



SciDAC plasma-based team:

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 - **F.S.Tsung**
 - **CK. Huang**
 - **V.K.Decyk**
- **D.Bruhweiler** **TechX**
 - **D.Dimitrov**
- **E.Esarey** **LBL**
 - **B.Shadwick**
 - **G.Fubiani**
- **T.Katsouleas** **USC**
 - **S.Deng**



Advanced accelerator effort is highly leveraged:
Big bang for the buck

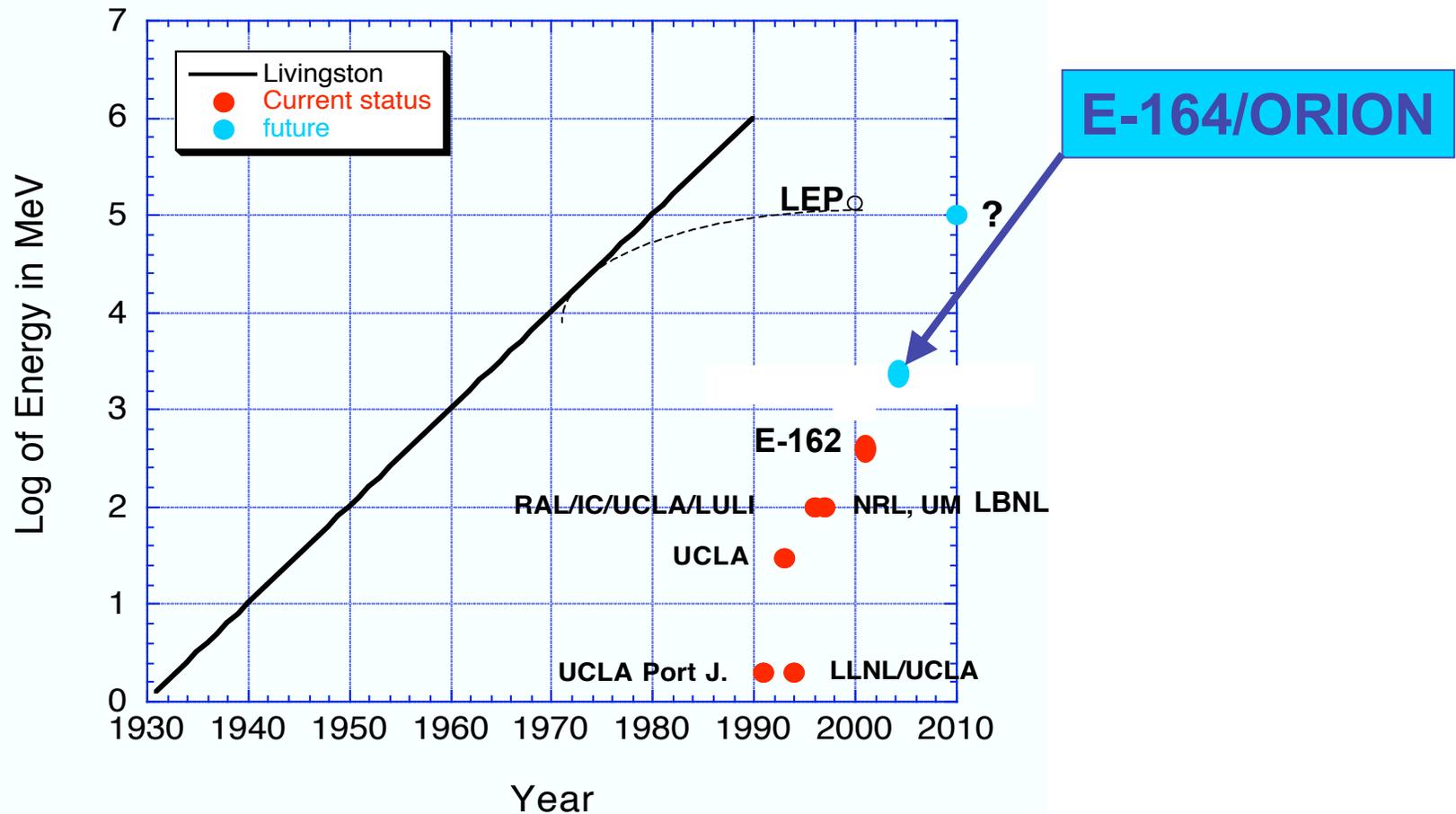
Institution	2002	2003
UCLA	60K (125K)	70K (144K)
Tech-X	50K	60K
USC	20K	25K
LBNL	20K	25K

Why and what is plasma-based acceleration

Long term future of High-Energy physics requires the need for new high-gradient technology

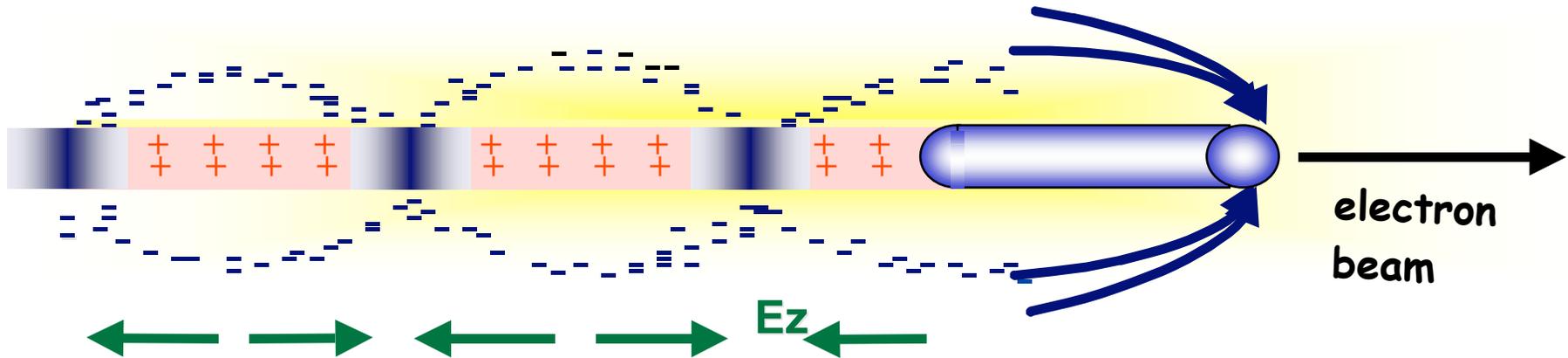
Gradients from 1GeV/m to 100 TeV/m are possible from relativistic plasma waves

Experimental progress



Physical Principles of the Plasma Wakefield Accelerator

- Space charge of **drive beam** displaces **plasma electrons**



- **Plasma ions** exert restoring force => **Space charge oscillations**

- Wake Phase Velocity = Beam Velocity (like wake on a boat)

- Wake amplitude N_b / σ_z^2 (for $2\sigma_z \ll \lambda_p$ $\frac{1}{\sqrt{n_0}}$)

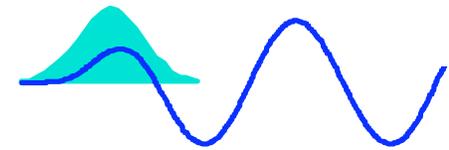
- Transformer ratio $E_{z,acc.} / E_{dec.beam}$

Concepts For Plasma Based Accelerators

Pioneered by J.M.Dawson

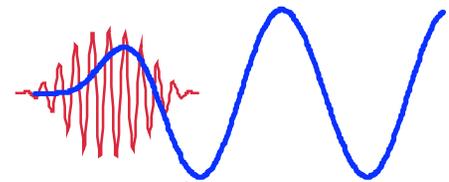
- Plasma Wake Field Accelerator(PWFA)

A high energy electron bunch



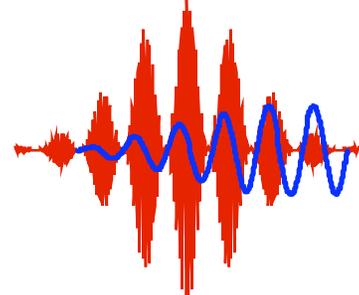
- Laser Wake Field Accelerator(LWFA)

A single short-pulse of photons



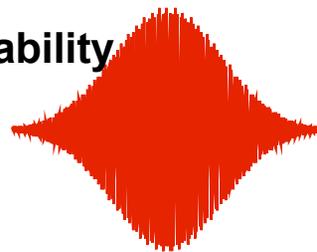
- Plasma Beat Wave Accelerator(PBWA)

Two-frequencies, i.e., a train of pulses

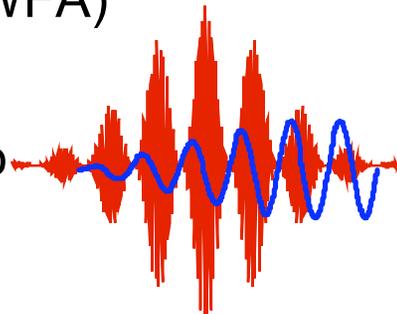


- Self Modulated Laser Wake Field Accelerator(SMLWFA)

Raman forward scattering instability



evolves to



Mission

Develop high fidelity parallelized software (at least two distinct codes): primarily particle based models

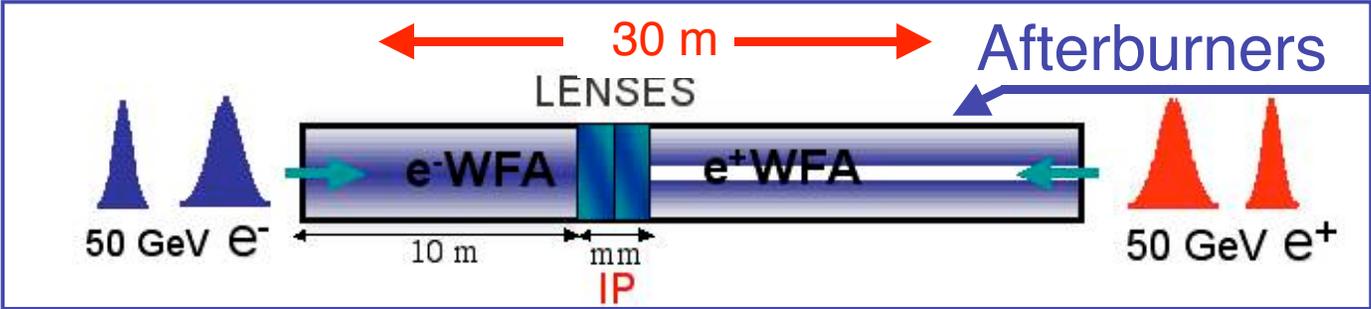
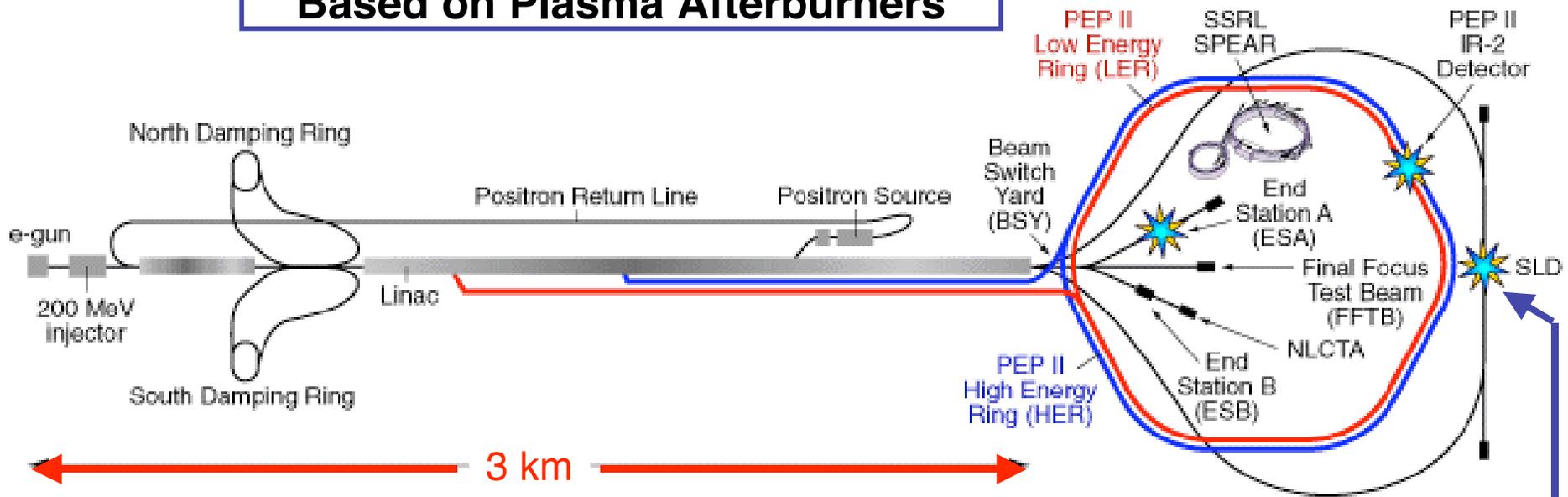
Model the full-scale of current experiments ~100MeV - 1GeV

Enable full-scale modeling of 100+ GeV plasma-based colliders

Transfer plasma models to conventional accelerator modeling

Enable scientific discovery

**A goal is to build a virtual
 accelerator:
 A 100 GeV-on-100 GeV
 e^-e^+ Collider
 Based on Plasma Afterburners**



Computational challenges for modeling plasma-based acceleration (1 GeV Stage): 1000hours/GFlop

Beam-driven wake*	Fully Explicit
Δz	$\Delta z \approx .05 c/\Delta t_p$
$\Delta y, \Delta x$	$\Delta x, \Delta y \approx .05 c/\Delta t_p$
Δt	$\Delta t \approx .02 c/\Delta t_p$
# grids in z	≥ 350
# grids in x, y	≥ 150
# steps	$\geq 2 \times 10^5$
$N_{\text{particles}}$	$\sim .25-1. \times 10^8$ (3D)
Particles x steps	$\sim .5 \times 10^{13}$ (3D) - $\geq 10,000$ hrs at $\sim .1$ GFlops

*Laser-driven GeV stage requires on the order of $(\Delta z/\Delta z_p)^2 = 1000$ x longer, however, the the resolution can usually be relaxed.

Community of parallel PIC codes and algorithms exist: PIC codes make “minimal” physics approximations

- ❑ Parallel Full PIC

 - ❑ OSIRIS

 - ❑ Vorpal/OOPIC

- ❑ Parallel quasi-static PIC

 - ❑ quickPIC

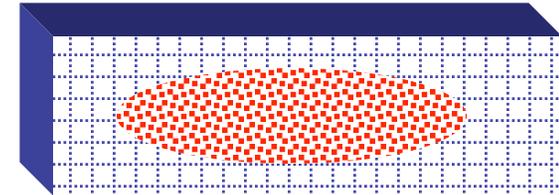
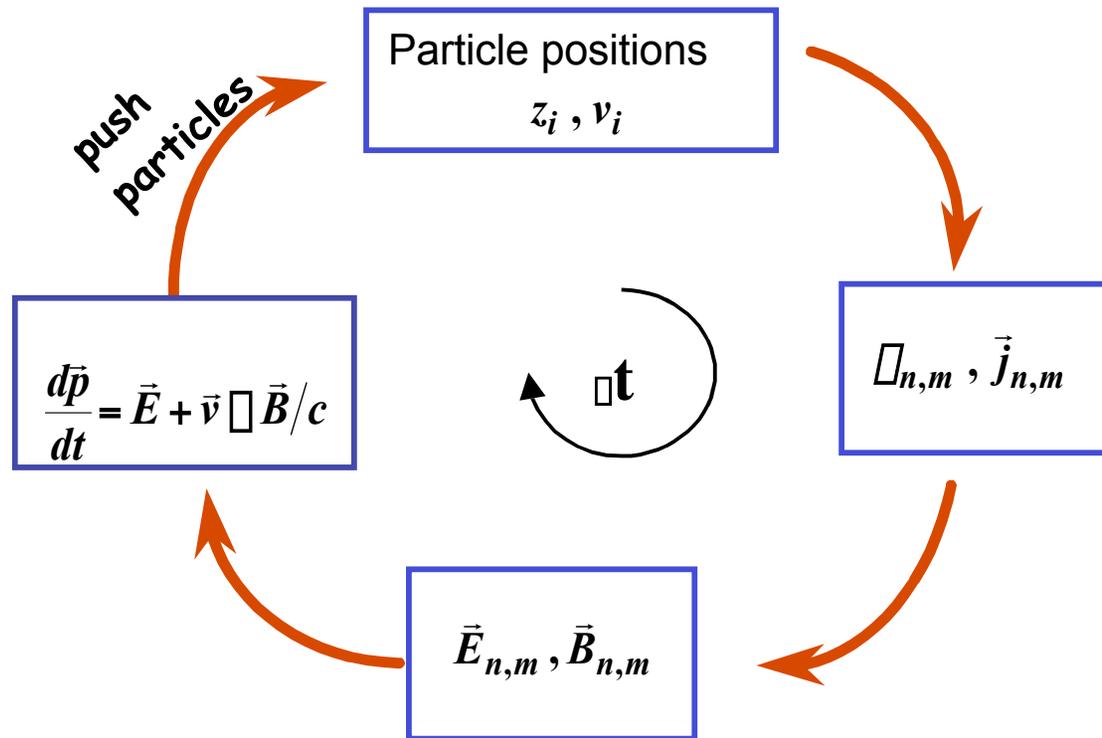
- ❑ Fluid (quasi-static and full)

 - ❑ To model a plasma stage including beam loading will require particle models

What Is a Fully Explicit Particle-in-cell Code?

