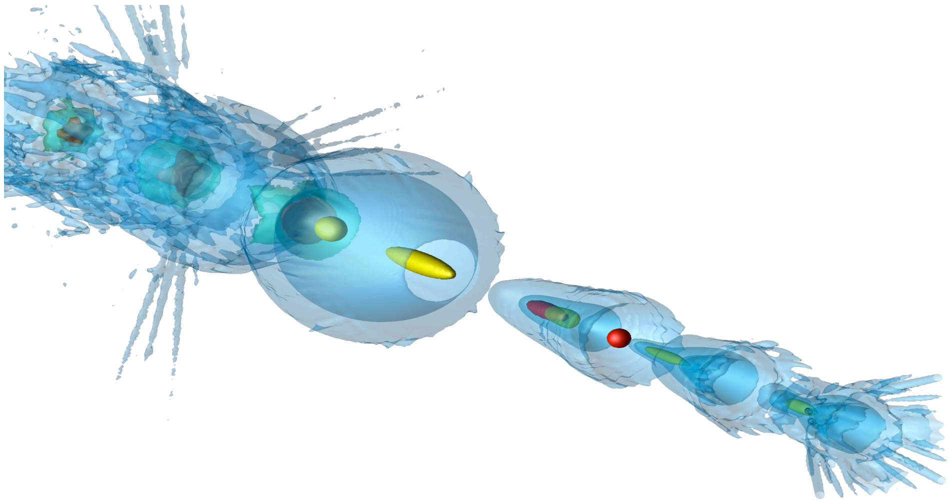
Status and plans for advanced accelerator work under Compass



- UCLA: W. B. Mori, F. S. Tsung, C. K. Huang, V.K.Decyk, W. Lu, M. Tzoufras, M Zhou
- Tech-X: D. Bruhwiler, J. Cary, P. Messner, D. A. Dimitrov, C. Neiter
- USC: T. Katsouleas
- LBL: E. H. Esarey, C. Geddes, E. Michel[1], W.A. Isaacs
- U. Maryland: T. M. Antonsen Jr.

[1]also U. Nevada, Reno

Outline

- Status:
  - Experiment
  - Code and algorithm development
  - Code comparison
  - Code validation
- Science goals:
  - Accelerate development of new accelerator technology
    - Model 250-500 GeV PWFA Afterburner Stages
    - Model 100+GeV LWFA Stages
    - Model LWFA and PWFA experiments
    - Provide real-time feedback for experiments
- Petascale modeling is required
  - **What is need to achieve petascale computing**

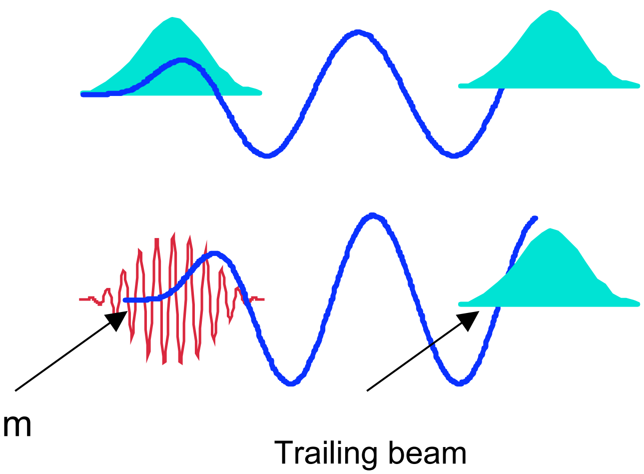
Status of experiments: Incredible progress

Plasma Wake Field Accelerator(PWFA)

A high energy electron bunch

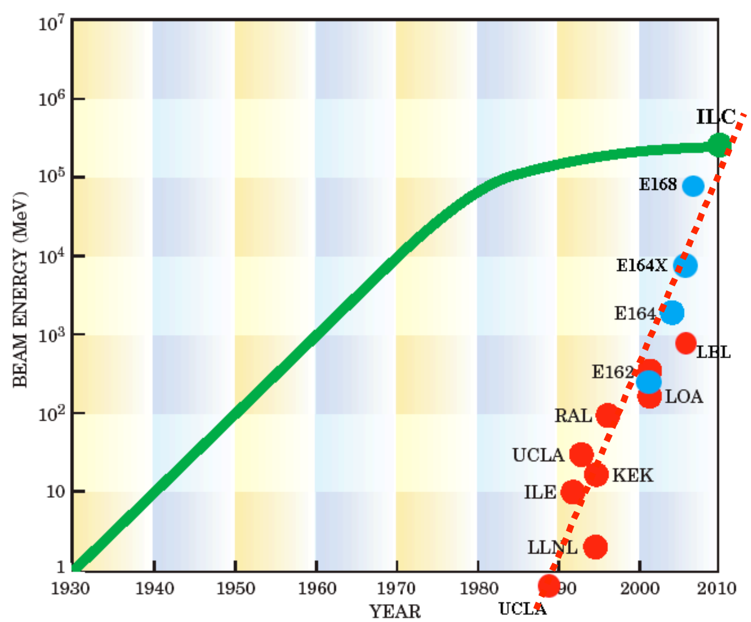
Laser Wake Field Accelerator(LWFA, SMLWFA)

A single short-pulse of photons -- wasn't available in 1979



The Livingston curve traces the history of electron accelerators from Lawrence's cyclotron to present day technology.

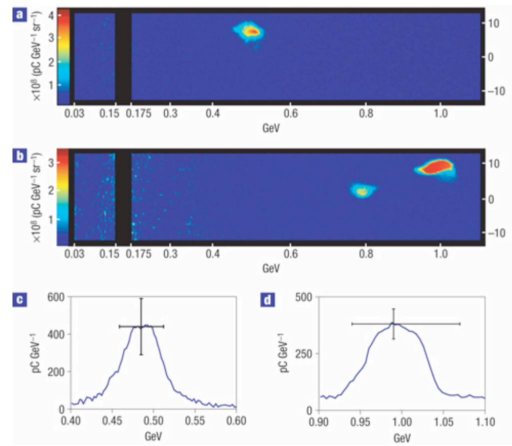
When energies from plasma based accelerators are plotted in the same curve, it shows the exciting trend that within a few years it is will surpass conventional accelerators in terms of energy.



