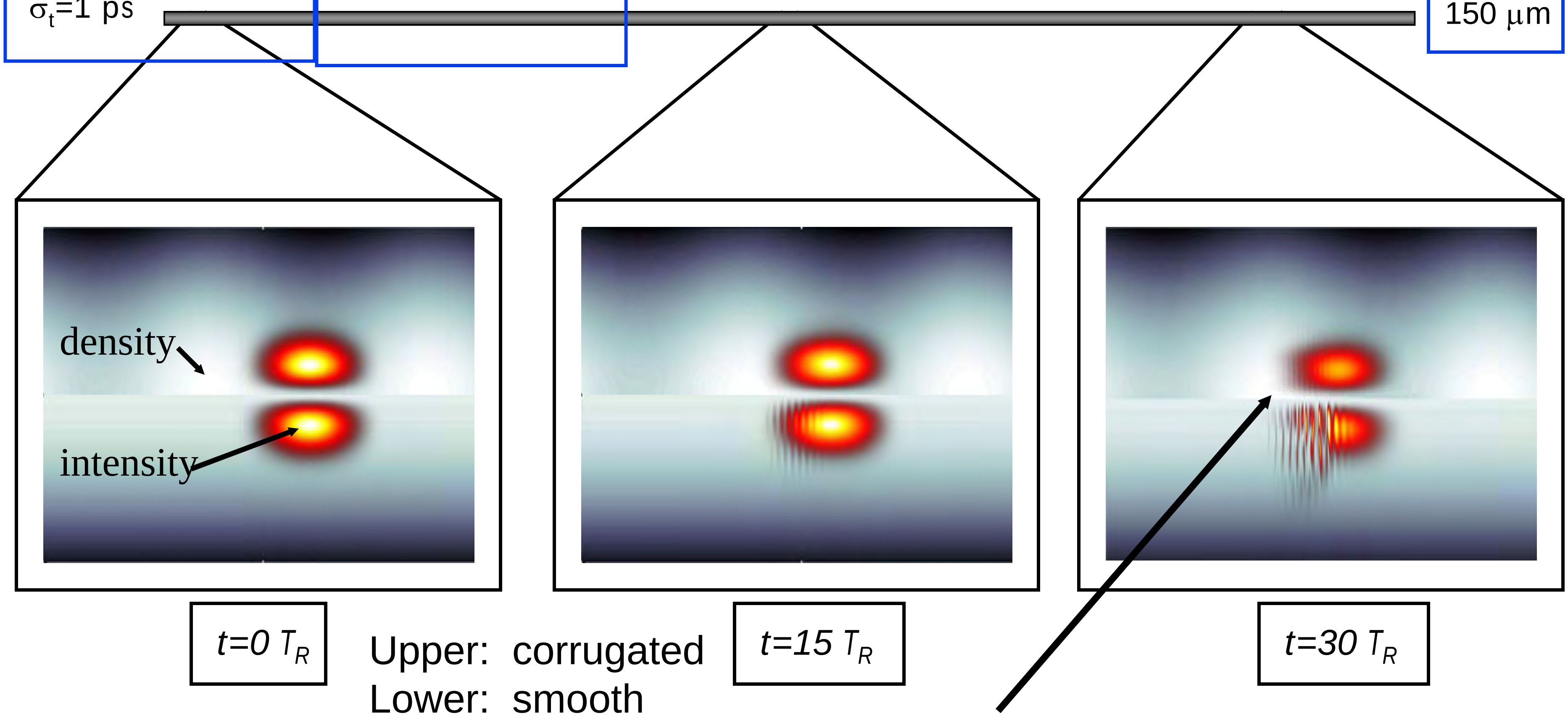
See WG #1 B. Layer Wed. PM, J. Palastro Thu. AM