Computational cycle

(at each step in time)



- Maxwell's equations for field solver
- Lorentz force updates particle's position and momentum

Typical simulation parameters:

$\sim 10^7$ - 10^9 particles

$\sim 10^4$ time steps

~ 1 - 100 Gbytes

$\sim 10^2$ - 10^4 cpu hours

SciDAC collaborative approach

- ❑ Multiple codes
- ❑ Benchmarking against each other and against reduced numerical models and analytic theory
- ❑ Validation against experiment
 - ❑ E-162/E-164
 - ❑ L'OASIS
- ❑ Modeling future experiments
 - ❑ E-164/E-164x
 - ❑ L'OASIS
- ❑ A path towards a virtual accelerator
- ❑ SCIENTIFIC DISCOVERY ALONG THE WAY

Parallel Code Development

OSIRIS: full PIC

Uorpal/OOPIC: full PIC

quickPIC: reduced PIC

UPIC: parallel PIC framework



OSIRIS.framework

Basic algorithms are mature and well tested

- **Fully relativistic**
- **Choice of charge-conserving current deposition algorithms**
- **Boris pusher for particles, finite field solver for fields**
- **2D cartesian, 2D cylindrical and 3D cartesian**
- **Arbitrary particle initialization** and external fields
- **Conducting and Lindmann boundaries for fields; absorbing, reflective, and thermal bath for particles; periodic for both**
- **Moving window**
- **Launch EM waves: field initialization and/or antennas**
- **Launch particle beam**
- **particle sorting and ion subcycling**
- **Extended diagnostics using HDF file output:**
 - Envelope and boxcar averaging for grid quantities
 - Energy diagnostics for EM fields
 - Phase space, energy, and accelerated particle selection diagnostics for particles

**Ionization modules are being added:
Both in 2D and 3D**

Ionization modules were added in 2D (slab and cylindrical) and 3D

Monte Carlo impact ionization model was used: particles are born at rest

Monte Carlo field ionization model was used: particles are born at rest

Various cross sections and tunnel rates are being tested: benchmarking with the help of OOPIC

Effort was made to improve speed and maintaining parallel efficiency:

2D 128x128 with 16 particles/cell per processor and $V_{th} = .1c$

CPU #	Speed μ s/ps	Push %	BCpart	BCcurr	Field Solve	BC Field	other	Efficiency
1	2.1	95	4.2	.03	.56	.03	.19	100
4	2.13	95	3.89	.09	.59	.1	.31	99.48
16	2.2	92.8	4.91	.53	.71	.38	.68	95.82
64	2.3	89.3	6.87	1.28	.57	1.09	1.09	91.82
256	2.29	88.7	6.97	1.29	.55	1.39	1.15	92.16
512	2.37	85.2	7.42	1.27	.54	1.87	3.72	88.52
1024	2.45							85

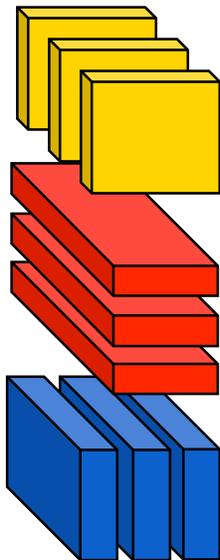
Speed in 3D: 3.2 μ s/ps with 80% efficiency on 512 processors
And 60% on 1024 processors

OSIRIS Algorithms

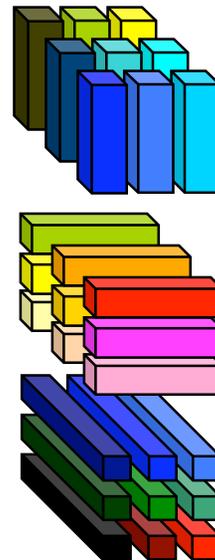
Domain Decompositions

- *OSIRIS* currently allows distribution of the simulated space into evenly partitioned domains along any axis
- next steps in extending the code will be to introduce an uneven distribution of domains and dynamic load balancing: follow concepts in PLIB

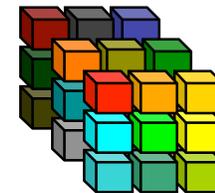
1D Decomposition



2D Decomposition



3D Decomposition



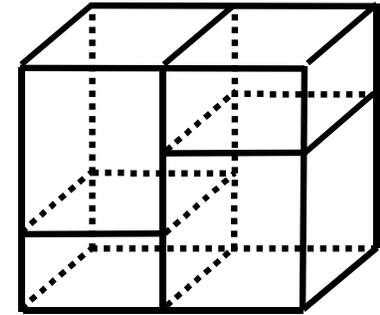
VORPAL – Multi-dimensional hybrid code

- Achieves great flexibility with negligible run-time penalty
 - Multi-dimensional (2D or 3D, with Cartesian geometry)
 - can switch from 2D to 3D with same code and input file
 - enabled by “generic programming” paradigm of C++
 - Runs in serial or parallel (using MPI)
 - flexible 2D and 3D domain decomposition
 - good scaling up to 500 processors has been demonstrated
 - Cross-platform: Linux, IBM SP, Windows, Solaris
- Combines multiple fluid and PIC algorithms seamlessly
 - finite-difference time domain (FDTD) on structured Yee mesh
 - Particle-in-Cell
 - standard Boris particle push
 - charge-conserving current deposition
 - Cold fluid algorithms
 - multiple flux-corrected transport (FCT) algorithms for positive density



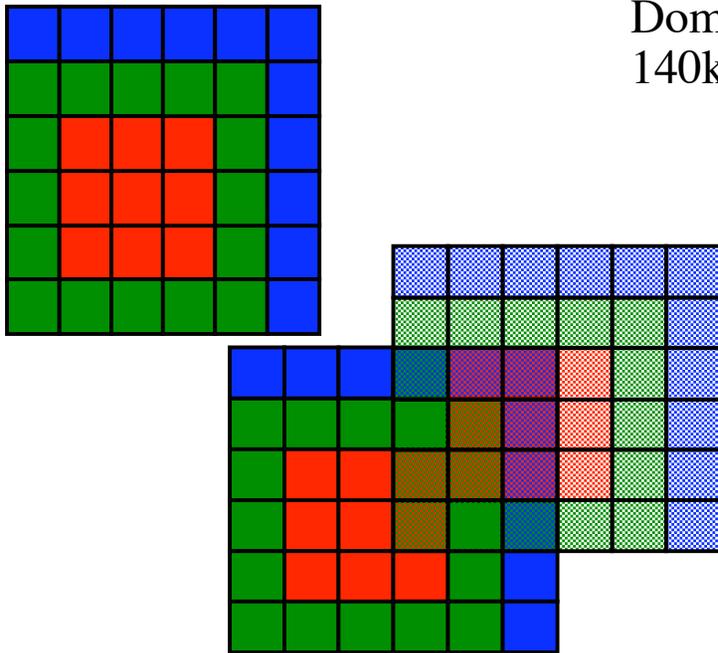
VORPAL's flexible domain decomposition allows full load balancing, good scaling

- Beowulf: 1.2GHz Athlons, fast ethernet
- Have seen good scaling on 128-256 SP processors

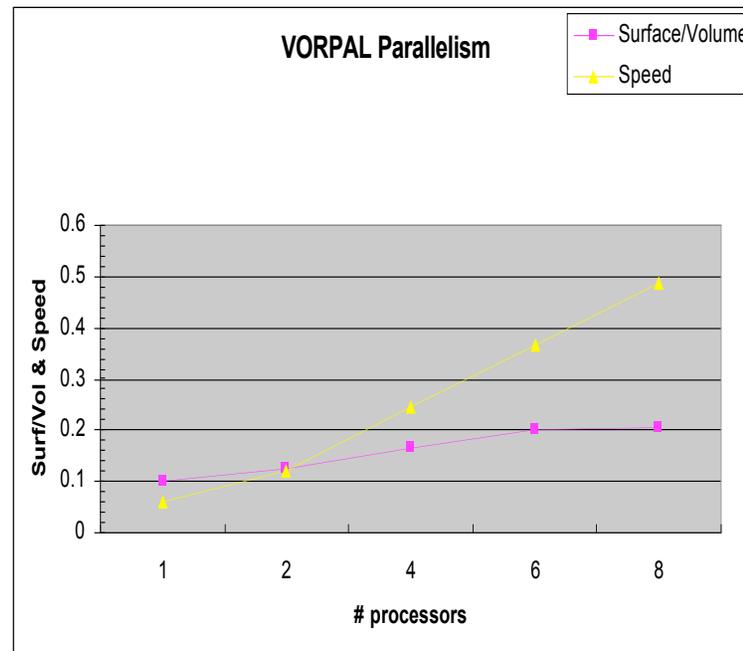


General decomposition *allows* load balancing

Domains down to 45x25x25 with 140k particles, 20% surf/vol

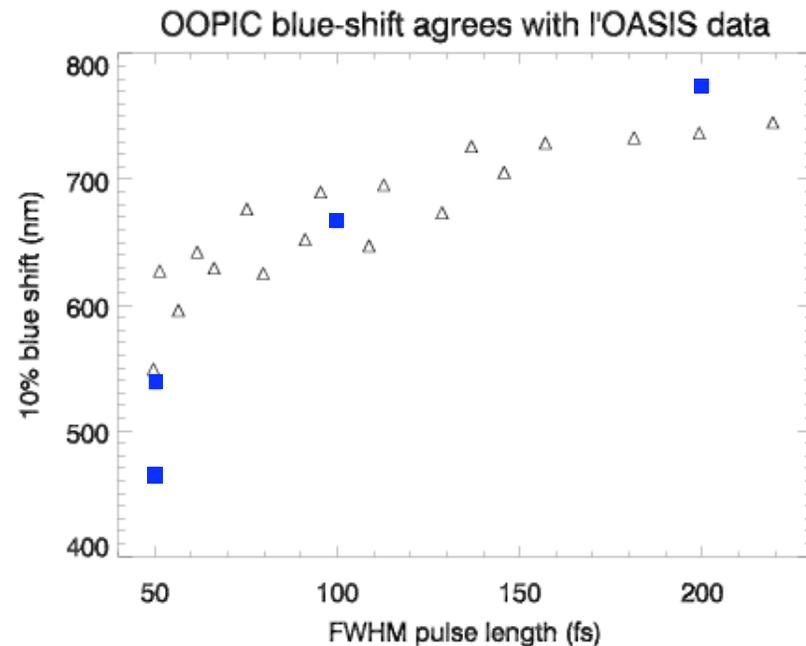


Set theory based messaging



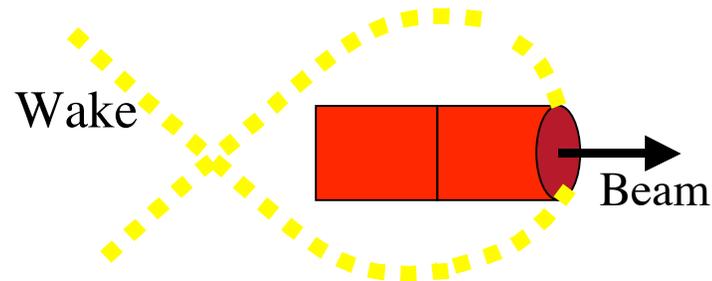
Moving Ionization Algorithms from OOPIC to VORPAL

- OOPIC is a 2-D (x-y & r-z) electromagnetic PIC code
 - Includes Monte Carlo collision (MCC) models
 - These enabled rapid implementation of relativistic electron-impact and field-induced tunneling ionization algorithms
 - Uses MPI for parallel computing (1-D domain decomposition)
- These ionization algorithms are being ported to VORPAL
- OOPIC ionization algorithms have been validated against data from the l'OASIS lab at LBNL:



quickPIC

- Quasi-static approximation: driver evolves on a much longer distances than wake wavelength
 - Frozen wakefield over time scale of the bunch length



- $\Rightarrow \lambda \text{ and/or } x_R \gg \lambda_z$ (very good approximation!)

Basic equations for approximate QuickPIC

- **Quasi-static or frozen field approximation converts Maxwell's equations into electrostatic equations**

Maxwell equations in Lorentz gauge

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2\right) \mathbf{A} = \frac{4\pi}{c} \mathbf{j}$$

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2\right) \phi = 4\pi \rho$$

Quasi-static approx.
 $\xrightarrow{\hspace{2cm}}$
 $\nabla \cdot \mathbf{A} = 0, A(z) = A(z - ct)$

Reduced Maxwell equations

$$\nabla^2 \mathbf{A} = \frac{4\pi}{c} \mathbf{j}$$

$$\nabla^2 \phi = 4\pi \rho$$

Local ρ, \mathbf{j} at any z-slice depend only on ρ, \mathbf{j} at that slice!