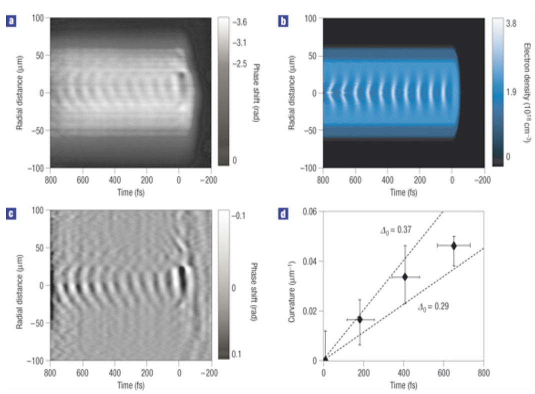
SciDAC is part of this progress (< Last 3 years)

”Dream Beam” (Nature, 2004)

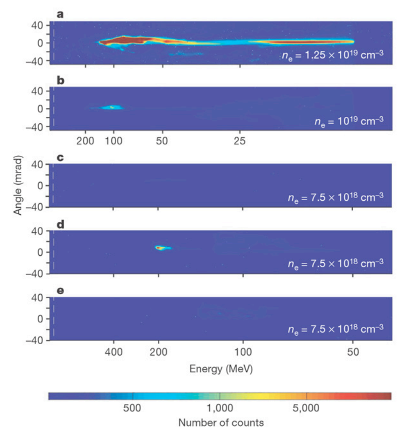
GeV PWFA (July 2005)



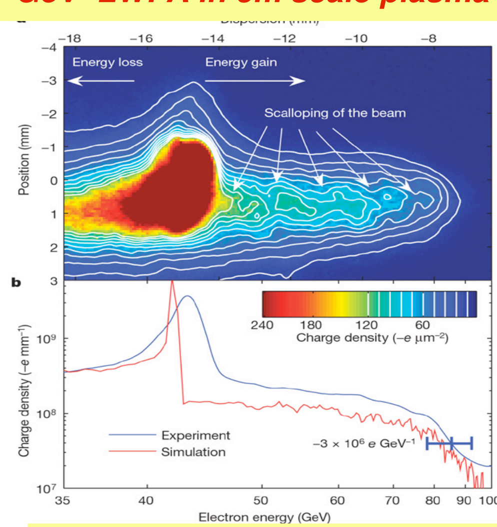
GeV LWFA in cm scale plasma



Snap shot of wakefield



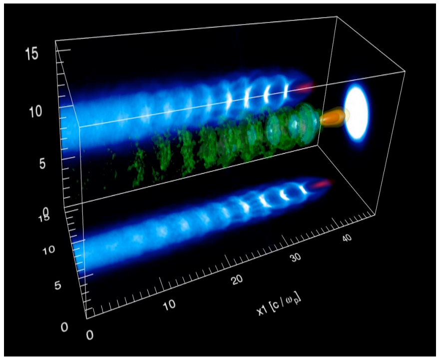
Controlled electron injection

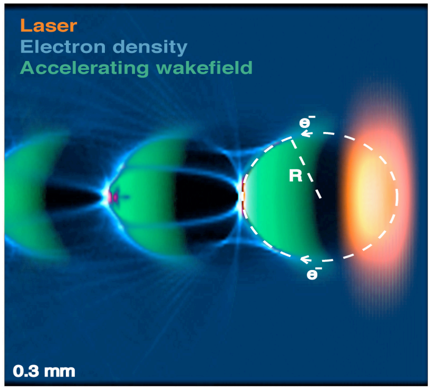


42 GeV in less than one meter!

OSIRIS:full parallel PIC for plasma accelerators

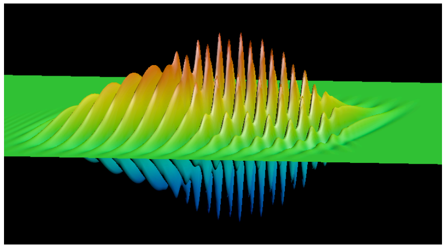
- Successfully applied to various LWFA and PWFA problems
  - Mangles *et al.,* Nature **431**, 538 (2004).
  - Tsung *et al*., Phys. Rev. Lett., **93**, 185002 (2004)
  - Blue et al., Phys. Rev. Lett., 90 214801 (2003)
- Code
  - Splines with <30% overhead
  - Open boundary conditions (PML)
  - Current and field smoothing
  - Field + Impact Ionization
  - Static load balance
  - Well tested and scales to 1000’s of processors
- Modern (object-oriented, Fortran 95 techniques)
  - Parallel (general domain decomposition) or Serial
  - Cross-platform (UNIX, Linux, AIX, OS X, MacMPIC)
  - Based on a well proven Fortran 77 code
  - Sophisticated 3D data diagnostics
- OSIRIS development team
  - UCLA(F. S. Tsung, J. W. Tonge), USC (S. Deng), IST (R. A. Fonseca and L. O. Silva), Ecolé Polytechnique (J. C. Adam), and RAL (R. G. Evans).
  - See http://exodus.physics.ucla.edu/



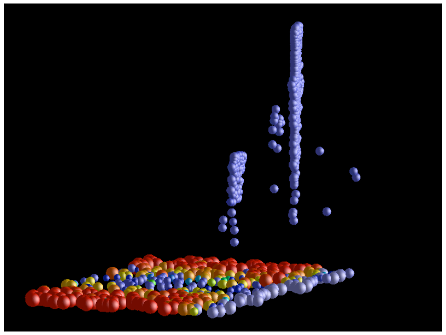


VORPAL – parallel PIC & related algorithms for advanced accelerators

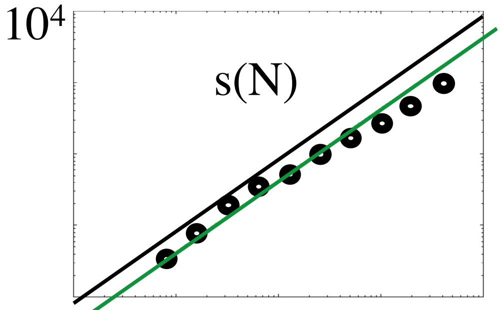
- Successfully applied to various LWFA problems
  - Geddes *et al.,* Nature **431**, 538 (2004).
  - Cary *et al*., Phys. Plasmas (2005), in press (invited).
- Recently implemented algorithms
  - Ponderomotive guiding center treatment of laser pulses
  - PML (perfectly matched layer) absorbing BC's
  - implicit 2nd-order & explicit 4th-order EM
  - Higher order splines
- Many other capabilites/algorithms (only a sample here):
  - Impact & field ionization; secondary e- emission
  - Fluid methods for plasmas; hybrid PIC/fluid
- Modern (object-oriented, C++ template techniques)
  - Parallel (general domain decomposition) or Serial
  - Cross-platform (Linux, AIX, OS X, Windows)
- VORPAL development team
  - J. Cary (Tech-X/CU), C. Nieter, P. Messmer, D. Dimitrov, J. Carlson, D. Bruhwiler, P. Stoltz, R. Busby, W. Wang, N. Xiang (CU), P. Schoessow, R. Trines (RAL)
  - See http://www.txcorp.com/technologies/VORPAL/
- Highly leveraged via SBIR funds: DOE, AFOSR, OSD