λ=800 nm
w_{ch}=15 μm
a_o=.35
σ_t=1 ps

n_o=7x10^{18} cm^{-3}
δ=.9
λ_m=.035 cm

3 cm ~ 90 corrugations ~ 40 T_R

150 μm



Upper: corrugated
Lower: smooth

Suppression of Raman Instability

ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

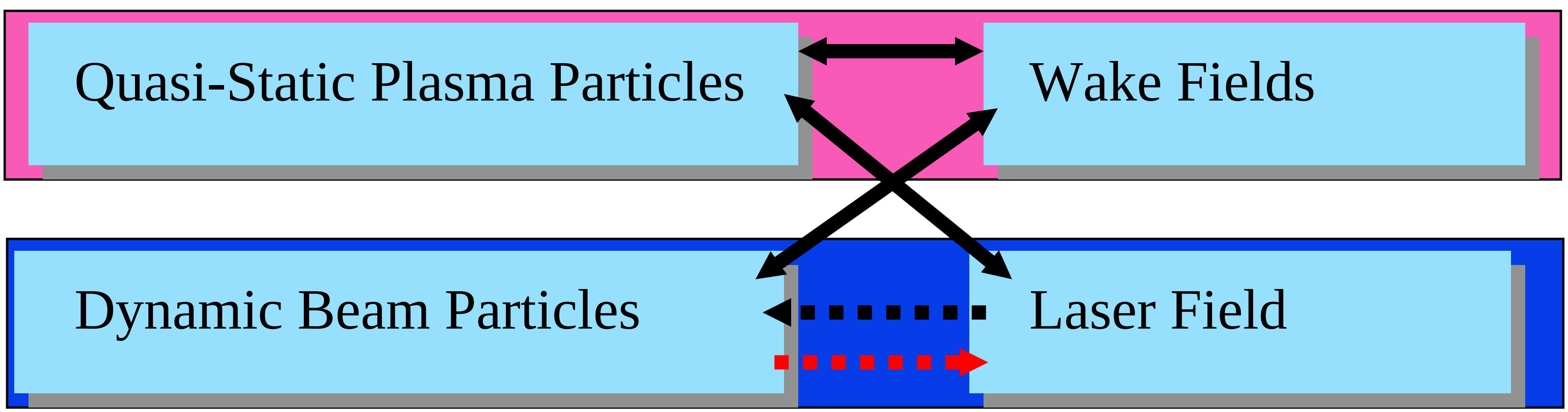
Journal of Computational Physics 217 (2006) 658–679