- $\mathbf{j} = \mathbf{j}_b + \mathbf{j}_e \approx \mathbf{j}_b = c n_b \hat{z}$ ($\mathbf{A} = A_{||} \hat{z}$)

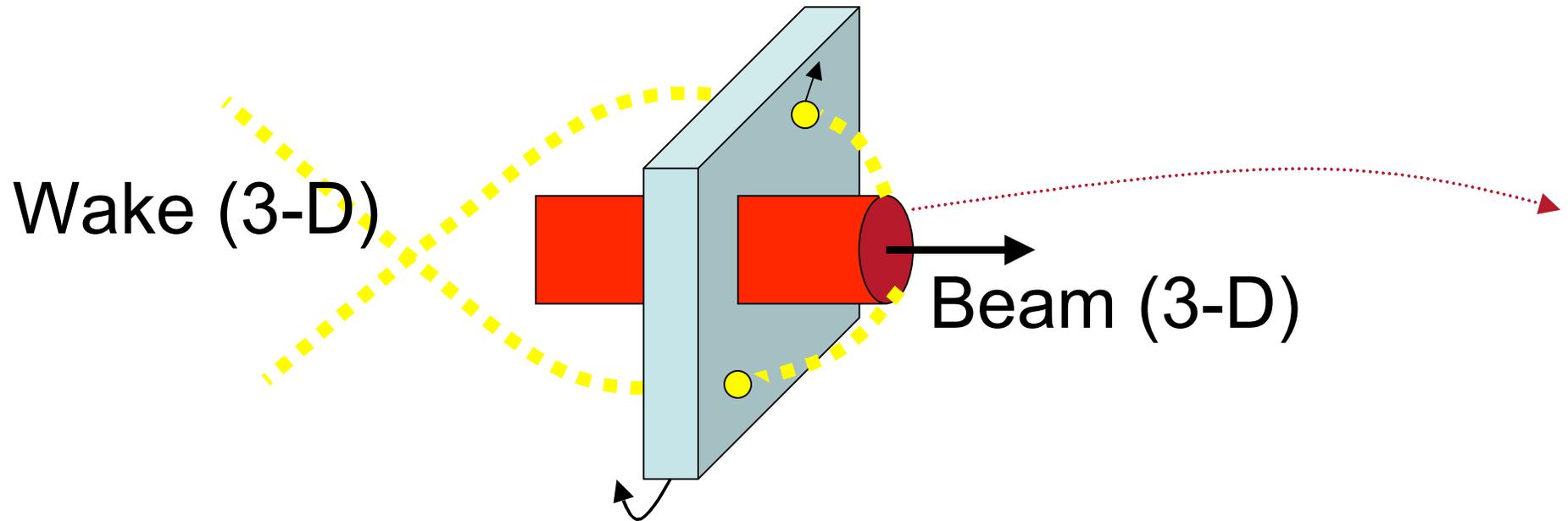
- $\phi = \int \rho A_{||}$

Forces :

plasma : $F_{e||} = -e n_e \phi$

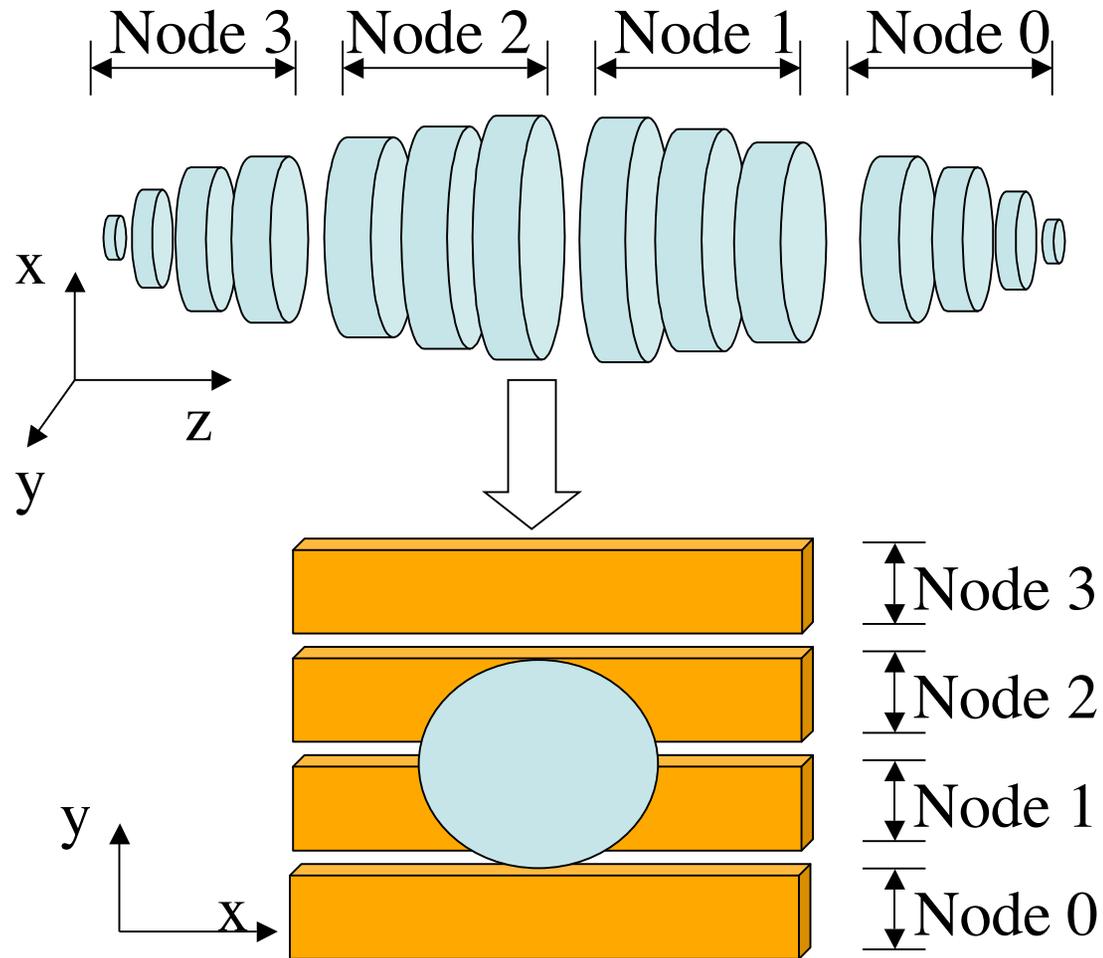
beam : $F_{b||} = e n_b \phi$

QuickPIC loop (based on UPIC): 2-D plasma slab



1. *initialize beam*
2. *solve $\nabla_{\perp}^2 \phi = \rho$, $\nabla_{\perp}^2 \psi = \rho_e - F_p$, $\nabla_{\parallel}^2 \chi = \rho_e - F_p$*
3. *push plasma, store ϕ*
4. *step slab and repeat 2.*
5. *use ϕ to giant step beam*

Parallelization of QuickPIC



Benchmarking

Full PIC: OSIRIS and OOPIC

particle drivers

laser drivers

Full PIC vs. quasi-static PIC: OSIRIS and quickPIC

particle drivers

PIC vs. Fluid:

Laser drivers

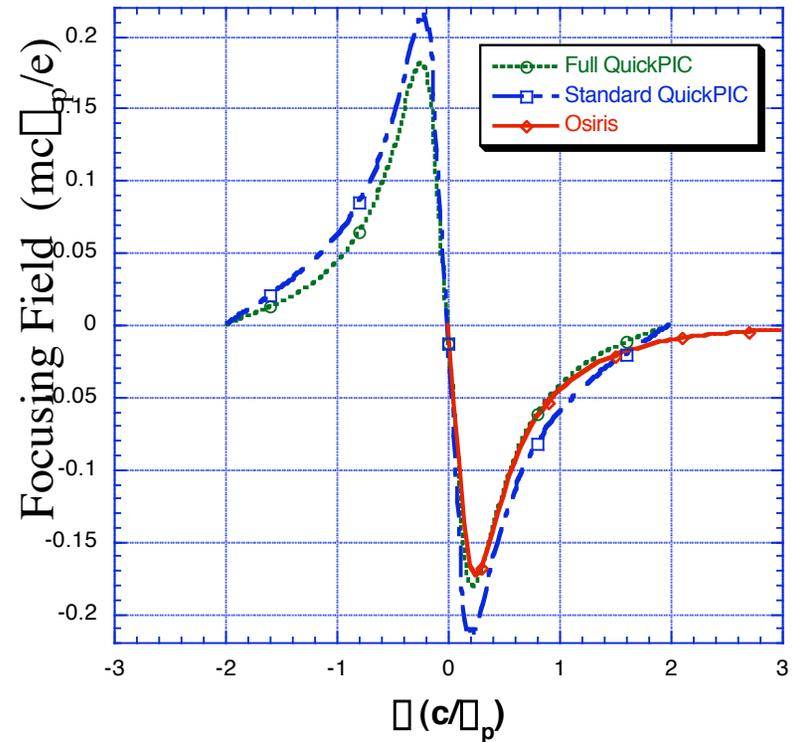
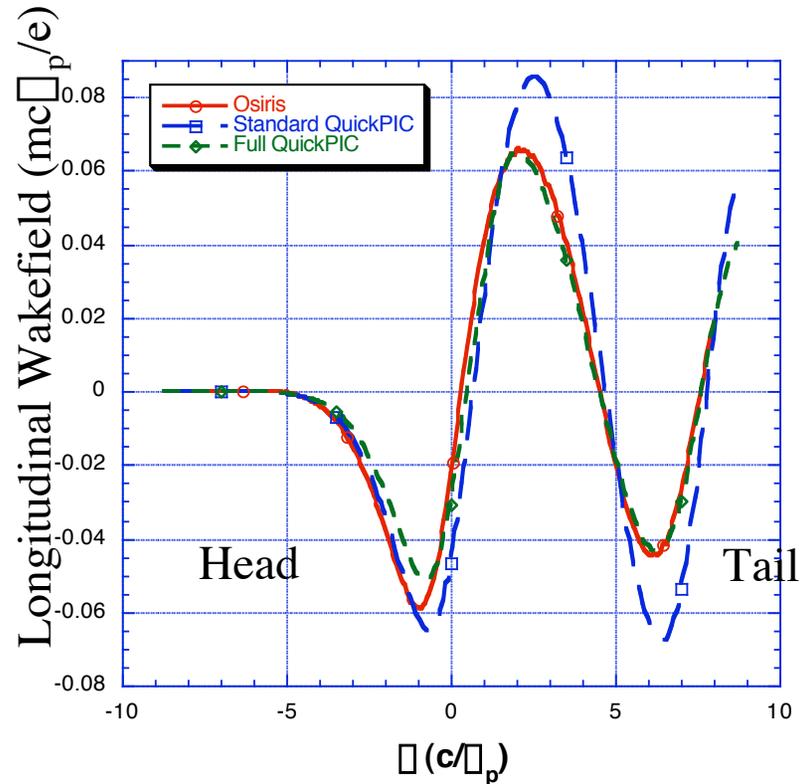
particle drivers

Simulation against theory

trapping mechanism in all optical injection

quickPIC vs. OSIRIS

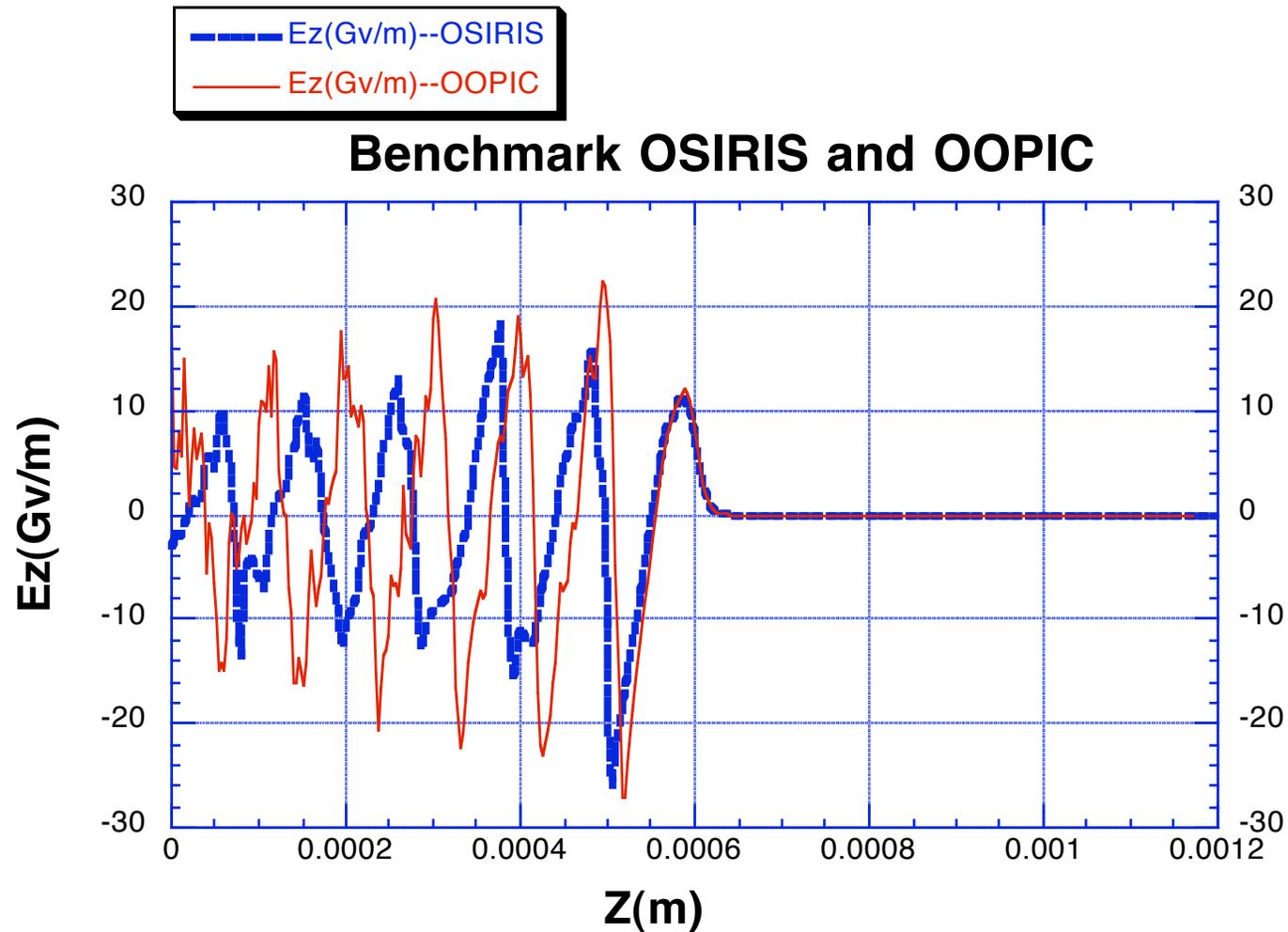
Positron driver



Plasma density = $2.1\text{E}14 \text{ cm}^{-3}$, Beam Charge = $1.8\text{E}10 \text{ e}^+$

Wakefield and focusing field from QuickPIC agree well with those from Osiris, and it is >100 times faster!

Benchmarking (2D) field ionization routines: OOPIC and OSIRIS



**Modeling experiments:
Code validation and interpretation of physics**

Plasma wakefield accelerator(PWFA)

E-157/E-162

electron acceleration/focusing

positron acceleration/focusing

Laser wakefield accelerator(LWFA/SMLWFA)