Colliding laser pulses



Particle beams



VORPAL scales well to 1,000's of processors

Code development: QuickPIC

Code features:

- Based on **UPIC** parallel object-oriented plasma simulation Framework.
- Underlying Fortran library is reliable and highly efficient
- Multi-platform, Mac OS 9/X, Linux/Unix.
- Dynamic load balancing

Model features:

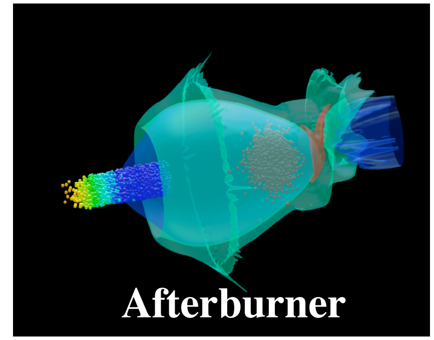
- Highly efficient quasi-static model for beam drivers
- Ponderomotive guiding center model for laser drivers.
- Can be 100 to 1000 times faster than conventional PIC with no loss in accuracy.
- ADK model for field ionization.

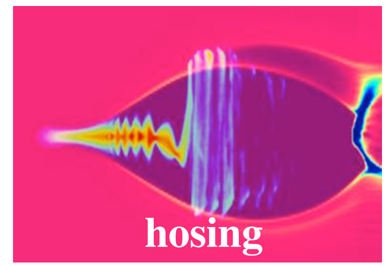
Applications:

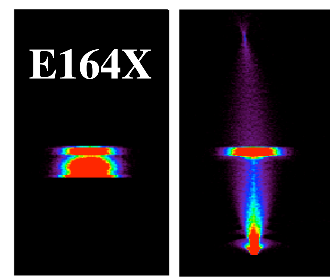
- Simulations for PWFA experiments, E157/162/164/164X/167
- Study of electron cloud effect in LHC.
- Plasma afterburner design

Scalability:

- With pipelining it currently scales to 1,000+ processors

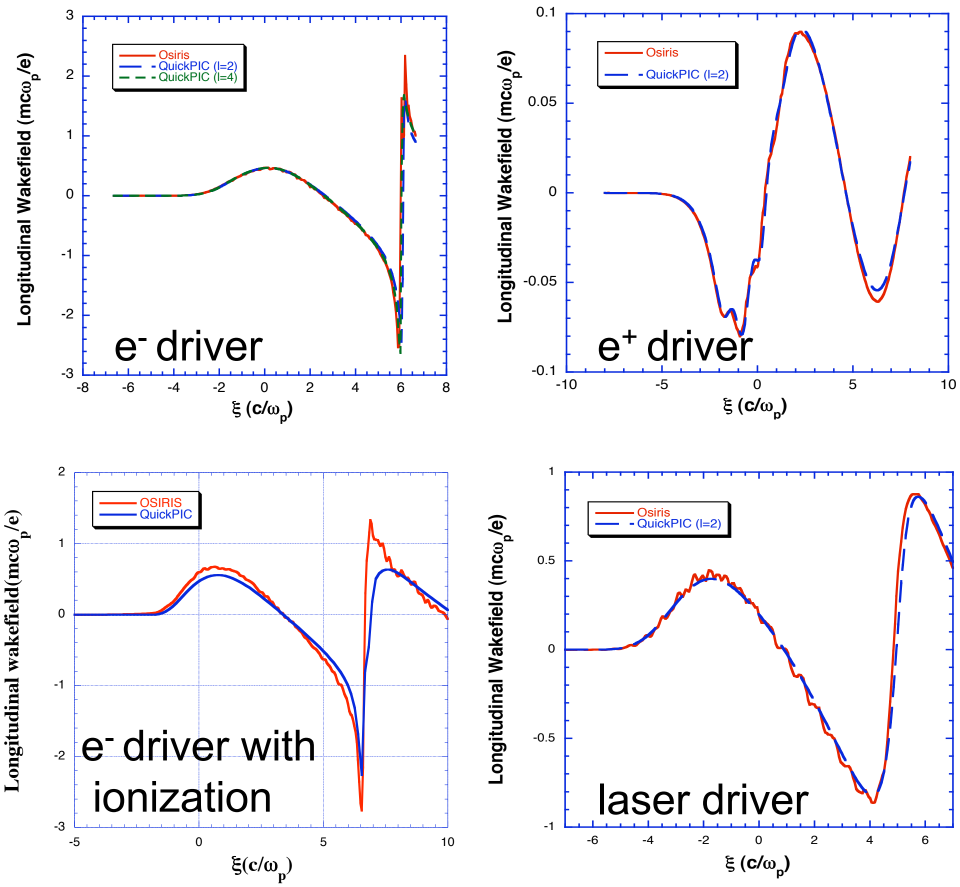






Algorithm validation: Full PIC vs. Quasi-static PIC

Benchmark for different drivers:
QuickPIC vs. Full PIC

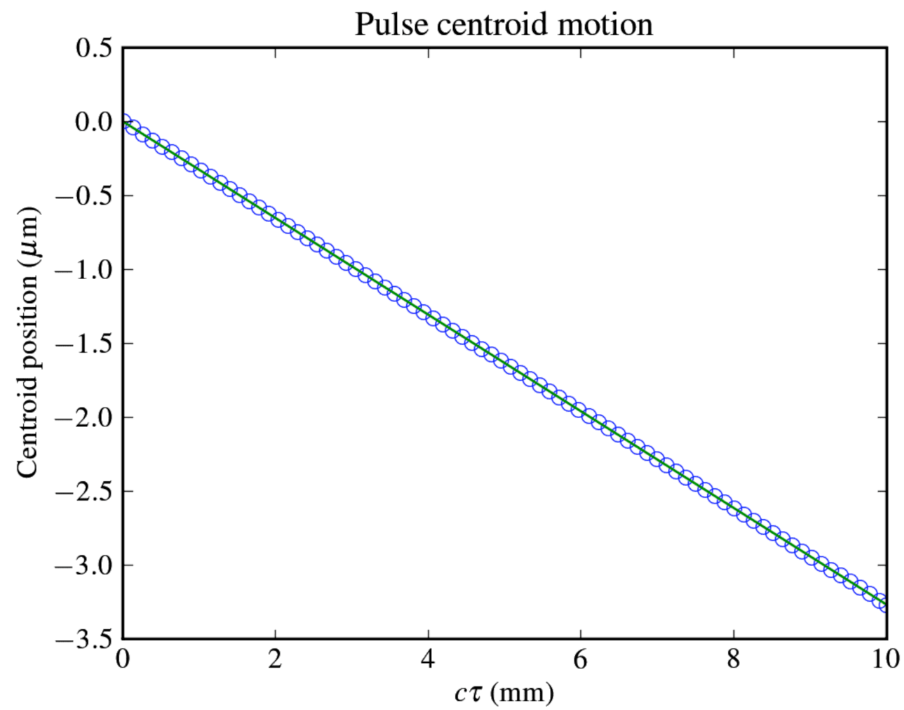


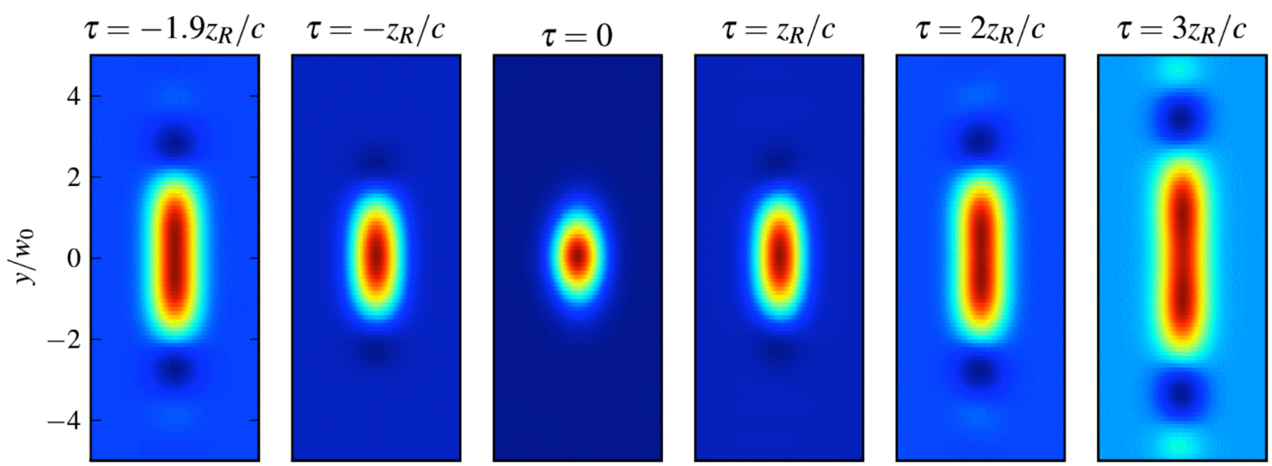
- Excellent agreement with full PIC code.
- More than 100 times time-savings.
- Successfully modeled current experiments.
- Explore possible designs for future experiments.
- Guide development on theory.

100+ CPU savings with "no" loss in accuracy

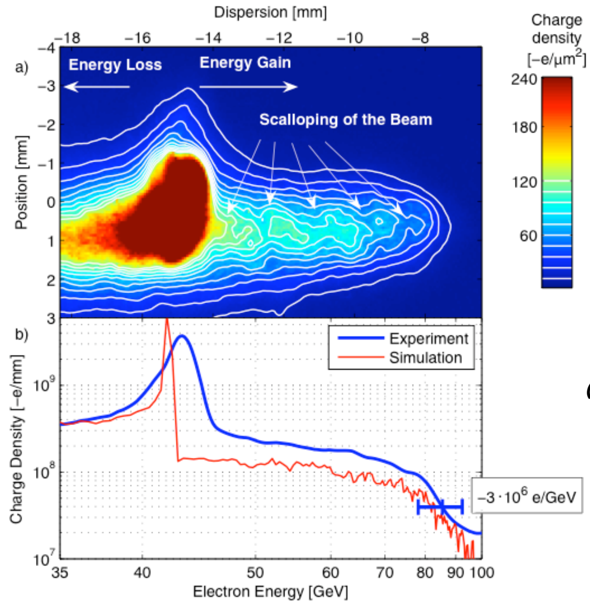
PGC/Envelope Laser Pulse propagates accurately over many Raleigh lengths (uses Trilinos)

- Numerical group velocity in a plasma channel:
  - $1\text{-}v_g$ = _3.2698 _ 10^{-4}
- Theoretical:
  - $1\text{-}v_g$ = _3.2756 _ 10^{-4}
- Maxwell:
  - $1\text{-}v_g$ = _3.2740 _ 10^{-4}
- to implement via PETSc
  - use 1,000 proc's by Year 1