JOURNAL OF COMPUTATIONAL PHYSICS

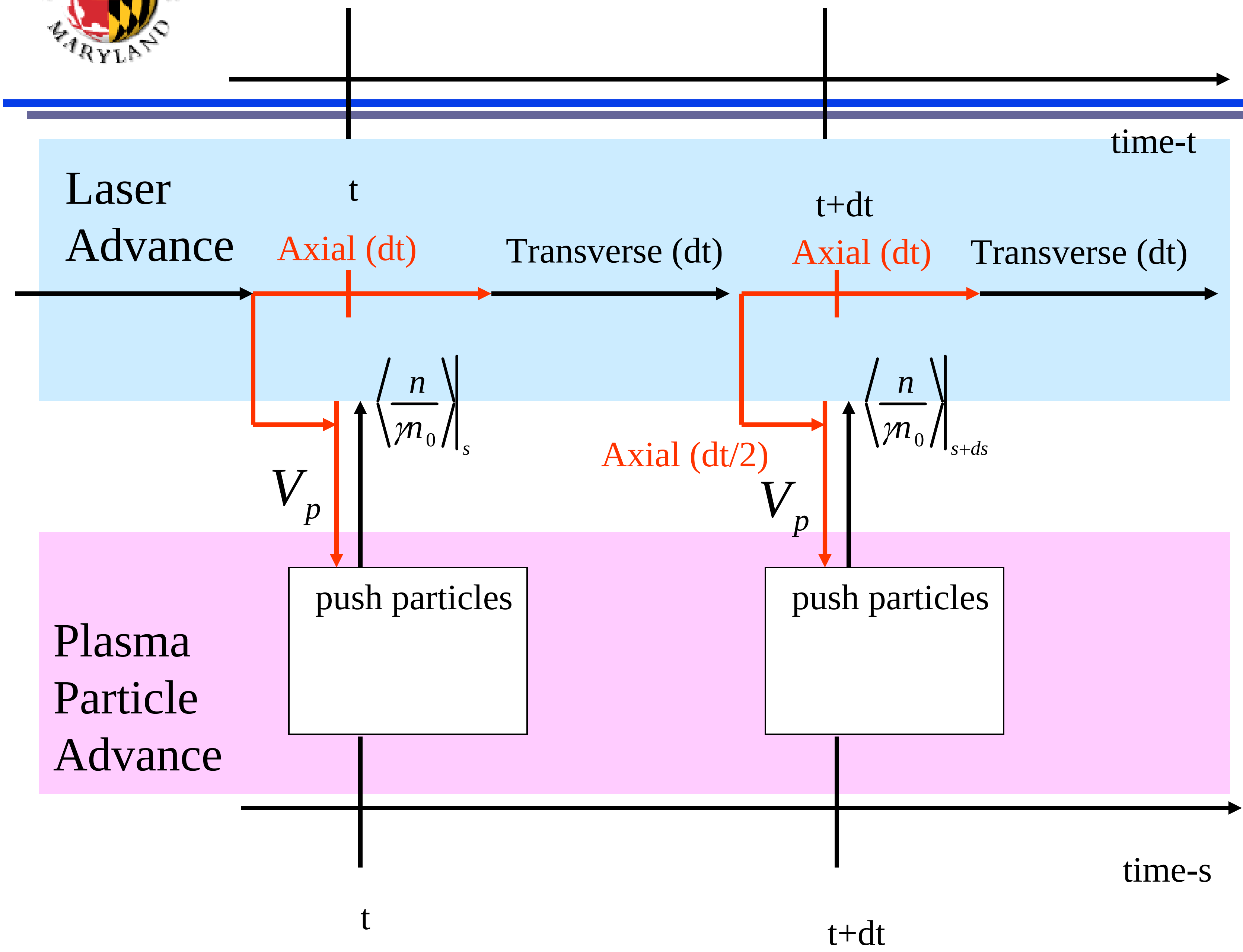
www.elsevier.com/locate/jcp

QUICKPIC: A highly efficient particle-in-cell code for modeling wakefield acceleration in plasmas

C. Huang [a,*], V.K. Decyk [a], C. Ren [a,1], M. Zhou [a], W. Lu [a], W.B. Mori [a], J.H. Cooley [b], T.M. Antonsen Jr. [b], T. Katsouleas [c]



Second Order Accurate Split-Step Scheme



QuickPIC: 3D quasi-static particle code

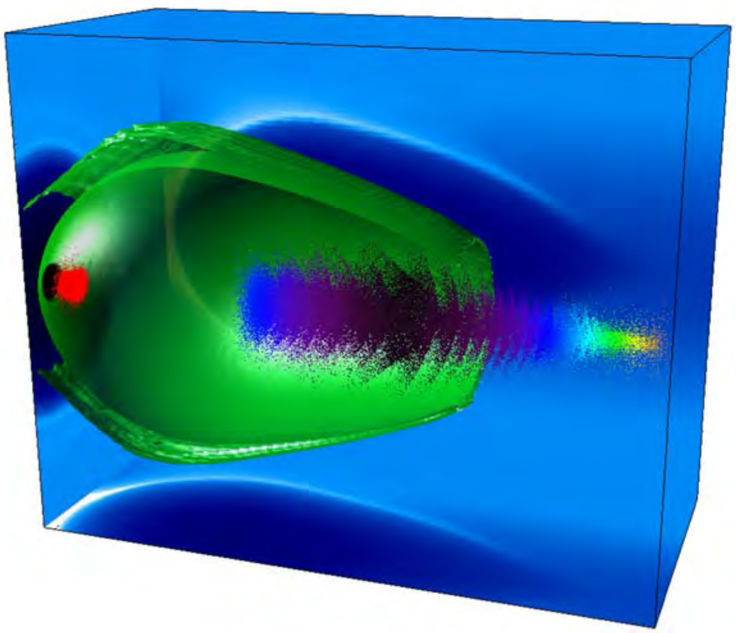
Description

- Massivelly Parallel, 3D Quasi-static particle-in-cell code
- Ponderomotive guiding center for laser driver
- 100-1000+ savings with high fidelity
- Field ionization and radiation reaction included
- Simplified version used for e-cloud modeling
- Developed by UCLA + UMaryland + IST