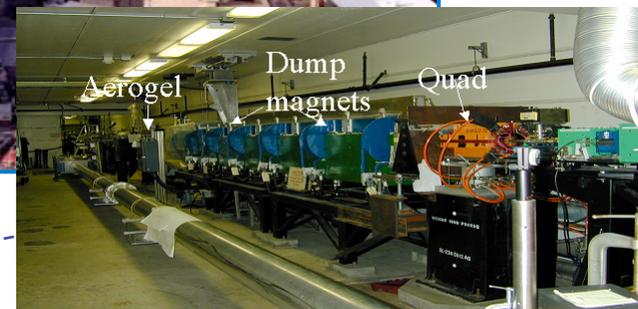
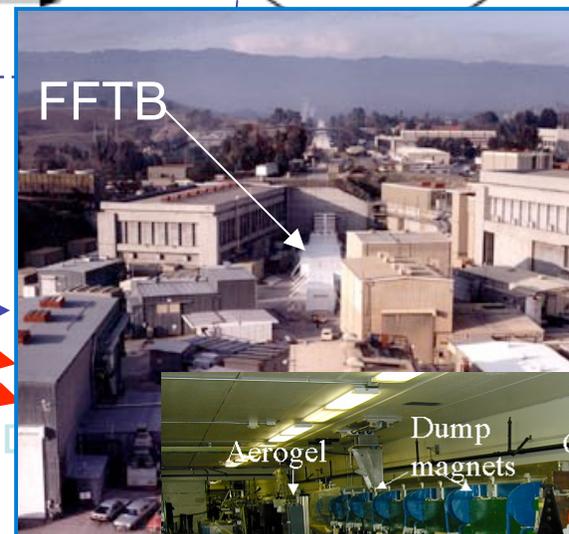
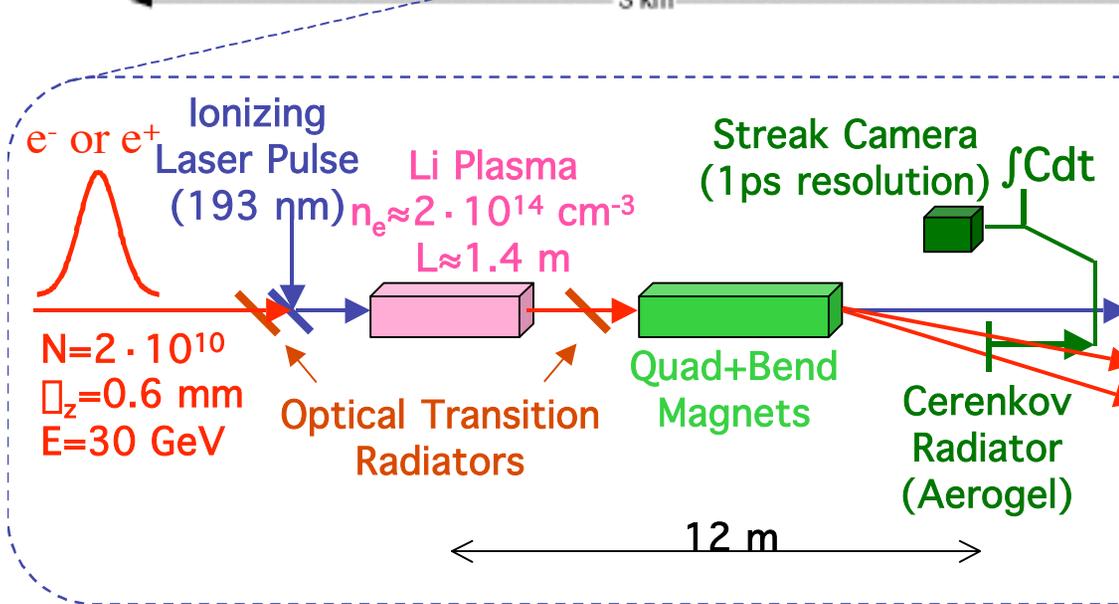
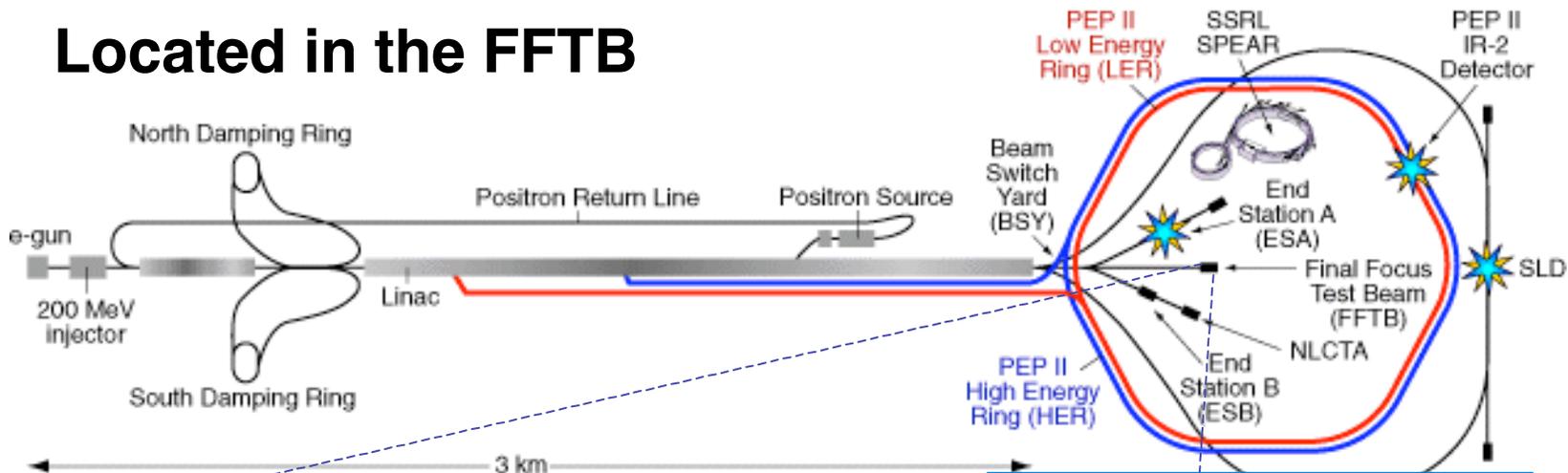
L'OASIS(LOA)

Blue shifts

self-trapped electrons



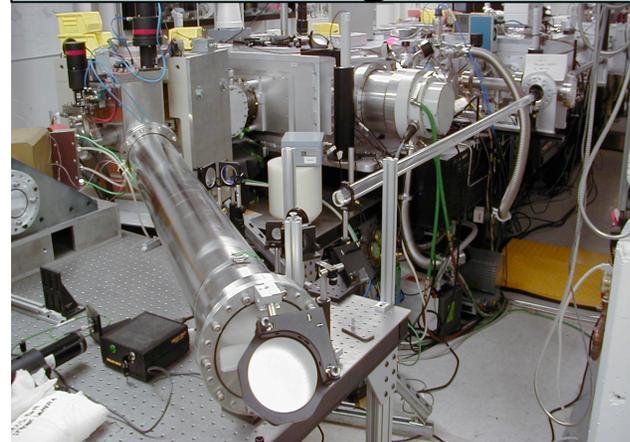
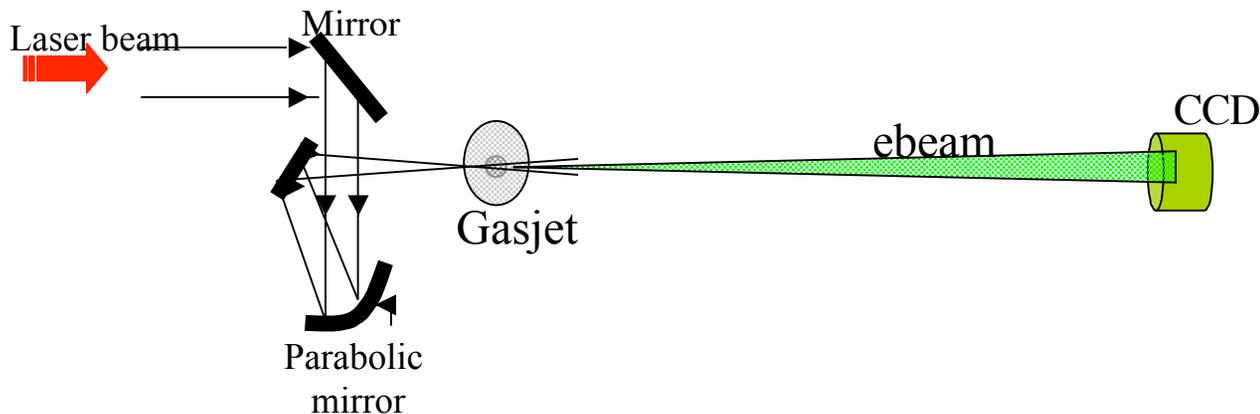
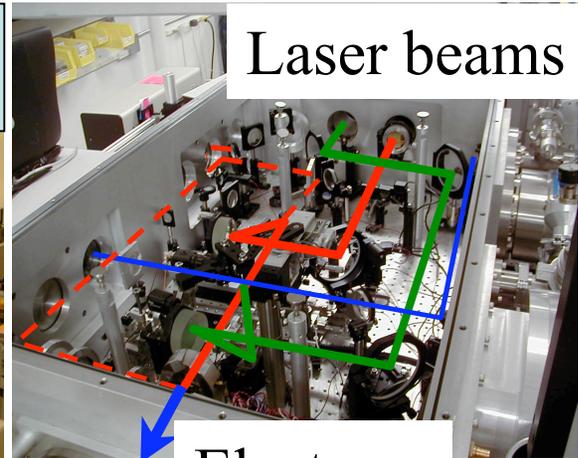
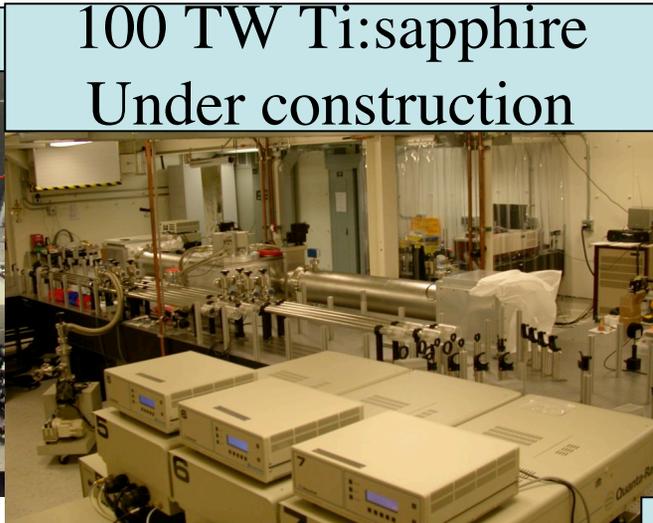
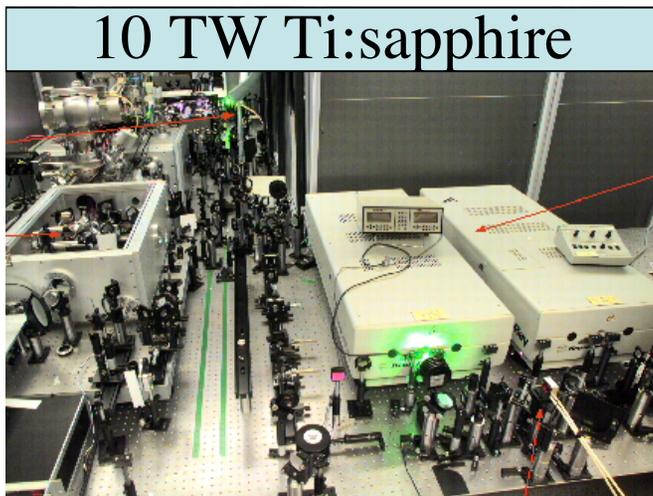
Located in the FFTB





Laser-plasma accelerator R&D at l'OASIS lab

- Test bed for R&D concepts towards 1 GeV module of a laser accelerator and applications
- Facility includes 10 TW, 50 fs laser system @ 10 Hz (100 TW under development)
- Laser, plasma and beam diagnostics; radiation shielded experimental bays
- Training ground for students and postdocs

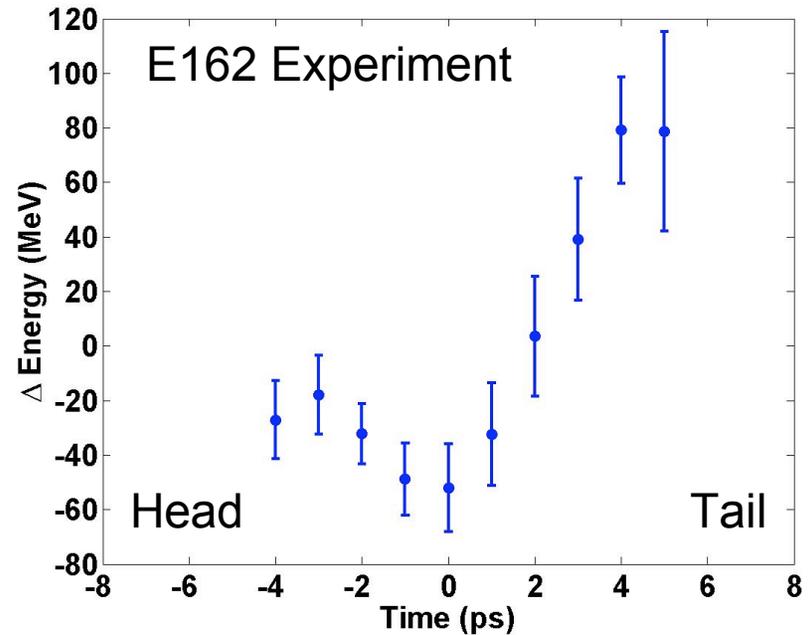
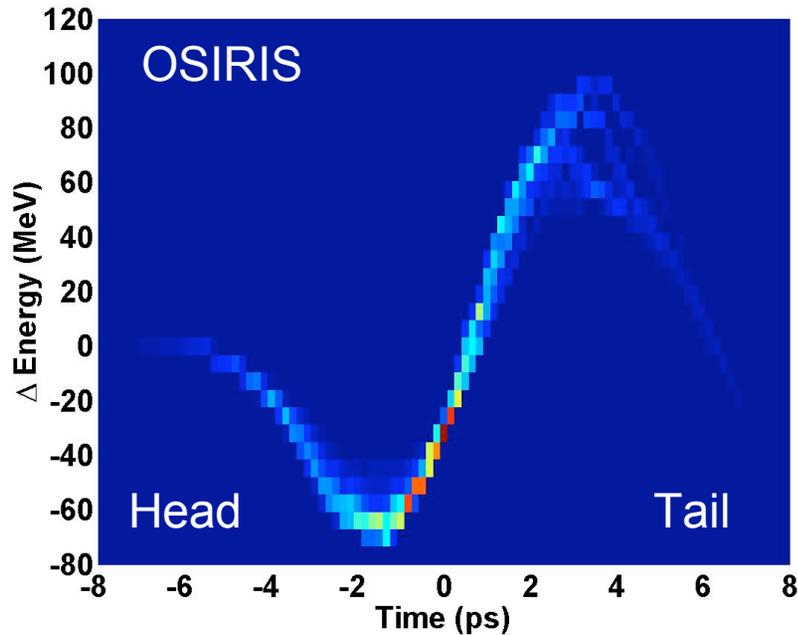


Excellent agreement between simulation and experiment of a 28.5 GeV positron beam which has passed through a 1.4 m PWFA

OSIRIS Simulation Prediction:
Experimental Measurement:

Peak Energy Loss
64 MeV
65±10 MeV

Peak Energy Gain
78 MeV
79±15 MeV

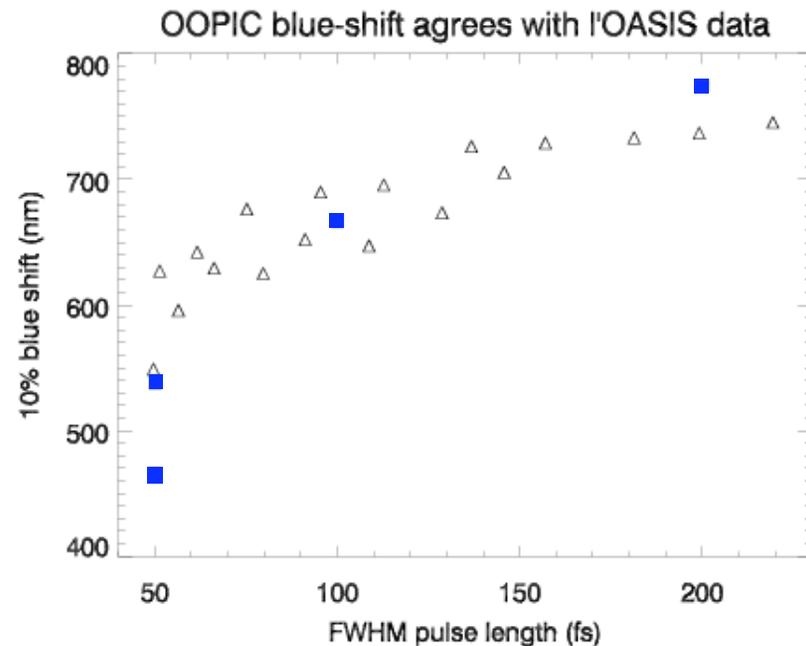


5×10^8 e⁺ in 1 ps bin at +4 ps

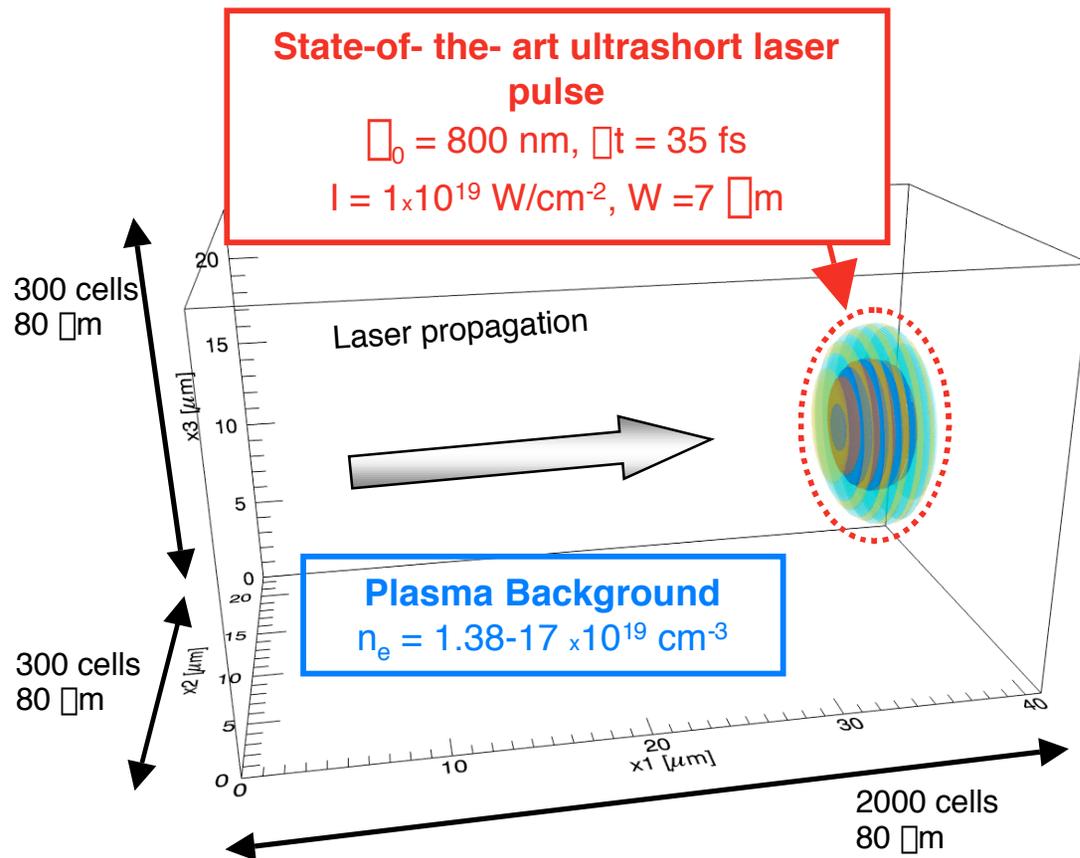
Moving Ionization Algorithms from OOPIC to VORPAL