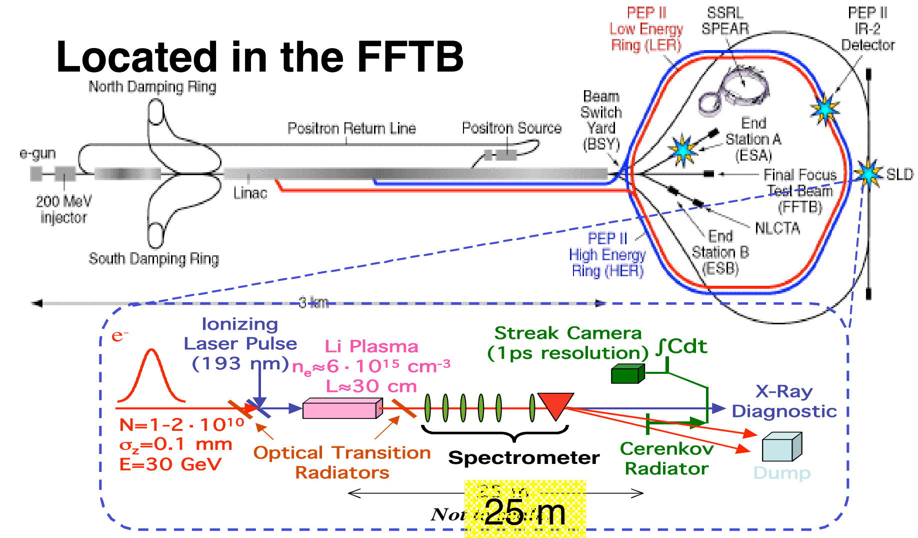


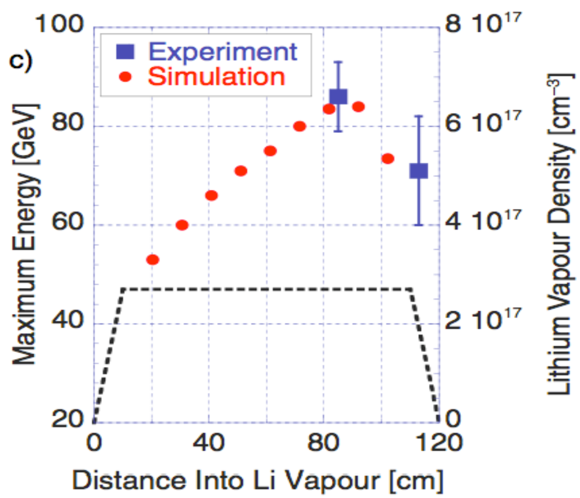


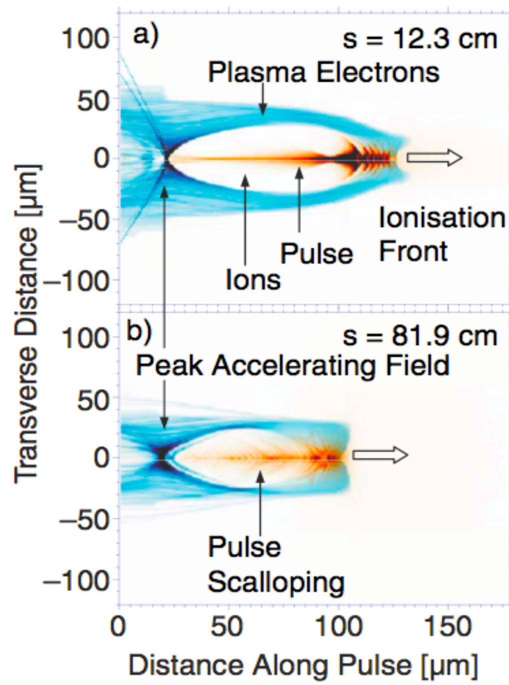
Modeling self-ionized PWFA experiment with QuickPIC



(Nature, Vol. 445, No. 7129, p741)







Simulations suggest “ionization-induced head erosion” limited further energy gain.

Direct comparison to experiment: OSIRIS 3D PIC vs. LBL Nature experiment

Total # of electrons:

Simulation: 1.8 10^9

Experiment: 2x10^9

Central energy:

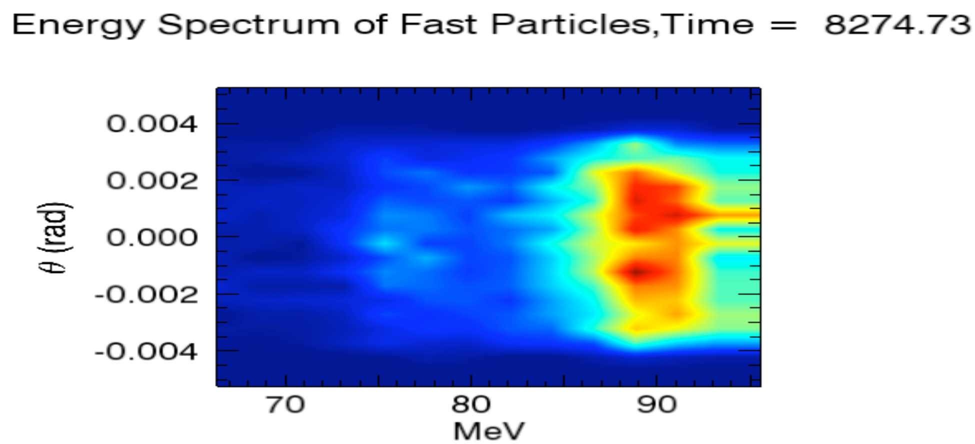
Simulation: 90 MeV

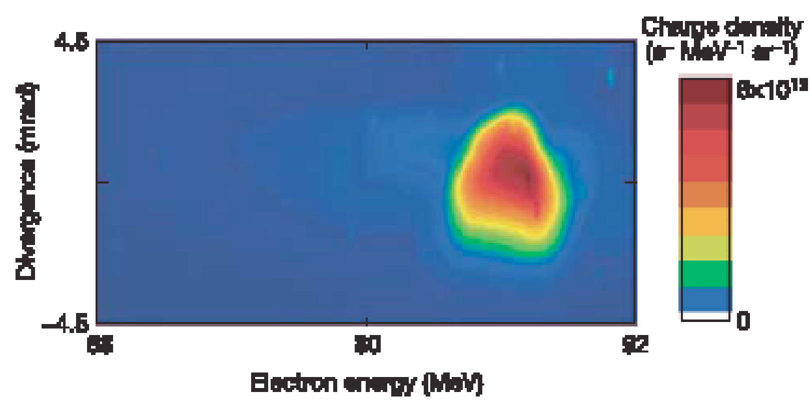
Experiment: 86

Energy spread:

Simulation: 10 MeV

Experiment: 1.8 MeV

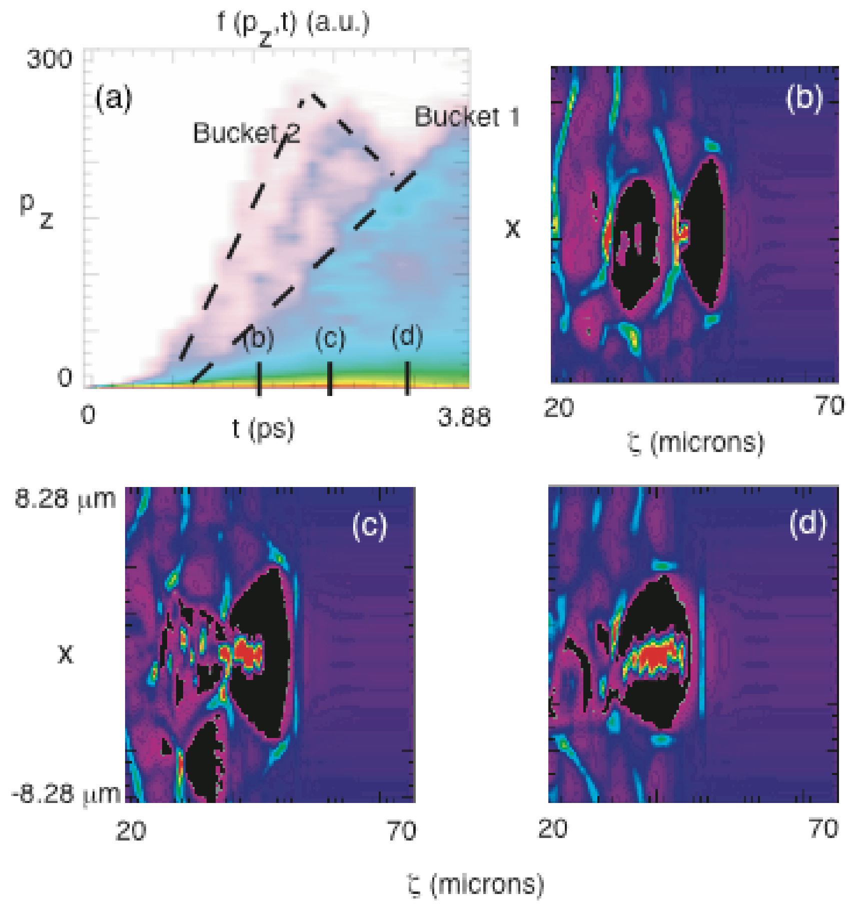




Interaction of two buckets -- LBL

Because of the initial pulse length of the laser, there are two groups of trapped electrons in this simulation. The first group resides initially in the 2nd bucket, and the second group is trapped in the first bucket.