Examples of applications

- Simulations for PWFA experiments, E157/162/164/164X/167 (Including Feb. 2007 Nature)
- Study of electron cloud effect in LHC.
- Plasma afterburner design up to TeV
- Efficient simulation of externally injected LWFA
- Beam loading studies using laser/beam drivers

Chengkun Huang:
huangck@ee.ucla.edu
http://exodus.physics.ucla.edu/
http://cfp.ist.utl.pt/golp/epp

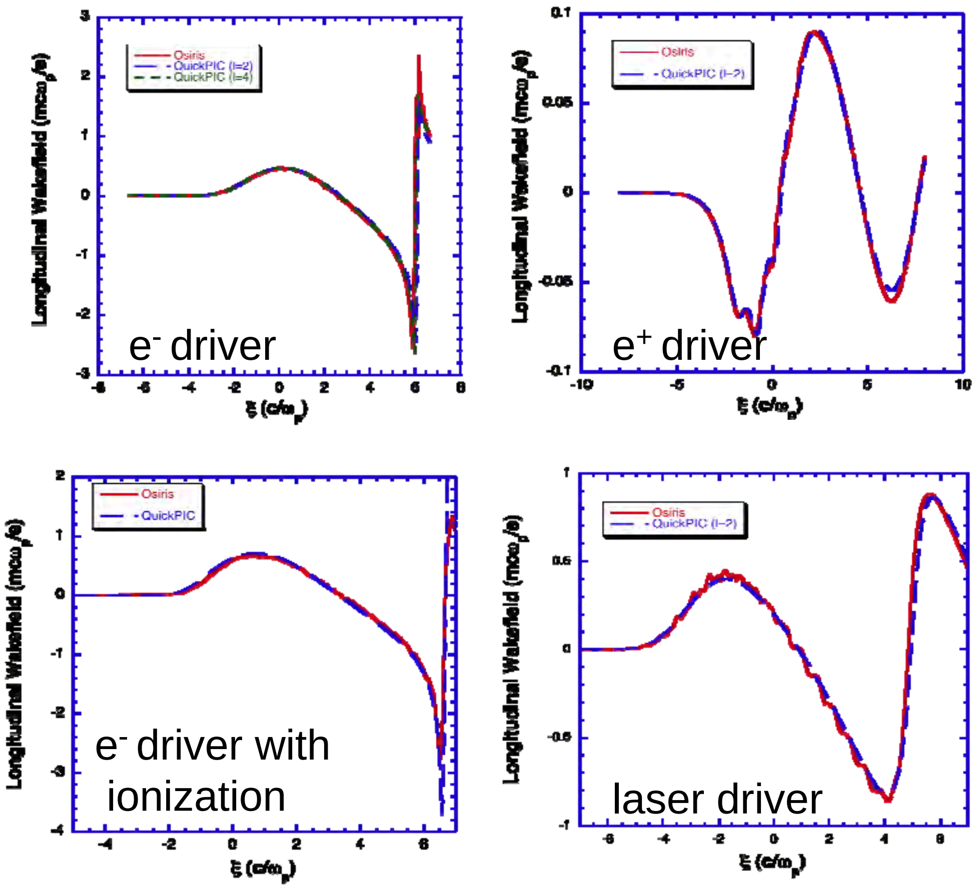


New Features

- Particle tracking
- Pipelining
- Parallel scaling to 1,000+ processors
- Beta version of enhanced pipelining algorithm: enables scaling to 10,000+ processors and unprecedented simulation