- OOPIC is a 2-D (x-y & r-z) electromagnetic PIC code
 - Includes Monte Carlo collision (MCC) models
 - These enabled rapid implementation of relativistic electron-impact and field-induced tunneling ionization algorithms
 - Uses MPI for parallel computing (1-D domain decomposition)
- These ionization algorithms are being ported to VORPAL

- OOPIC ionization algorithms have been validated against data from the l'OASIS lab at LBNL:



Full scale 3D LWFA and SMLWFA simulations: L'OASIS parameters



•Simulation Parameters

–Laser:

- $a_0 = 3$
- $\lambda_l / \lambda_p = 3$ to 15

–Particles

- 1x2x2 particles/cell
- 200 million total

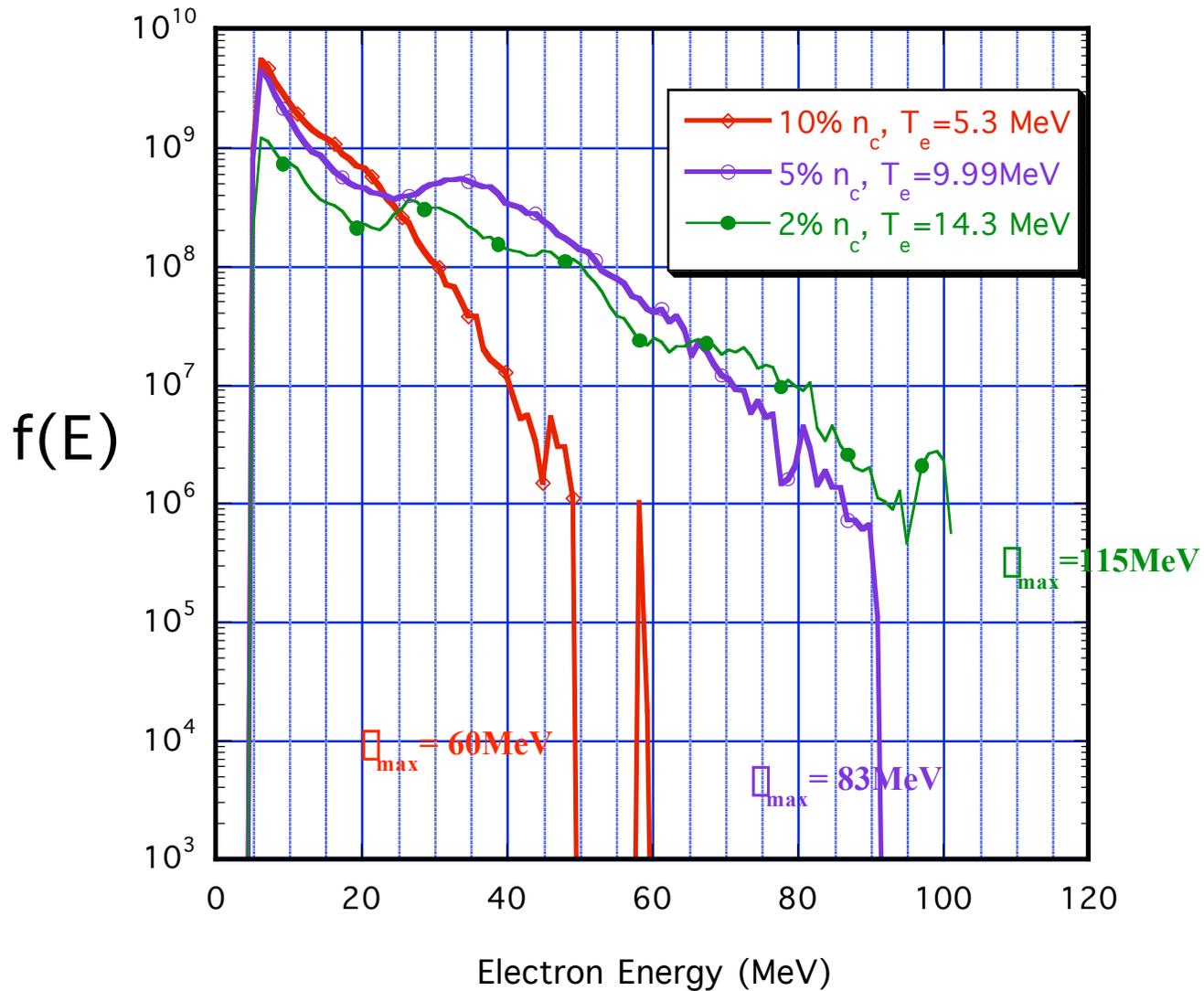
•The parameters are similar to those at LOA and **LBNL**

**Simulation ran for ~10000 time steps
(~3 Rayleigh lengths)**

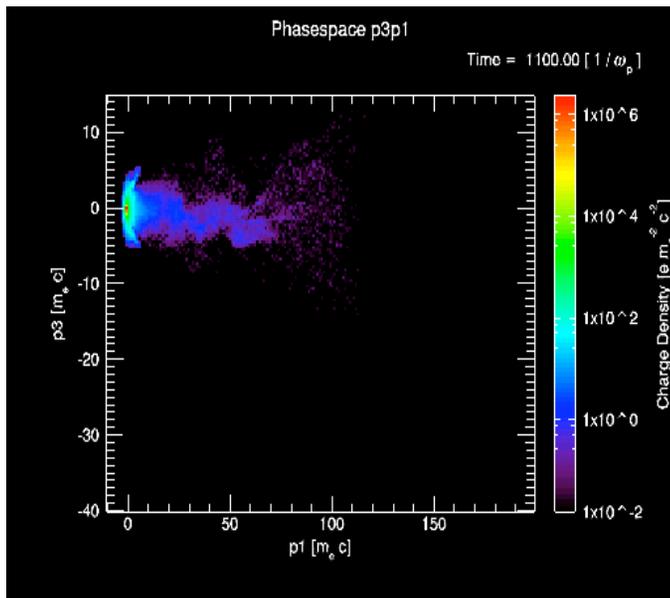
Electron spectra is **consistent** with results from LOA



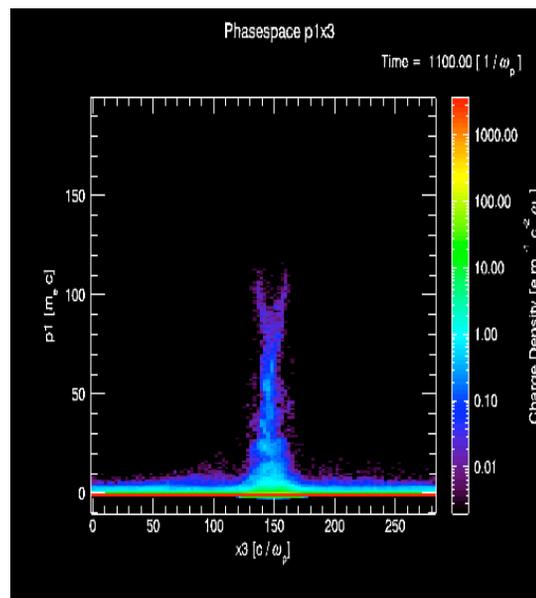
Energy Spectra of Fast Electrons



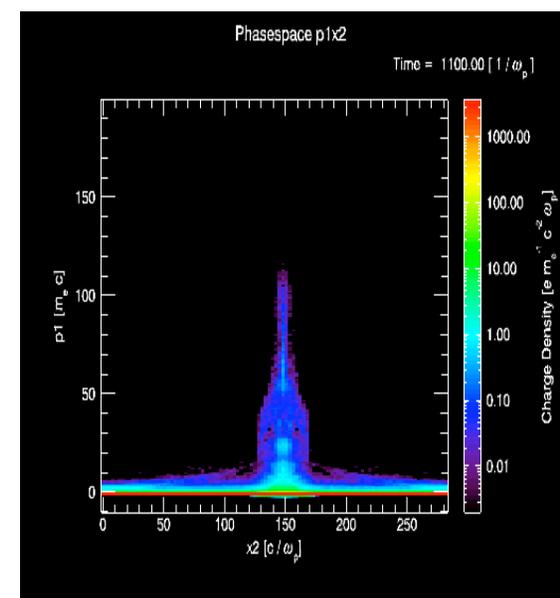
**In 3D the electrons have an asymmetric spot size in the plasma:
laser effects acceleration
what happens when they exit the plasma? (Electrostatic PIC combined with semi-analytical model: Fubiani)**



p3 vs. p1



p1 vs. x3



p3 vs. x2

**Modeling planned experiments:
Providing guidance**

Plasma wakefield accelerator(PWFA)

E-164/E-164x

high-gradient electron acceleration

bunch length scaling

ionization

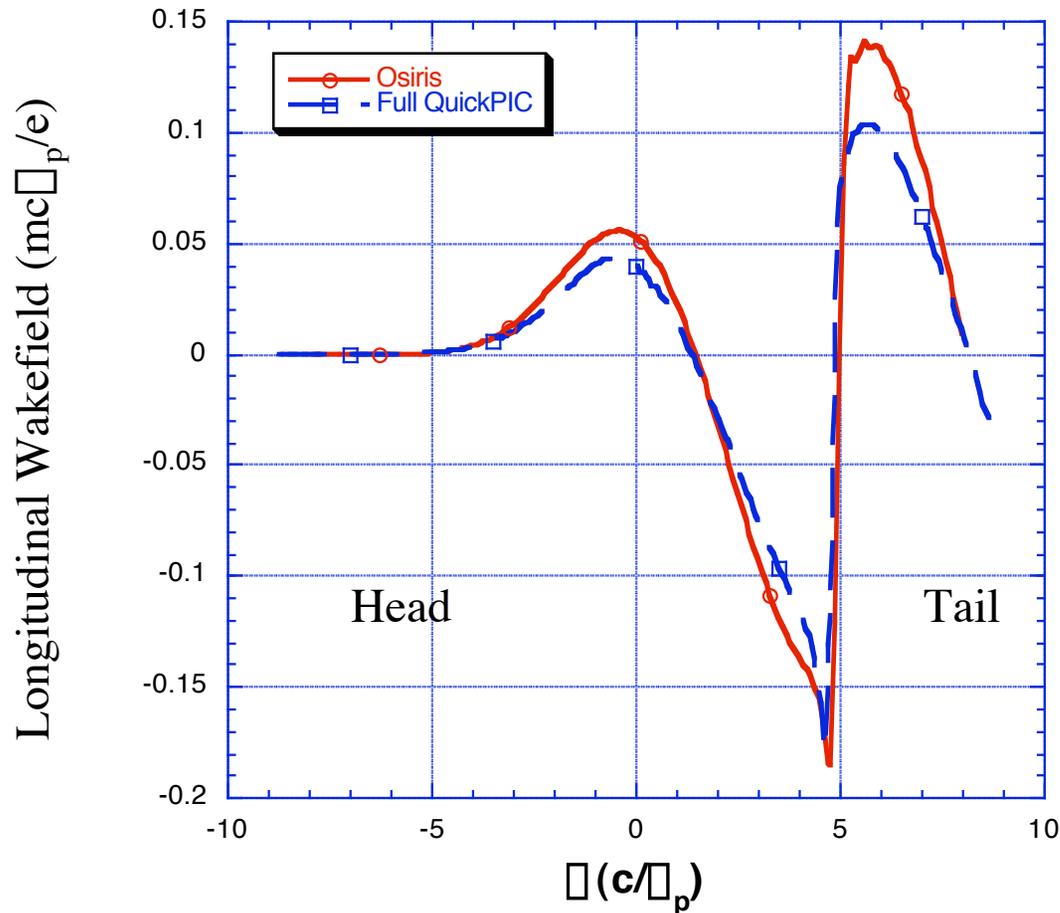
Laser wakefield accelerator(LWFA/SMLWFA)

L'OASIS(LOA)