The final monoenergetic beam consists of electrons from both buckets which have merged into a single bucket.



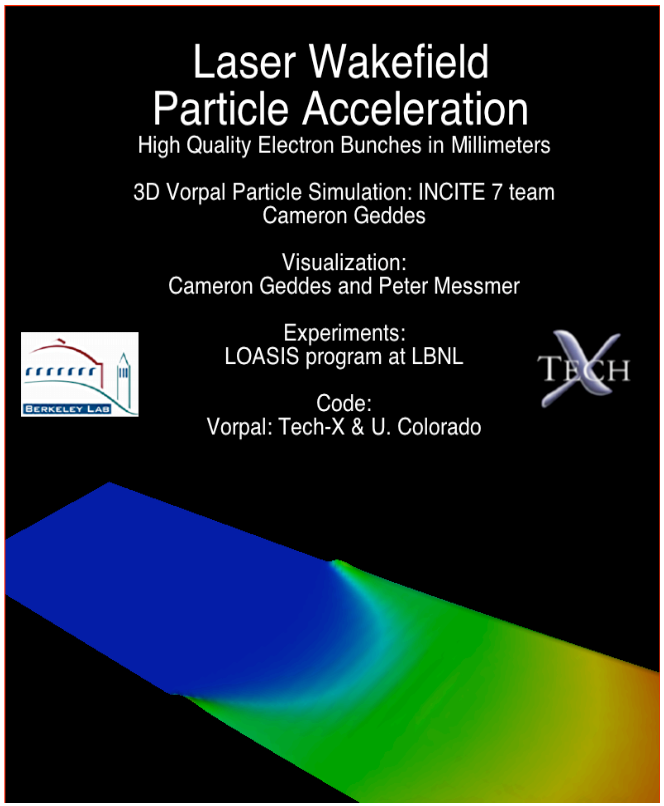
Detailed modeling to understand, plan experiments

MHour 3D runs backed by detailed 2d & numerical work

One-to-one simulation of LOASIS experiments

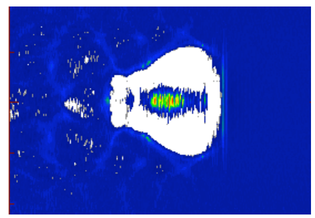
3d acceleration dynamics

Million hour scale simulations
10 TW, close to 90 MeV expt. Q, E

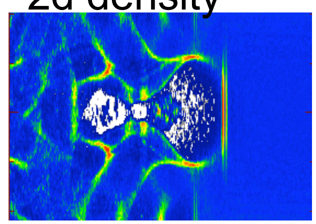


2d compensation

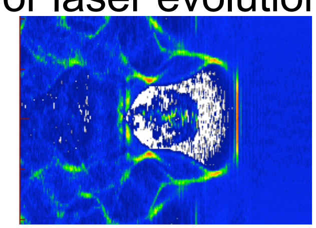
3d density



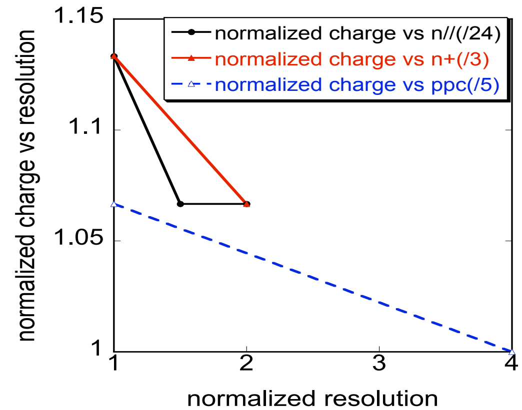
2d density



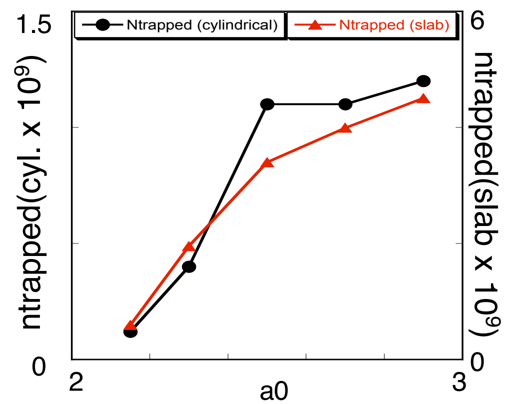
2d-compensated
for laser evolution



Numerical Convergence



Optimization

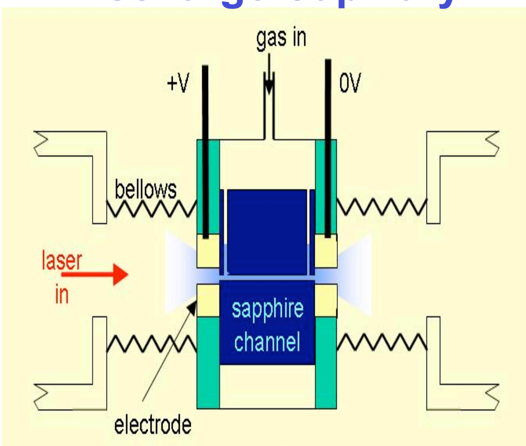


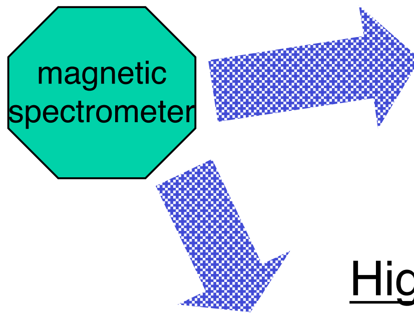
Experiments observe final state **Theory** gives general scaling

Simulations detail internal dynamics - quantitative understanding & engineering

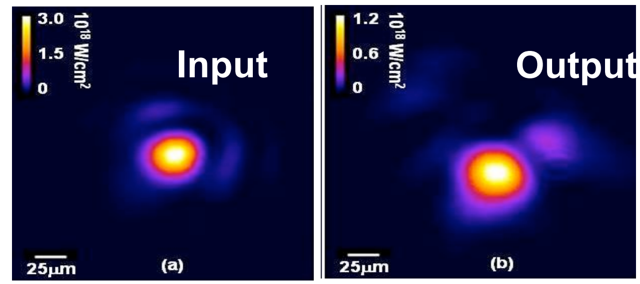
3 cm capillary channels at reduced density: increased laser v_{group} produces GeV ebeams