Verification : Full PIC vs. Quasi-static PIC

Benchmark for different drivers:
QuickPIC vs. Full PIC



- Excellent agreement with full PIC.
- 100 to 10000 times savings in CPU needs
- No noise issues and no unphysical Cerenkov radiation

100 to 10000 CPU savings with “no” loss in accuracy

Iteration of Electromagnetic Field

Parallel electric field $$E_z = \frac{\partial}{\partial \xi}(\phi - A_z) = -\frac{\partial}{\partial \xi}\psi$$

Electromagnetic portion $\tilde{\boldsymbol{E}}_\perp$

Transverse electric field $$\boldsymbol{E}_\perp = -\nabla_\perp \phi - \frac{\partial}{\partial \xi}\boldsymbol{A}_\perp = -\nabla_\perp \psi - \left(\frac{\partial}{\partial \xi}\boldsymbol{A}_\perp + \nabla_\perp A_z\right)$$

Iterate to find $\tilde{\boldsymbol{E}}_\perp$

Ampere's law $$\frac{4\pi}{c}\left(\nabla_\perp j_z + \frac{\partial}{\partial \xi}\boldsymbol{j}_\perp\right) = -\nabla_\perp^2 \tilde{\boldsymbol{E}}_\perp$$

Equation of motion $$\frac{d\boldsymbol{p}_\perp}{d\xi} = \frac{1}{c - v_z}\left[q\left(\boldsymbol{E} + \frac{\boldsymbol{v} \times \boldsymbol{B}}{c}\right) + \boldsymbol{F}_p\right]_\perp$$

Quasi-Static Field Representation

Lorenz

$$-\nabla_\perp^2 \boldsymbol{A} = \frac{4\pi}{c}\boldsymbol{j}$$

$$-\nabla_\perp^2 \phi = 4\pi\rho$$

Pro:

Simple structure

Compatible with 2D PIC

Con:

A carries "electrostatic" field

Transverse Coulomb

$$\nabla_\perp \cdot \boldsymbol{A}_\perp = 0$$

$$-\nabla_\perp^2 \boldsymbol{A} = \frac{4\pi}{c}\boldsymbol{j} - \nabla\left[\frac{\partial(\phi - A_z)}{\partial\xi}\right]$$

Pro:

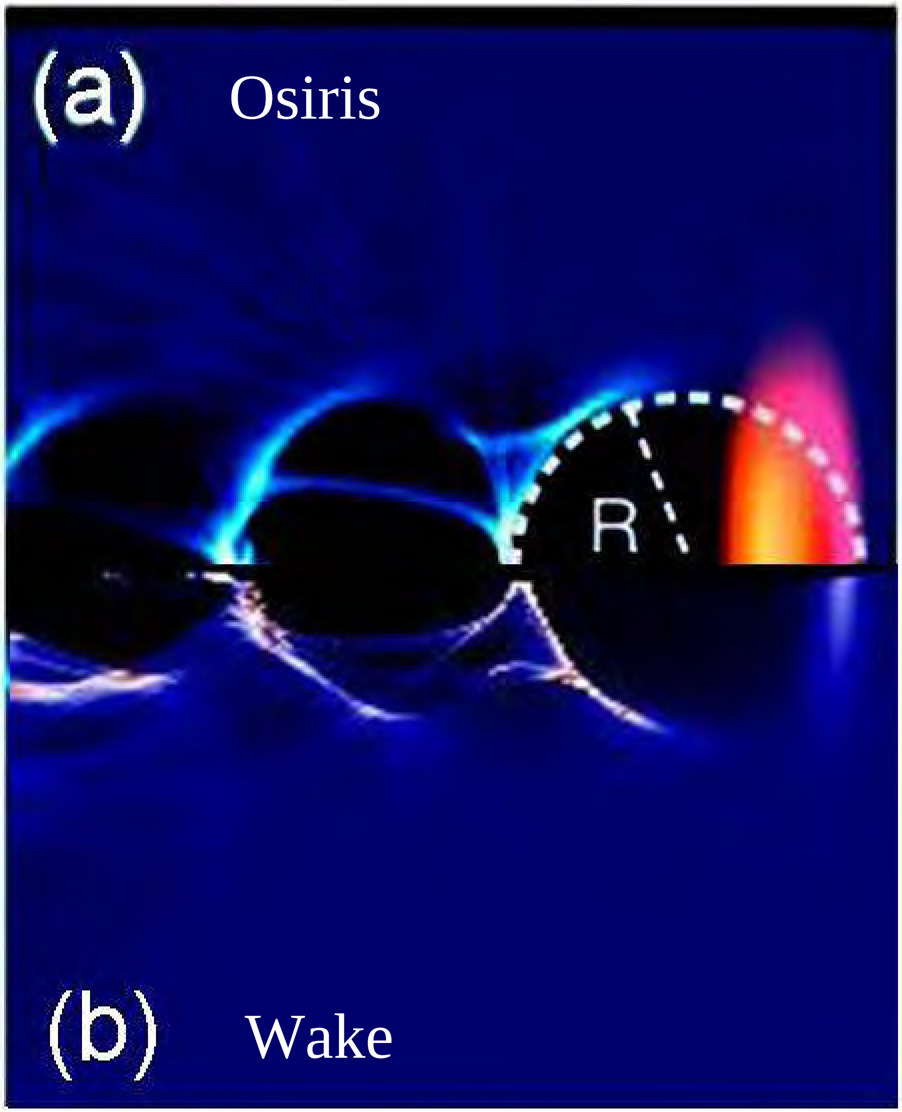
$\mathbf{A}_\perp = 0$ in electrostatic limit