all optical injection

acceleration in channels

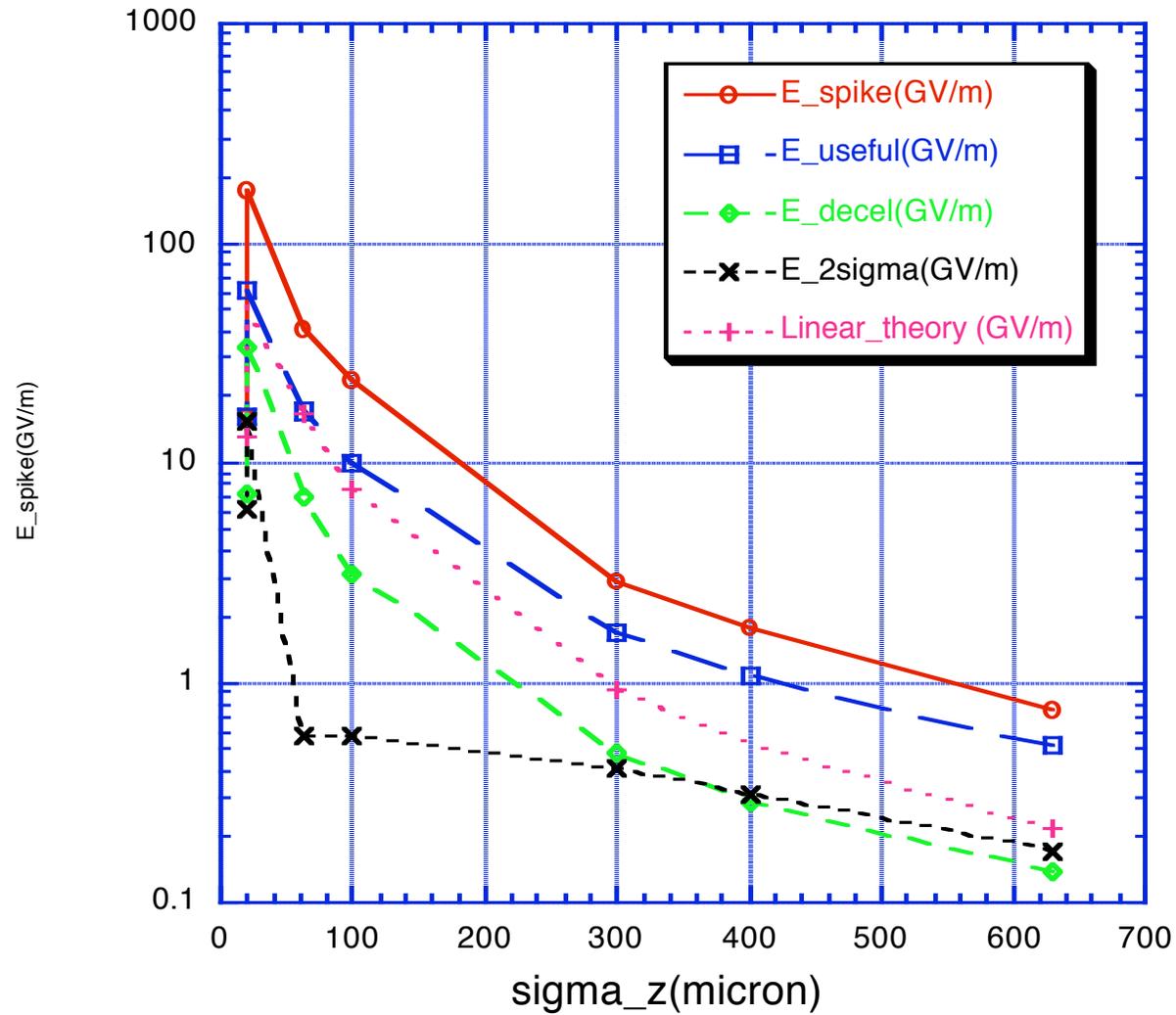
Benchmarking



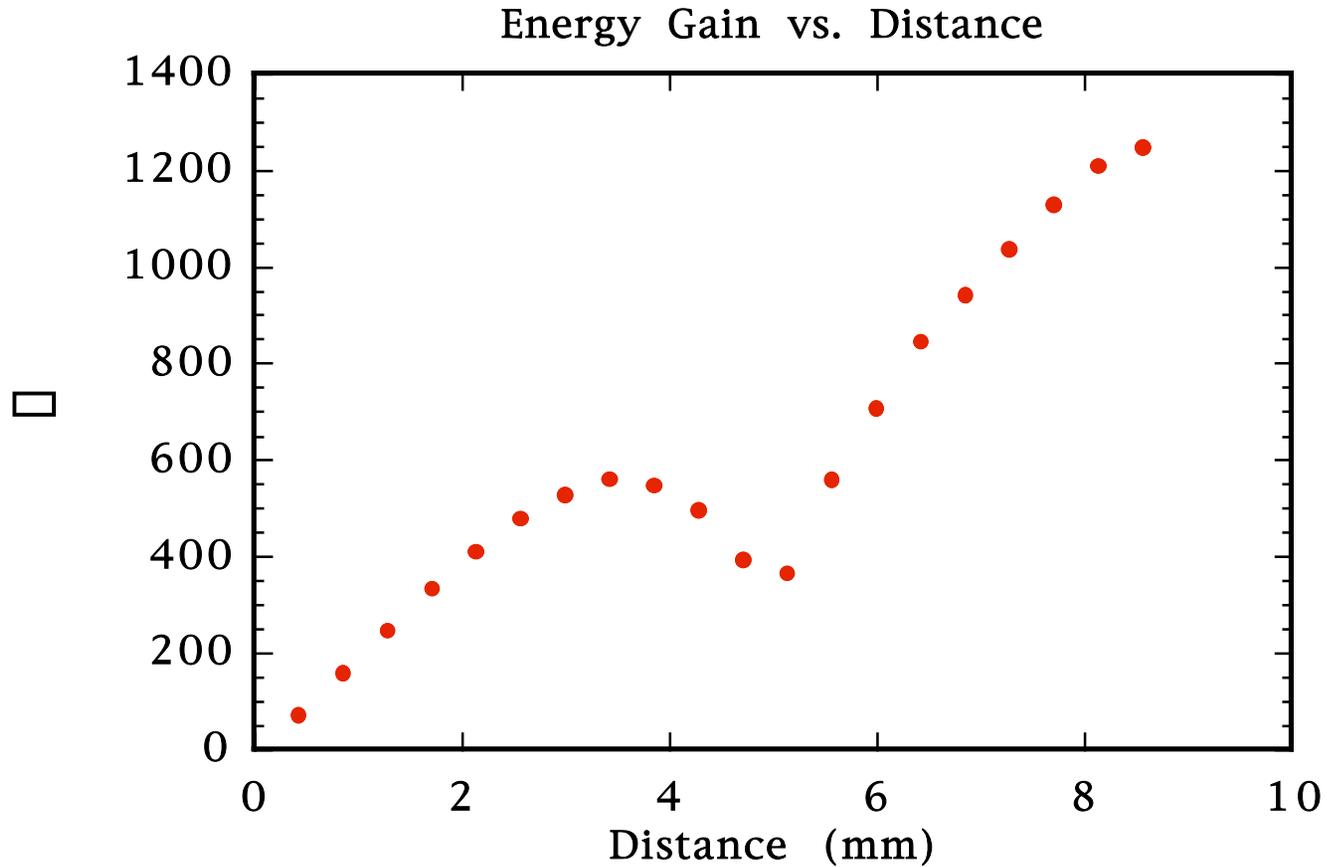
Result from benchmark run with plasma density = $2.1E14 \text{ cm}^{-3}$, beam charge = $1.8E10 \text{ e}^-$. QuickPIC run with periodic boundary, Osiris run with conducting boundary.

Bunch length scaling: E164 and Afterburner parameters

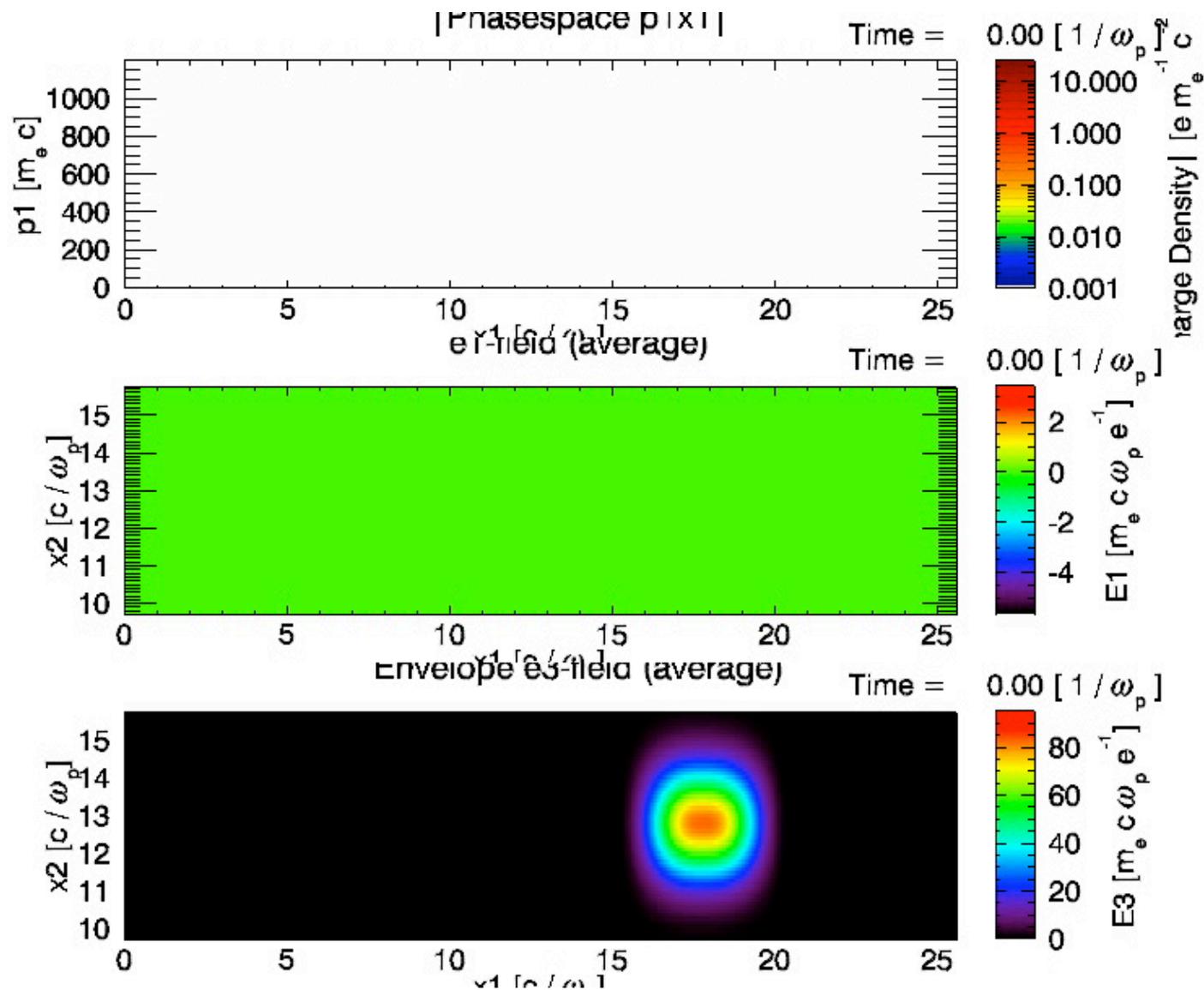
$\Sigma_r=25$ micron



Pulse distortion leads to a second phase of acceleration



Modeling a 5TW 50 fs laser propagating through 60 Raylengths in a plasma channel





Fluid Code: Laser pulse in a channel

- 2D Fluid-Maxwell Code
 - Relativistic and nonlinear
 - No averaging: laser oscillations resolved
 - Moving window
- Detailed comparisons to particle codes in progress
- Example: Laser pulse in a plasma channel
 - Wakefield generation
 - Laser pulse energy depletion
 - Frequency red-shifting
- Parameters: Achievable at the l'OASIS lab

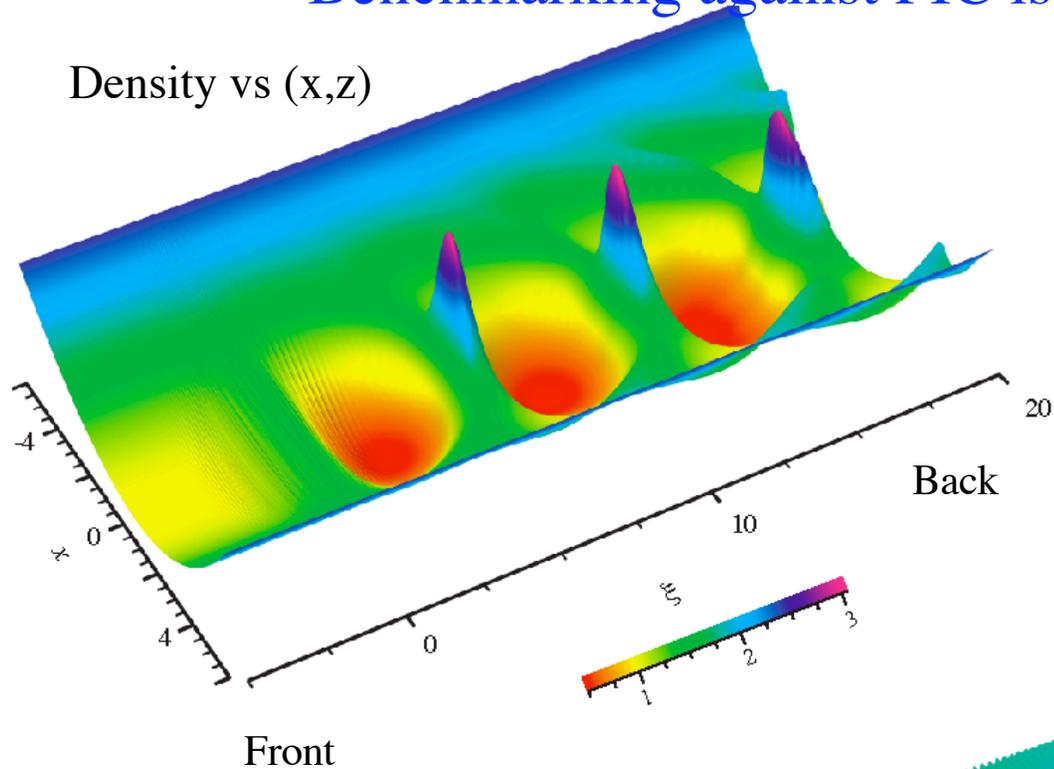
$$L_{\text{FWHM}} = 30 \text{ fs}, \lambda_0 = 0.8 \mu\text{m}, r_0 = 12 \mu\text{m}, Z_R = 565 \mu\text{m}, P = 4.84 \text{ TW}$$

$$\lambda_p = 24 \mu\text{m}, n_0 = 4.35 \times 10^{18} \text{ cm}^{-3}, \Delta n_c = 7.84 \times 10^{17} \text{ cm}^{-3}$$

$$L_D = 2.16 \text{ cm}, E_0 \approx 133 \text{ GV m}^{-1}, E_z|_{\text{max}} = 41.3 \text{ GV m}^{-1}$$

Laser Wakefields in Plasma Channel

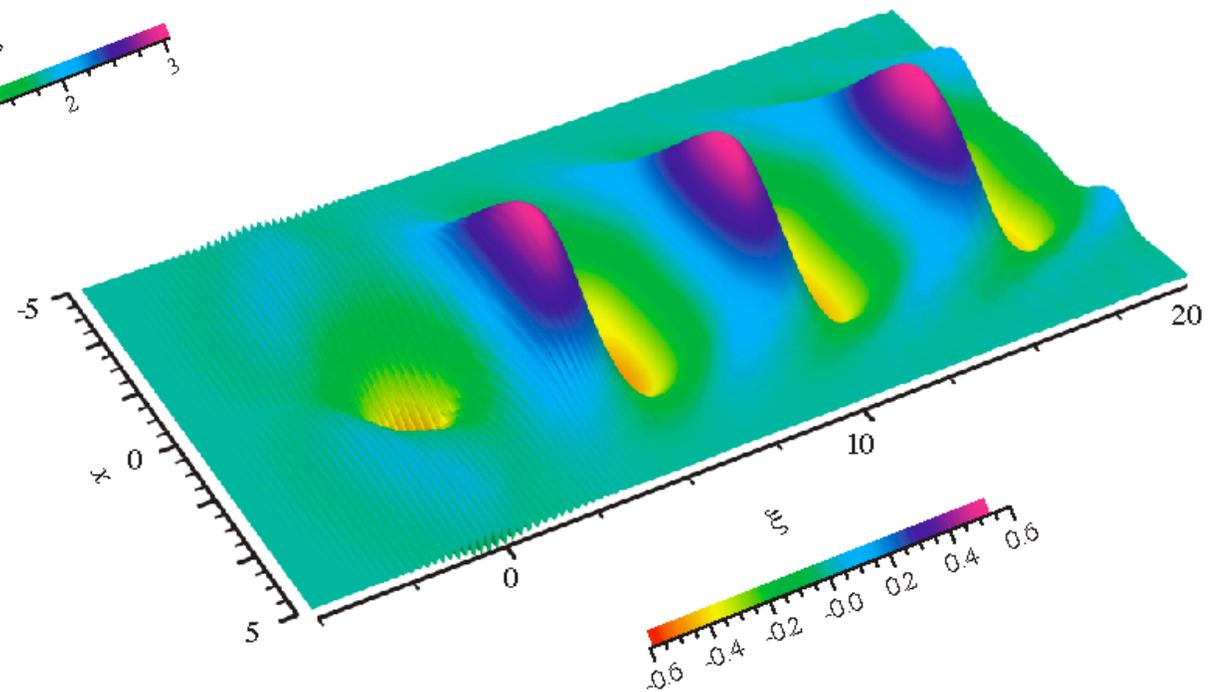
Benchmarking against PIC is beginning



Nonlinear plasma wave

$$\square_p t = 240 \text{ (0.9 mm)}$$

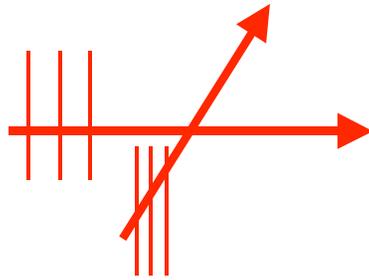
Longitudinal Electric Field vs (x,z)



Research focus: How can one inject particles into accelerating region of phase space?