Discharge Capillary

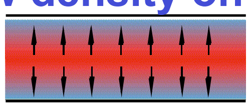




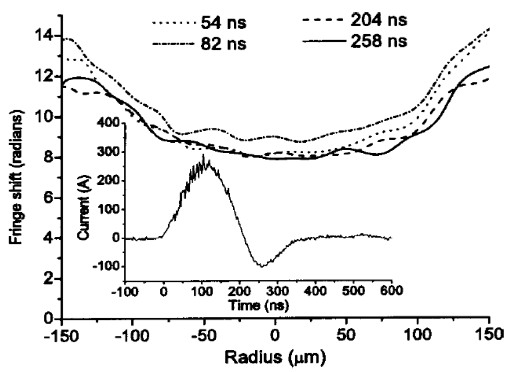
Guiding 40 TW over > 10 ZR ~ 3 cm at relativistic intensity



Pressure Balance-> low density on axis

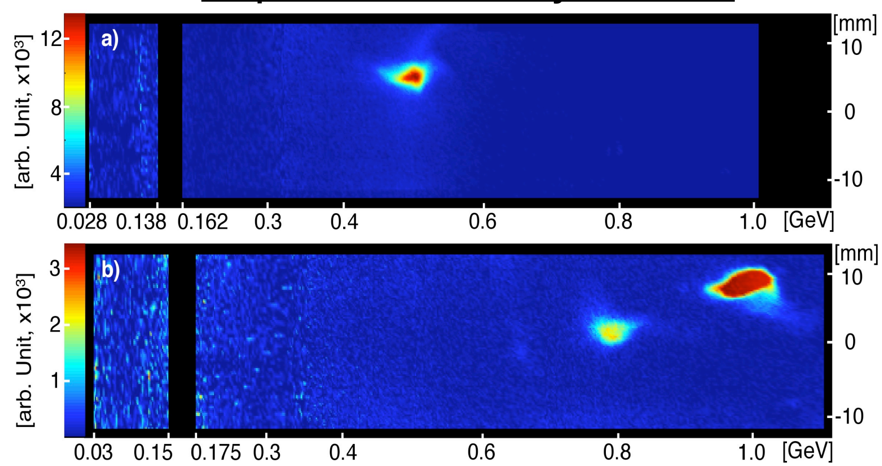


Channel Profile



From: Spence et al, JOSA-B, **20**,p138, 2003

High quality electron beams at plasma density ~ $4x10^{18}$



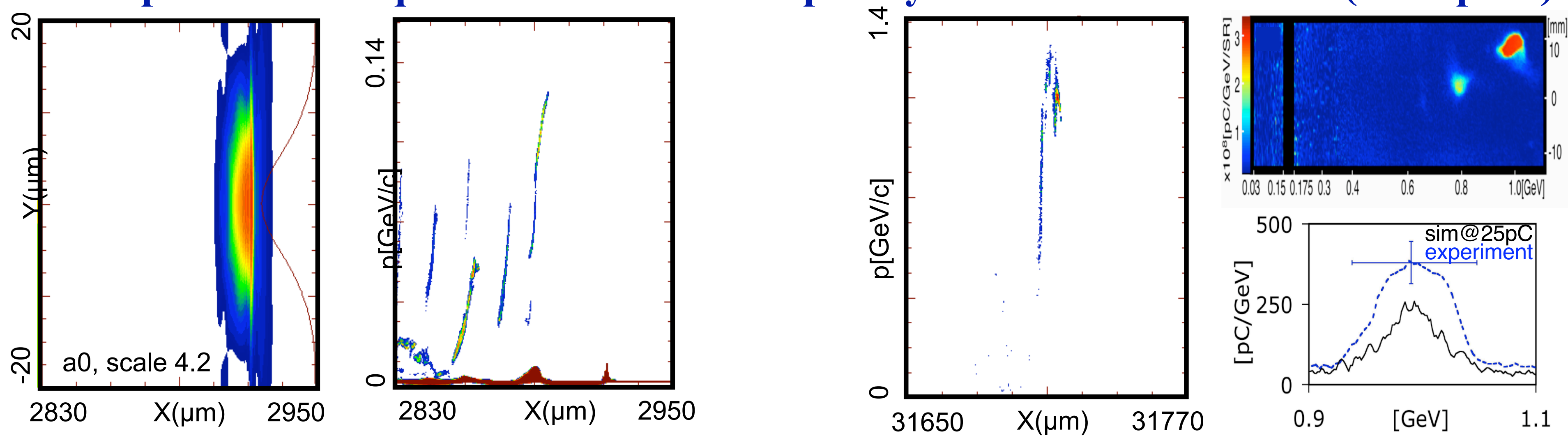
Energies up to 1 GeV

Stable operation at E ~ 0.5 GeV

Leemans et al, Nature physics,2006

GeV acceleration in 3cm capillaries
Simulation feedback to experiments

- **Computational requirements for 3cm capillary: several Mhour in 3d (4096 proc)**



Laser steepening yields injection@ 0.3cm

2d trapping requires increased density

Beam evolution, parameter tradeoffs

3D run @ 5mm - closer to experiment al trapping

60pC, 0.8 GeV, dE/E ~ 5%

2D Bunch@3.2 cm close to expt.*

Q	25-65 pC	(35 pc expt.)
E	1.03 GeV	(1.1 GeV expt.)
dE/E	7% FWHM	(8% expt.)
diverg.	2.5 mrad rms	(1.6mrad expt.)

3D run at experimental density under way

External injection would enable lower densities & higher energy

Laser depletes at ~ 1cm, beam decelerates - **Experiments confirming**

Density ~ 2e18cm^{-3} allows dephasing/depletion limited ~2 GeV beam

*Leemans et al Nature Physics 2006, Gonsalves et al Proceedings PAC 2007

QuickPIC Simulations: *simulation parameters*

Based on Lu et al., PRSTAB 10, 061301 2007

Initially used OSIRIS simulations (not shown)

$P(TW)$	$\tau(fs)$	$w_0(\mu m)$	$n_0(cm^{-3}$	$\langle \Delta W \rangle (GeV)$	$L_\phi(m)$	$\langle E_z \rangle (GeV/m)$	$\sigma_z(\mu m)$	$Q(pC)$
15	35.6	10.68	$2E+18$	0.4	0.0068	59.08	1.5	96
60	71.2	21.36	$5E+17$	1.6	0.0542	29.54	3	154
240	142.4	42.72	$1.25E+17$	6.4	0.4333	14.77	6	246
960	284.8	85.44	$3.125E+16$	25.6	3.4663	7.39	12	393
3840	569.6	170.88	$7.8125E+15$	102.4	27.7306	3.69	24	629
15360	1139.2	341.76	$1.95313E+15$	409.6	221.8450	1.85	48	1007
61440	2278.4	683.52	$4.88281E+14$	1638.4	1774.7598	0.92	96	1611