Con:

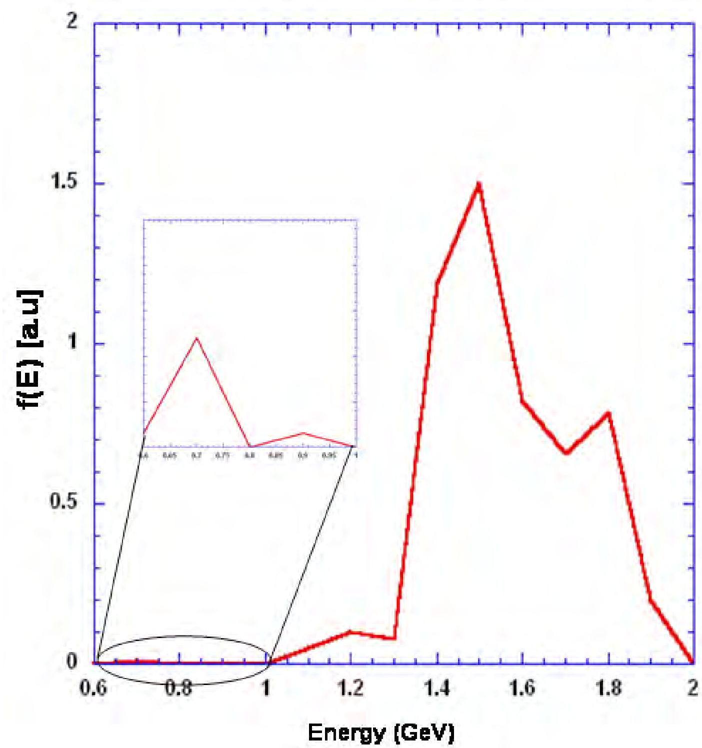
non-standard field equations

Particle Promotion in WAKE

S. Morshed PoP, to be published



"Plasma particles" for which quasi-static violated are promoted to "beam particles"



Conclusions

- Numerical simulation of Laser-Plasma interactions is a powerful tool

- A variety of models and algorithms exist
  - first principles
  - reduced modles

- Field is still advancing with new developments
  - Boosted Frame Calculations speed-up ~ γ^2
  - 3D Parallel Quasi-static speed-up ~ $[\omega_0/\omega_p]^2$
  - GPUs