Investigating multiple methods for optical inject, those of others and ours

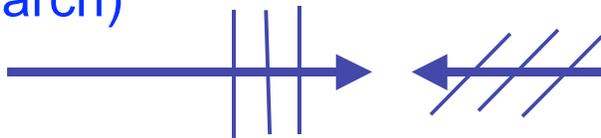
- LILAC



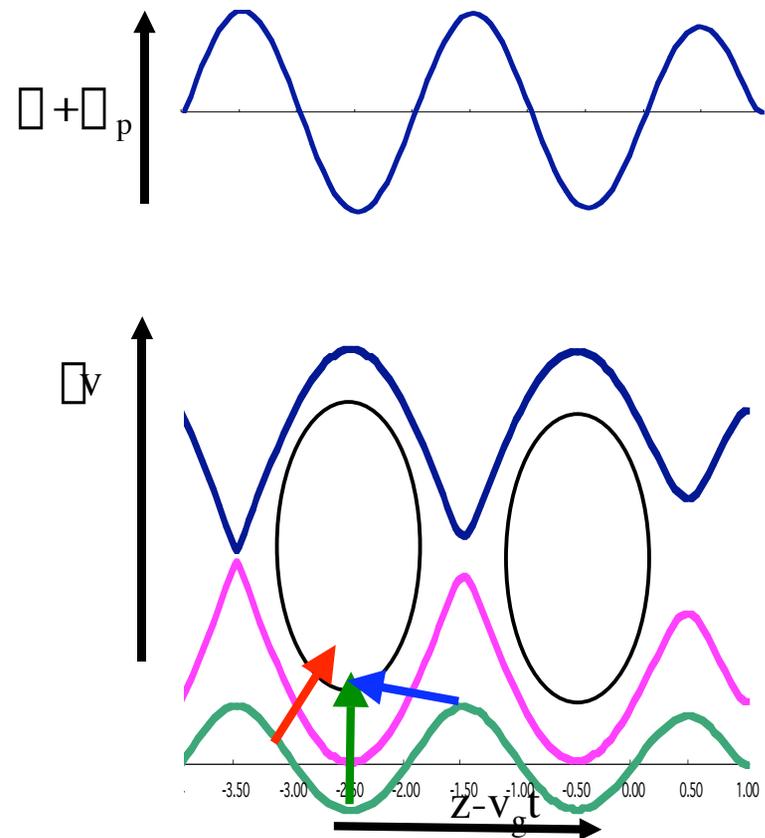
- Beat wave (LBNL)



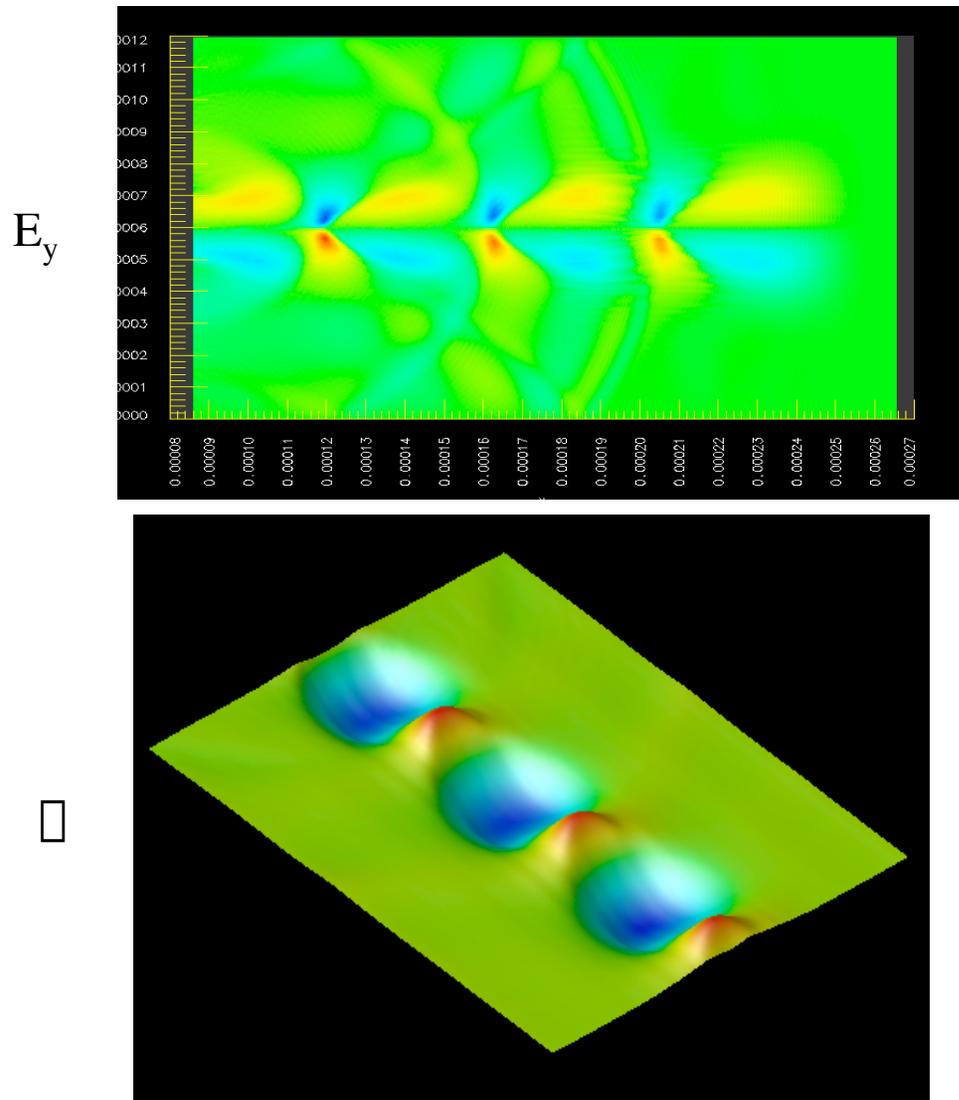
- Phase kick (result of this research)



All require moving particles to accelerating/focused region in phase space



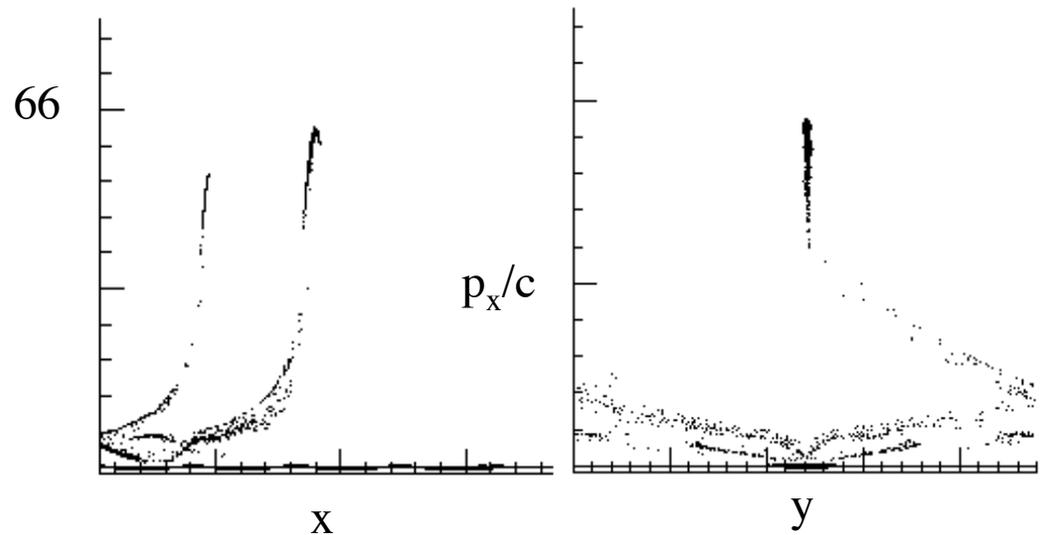
Discovery: The expansion of the focusing region for nonlinear wakes improves trapping mechanism



- Focusing region greatly expanded
- Focusing trajectories exists for positive potential
- Consequence: small phase kick can trap particles

Simulations show that focusing collimation forms the beam

- Region of negative potential energy is focusing
- Region of negative phase relative to minimum is accelerating
- Particles stay in this region while accelerating provided they are inside the F/D transition invariant curve
- Place large population of particles just inside this curve and dynamics forms beam after 1/4 of synchrotron (bounce) oscillation



Laser propagates along x

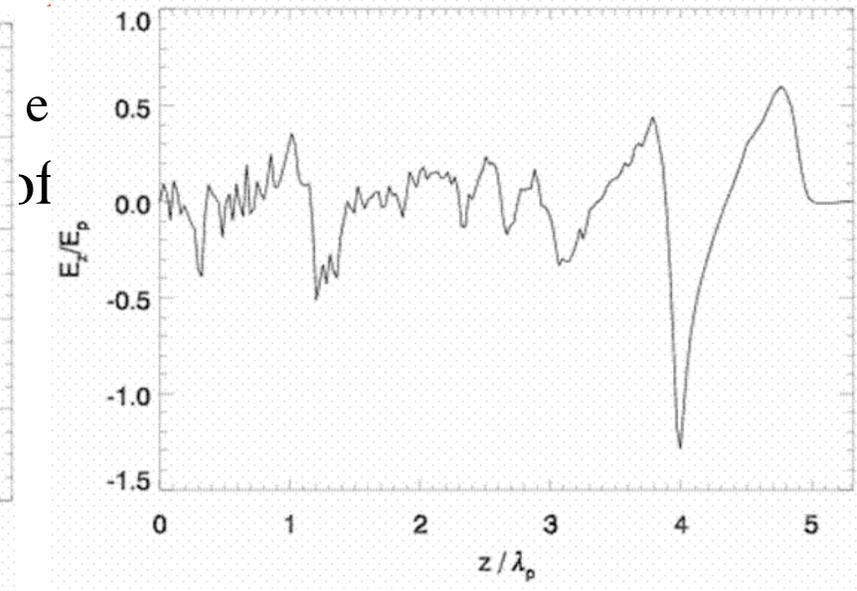
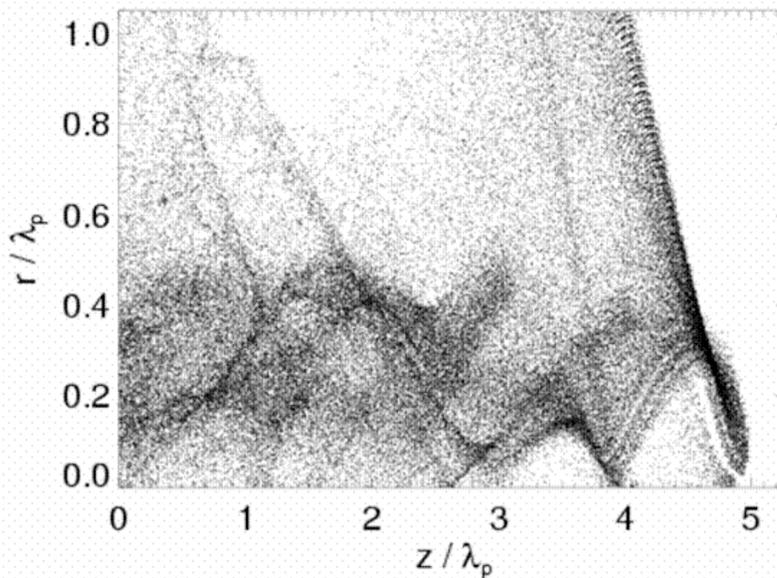
Overplotting shows beams worse than they are
Simulations showing secondary beams

**Beyond planned experiments:
Afterburner modeling**

Nonlinear wakes
preformed
self-ionized
Nonlinear beamloading
Stability: hosing
Final focusing

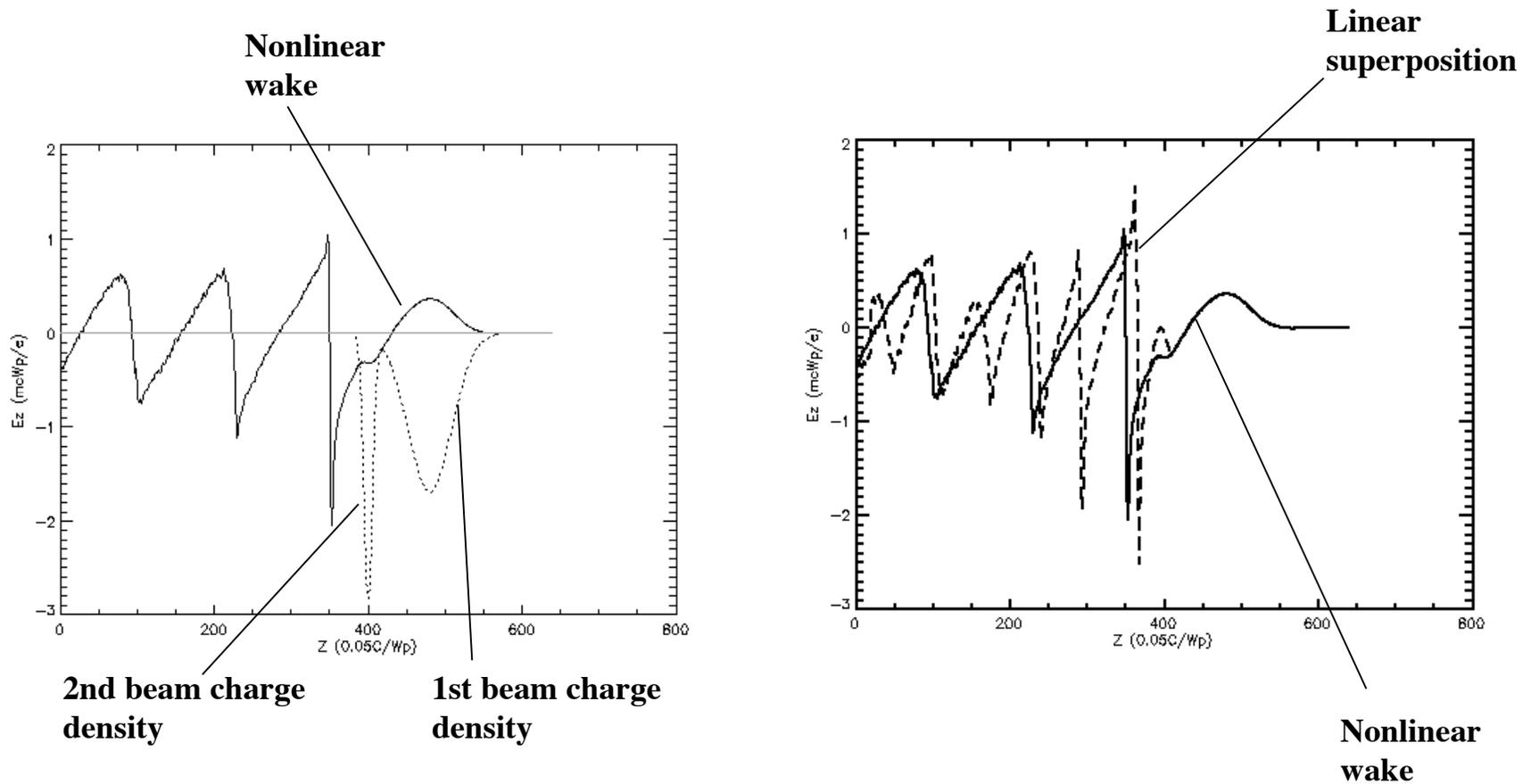
OOPIC shows that a PWFA e- driver can ionize neutral Li

- OOPIC simulations show that tunneling ionization plays a key role in the PWFA afterburner concept
 - The self-fields of the bunch can ionize Li or Cs
 - High particle density (i.e. large self-fields) is required to drive a strong wake
- In Li, a shorter afterburner drive beam could ionize the plasma by itself
 - *This approach would greatly simplify beam-driven wakefield*

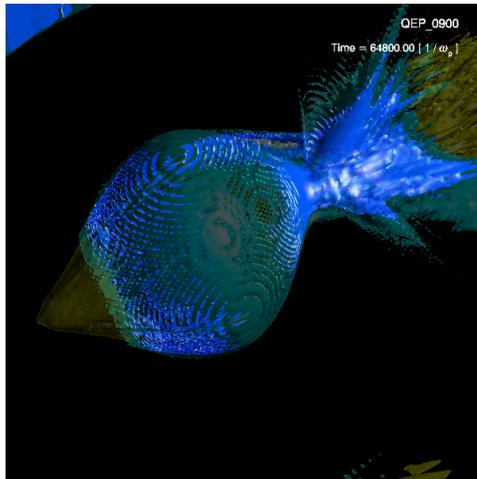
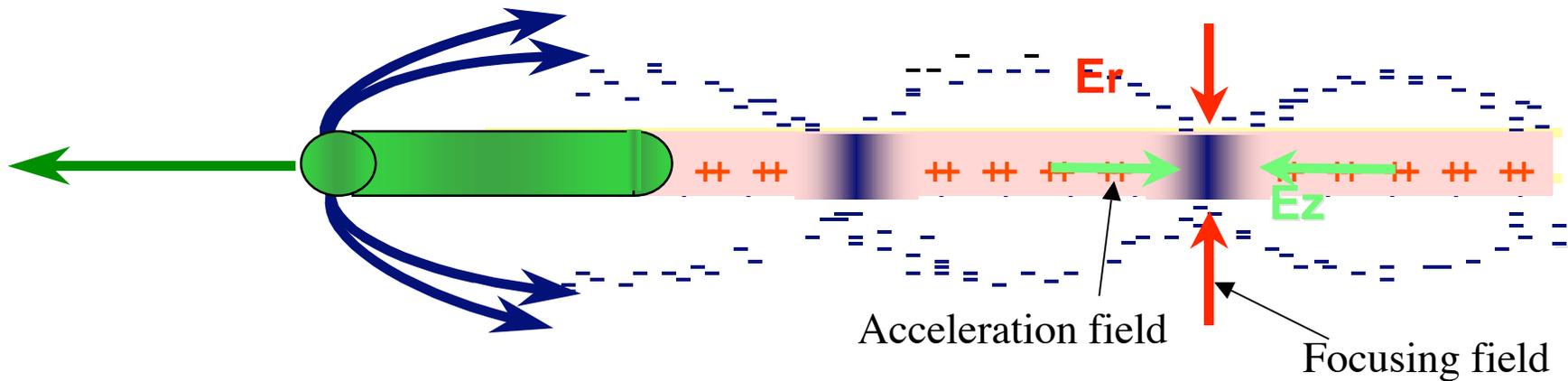


1+1 \neq 2:

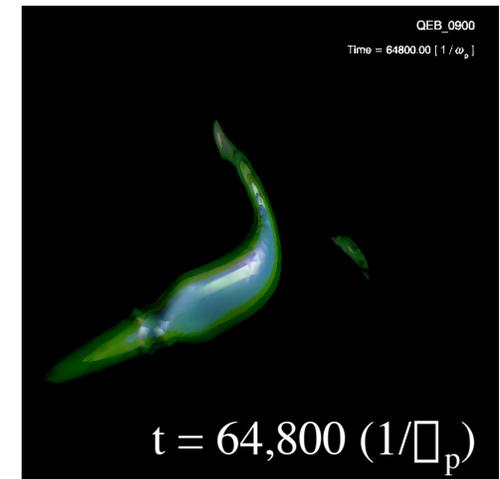
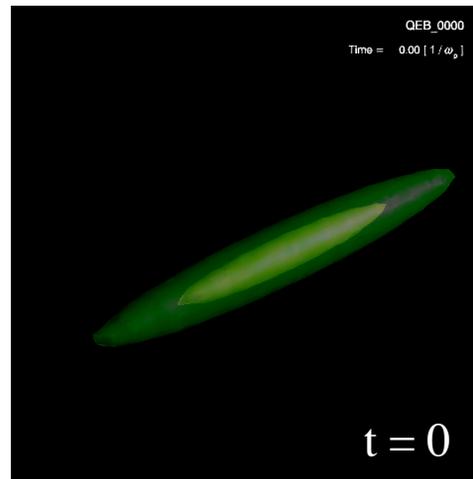
Superposition cannot be used for nonlinear beamloading



Hosing can be studied for afterburner parameters using quickPIC



3D image of the plasma charge density under blow-out regime



Electron drive beam hoses as it propagate over a long distance in the plasma

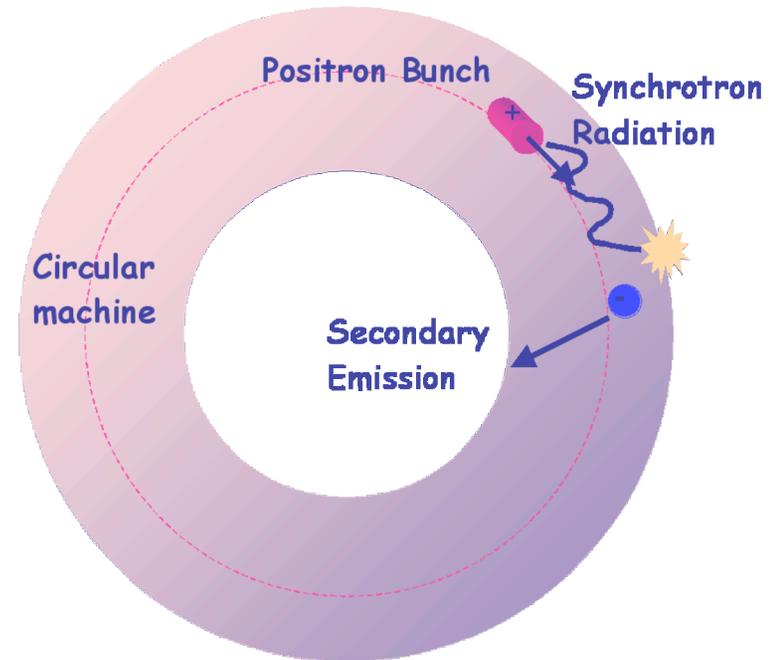
Connections to other areas in accelerator modeling

*electron-cloud modeling using plasma codes:
quickPIC*

***Beam-Beam codes use parts of UPIC:
UPIC is a parallel PIC Framework (it includes
PLIB) which is a general computer
science component to this project***

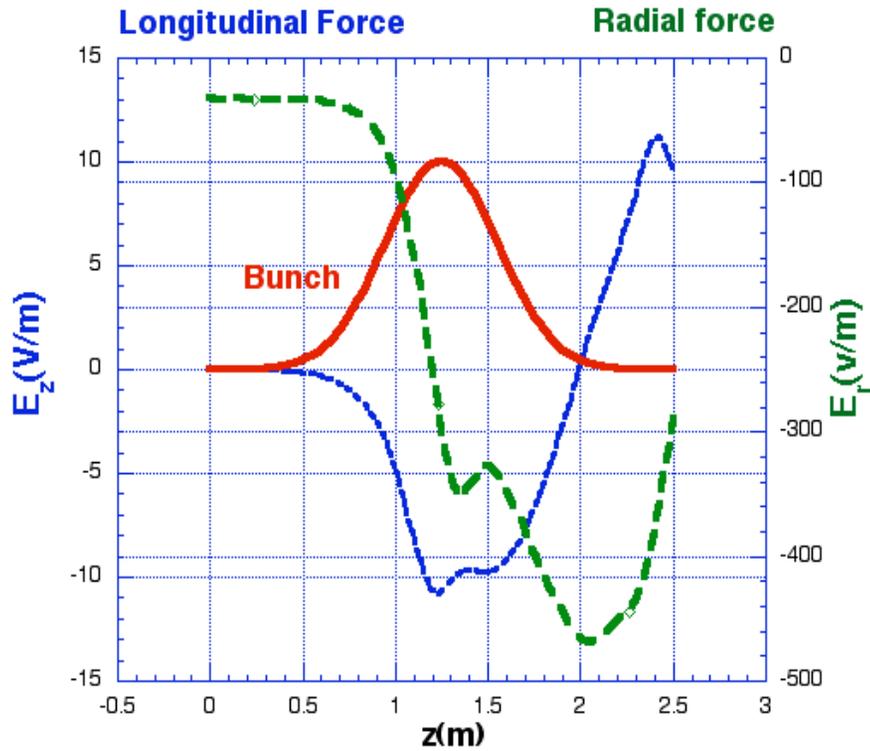
Plasma Modeling of Electron Cloud Instability

- E-cloud formation(Positron):
synchrotron radiation+secondary emission
- E-cloud formation(Proton):
halo scraping+secondary
- Observed in circular accelerators like:CERN-SPS and SLAC-PEP and KEKB
- Major concern in LHC Design, Fermilab upgrade

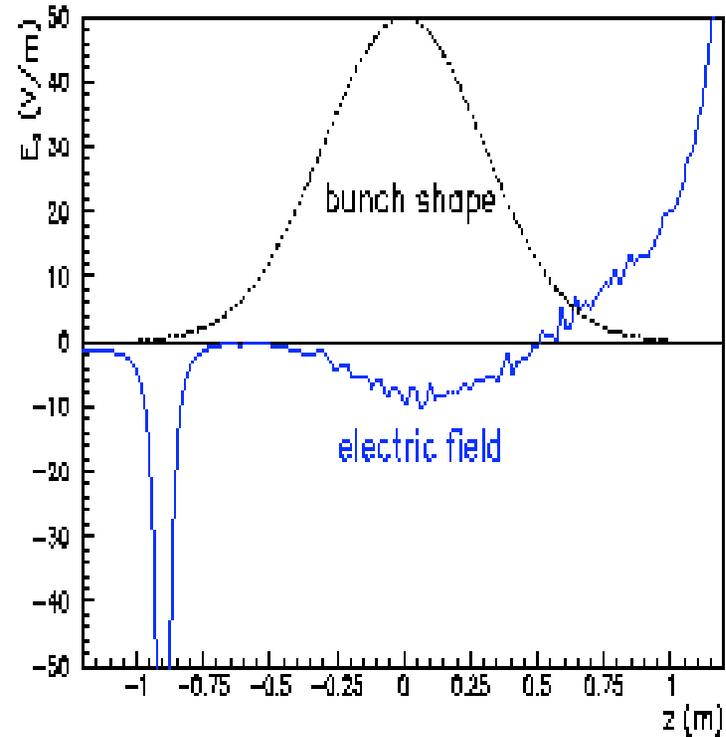


- e-cloud is a non-neutral plasma -- well suited to plasma wakefield PIC models
- Previous cloud models-- single node workstations
 - treat cloud as a **single kick once per orbit**
 - No image forces from beam pipe
 - No benchmarks-- poor agreement with experiments

Code Comparison

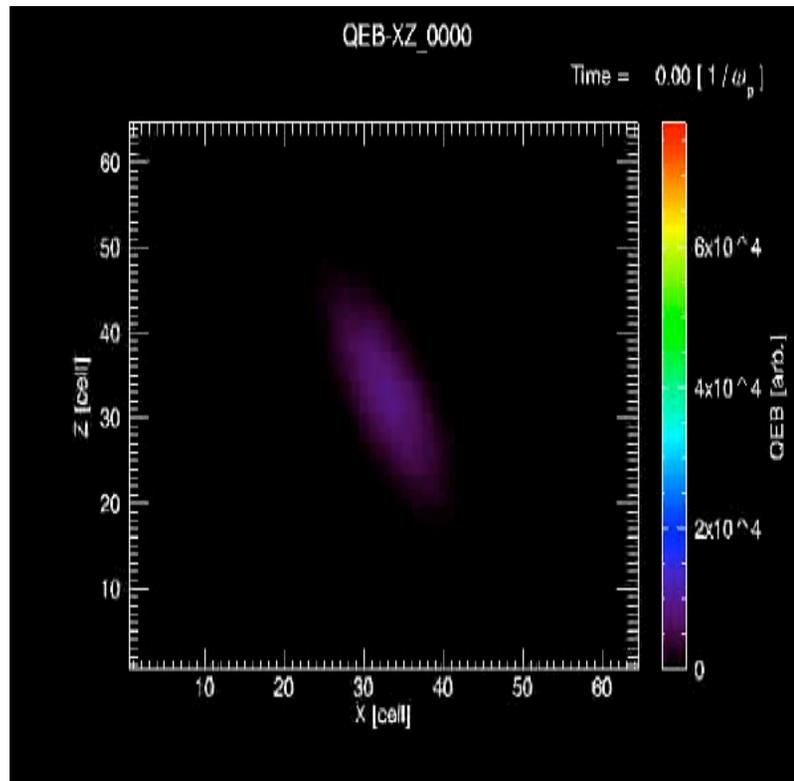


Transverse and Longitudinal wakes vs. z
(From QuickPIC)

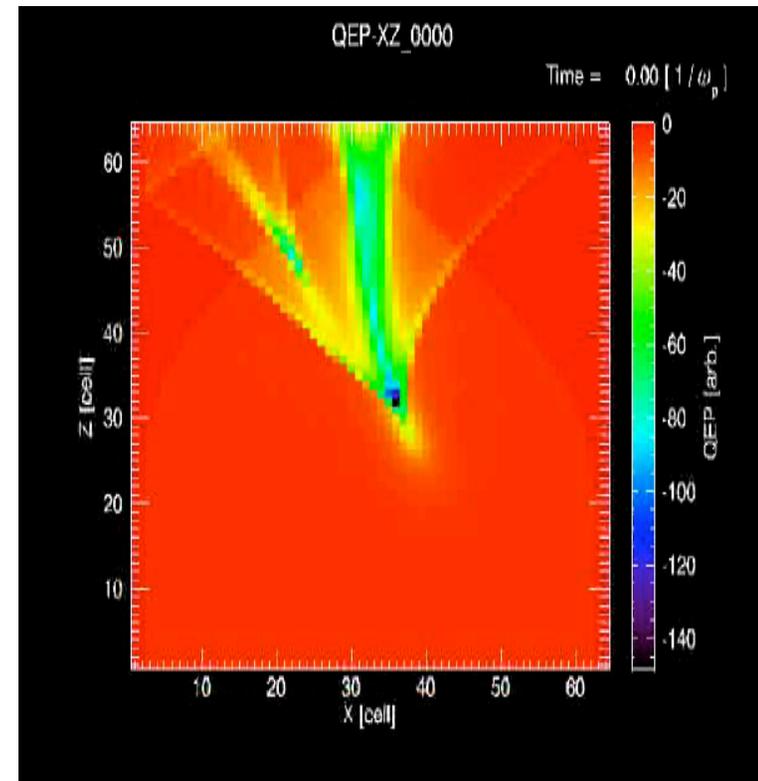


Longitudinal wake vs. z
unphysical divergence!
(From HEAD-TAIL)

QuickPIC Model of Beam & Cloud Evolution Through 40Km of SPS Proton Ring at CERN (6 turns)



**Beam
Density**



Cloud Density

Recently 700km (100 turns) was modeled

Connections with ISIC's

APDEC:

***Parallel Poisson solvers for elliptical conductors
for applying quickPIC to e-cloud***

Modeling gas jets

Laser-plasma experiments

**Strong educational component:
Includes those directly funded and those who are
closely coupled to the effort**

Graduate students:

CK.Huang, W.Lu, R.Narang (UCLA)

S.Deng, A.Z.Ghulam

G.Fubiani (LBNL)

J.Regele (UofColorado)

Young researchers:

F.S.Tsung (UCLA)

C.Nieter (UofColorado)

R.Giaconne

**SciDAC has greatly accelerated progress:
Collaboration, computational resources, applied math**

Code development:

- *benchmarking of codes against each other*
- *cooperation of ionization routine development*
- *rapid construction of new codes:*

Vorpal

quickPIC for e-cloud

Collaboration in science:

- *electron-cloud*
- *all-optical injection collaborative effort*

Enabling computational resources :

- *Full-scale modeling of SMLWFA experiments*
- *Full-scale modeling of E-162*
- *Modeling of LWFA in a channel*