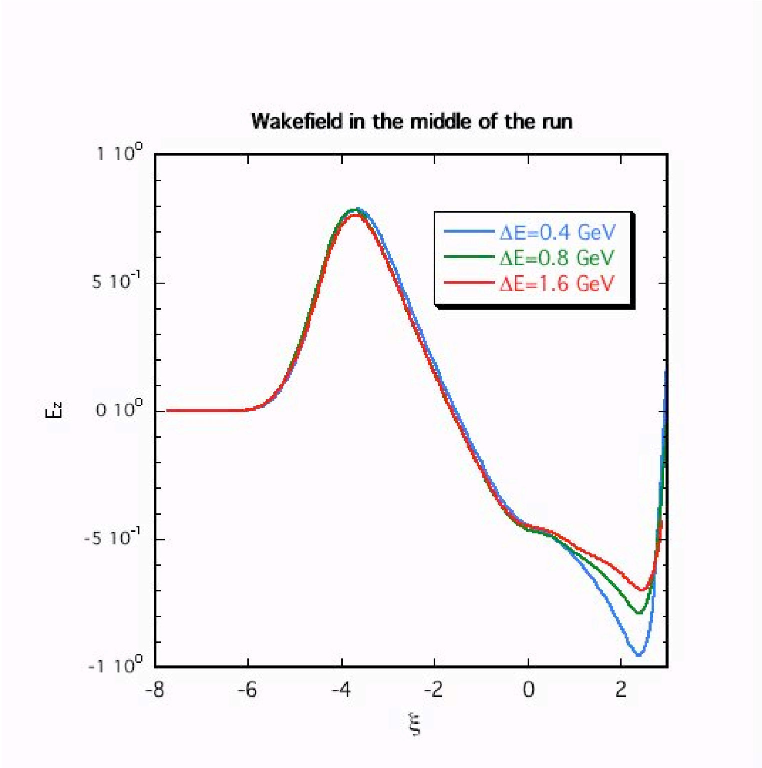
• The number of cells in the simulation box increases by a factor of 2 for every row in the table above. The simulation size increases by a factor of 4.

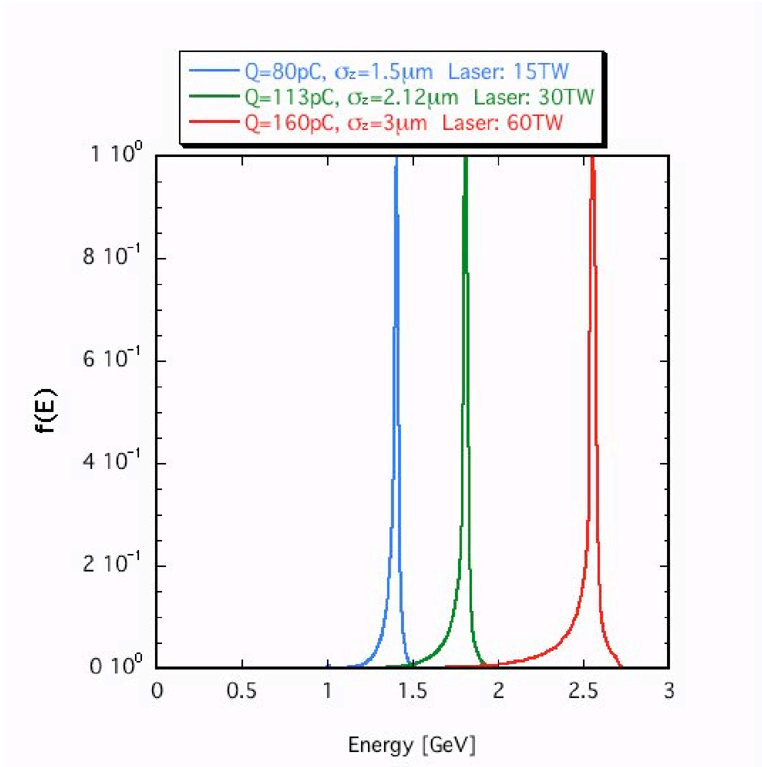
• For a_0=2, and as lasers with PW powers come online, availability of long plasma channels (see table) is an obstacle in creating 100GeV-TeV LWFA.Other obstacles are common to PWFA Afterburner: Hosing of trailing beam

QuickPIC Simulations:

scaling from 0.4GeV to 1.6GeV

- The wakefield from the simulation for three different cases scaled properly is nearly identical in normalized units.
- The energy scaling is excellent as well.



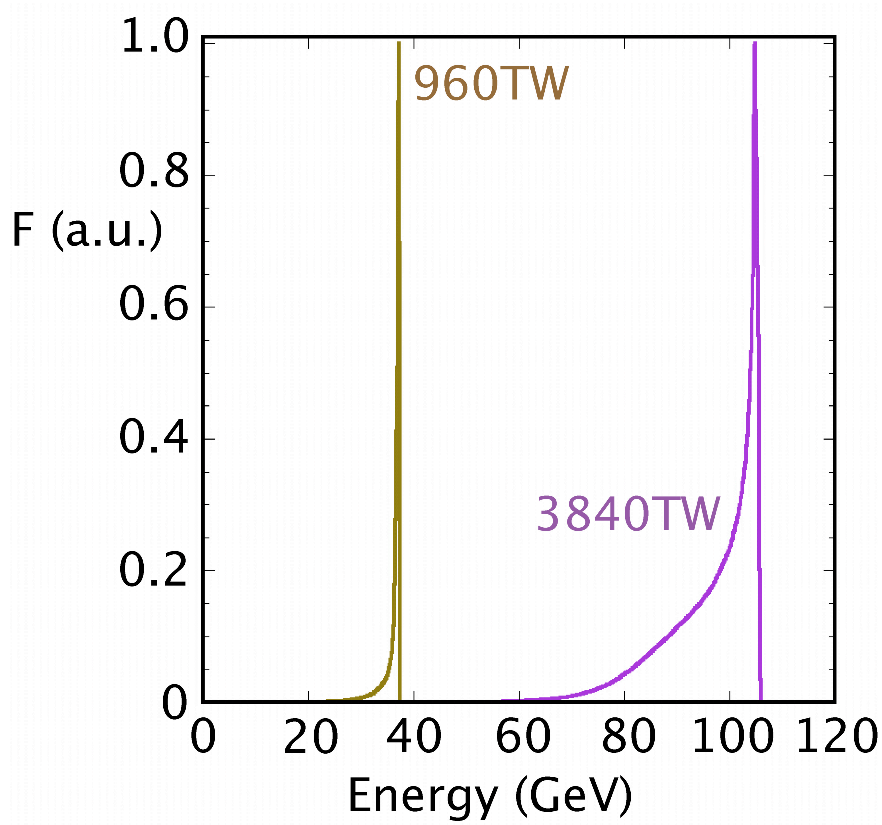


QuickPIC Simulations:

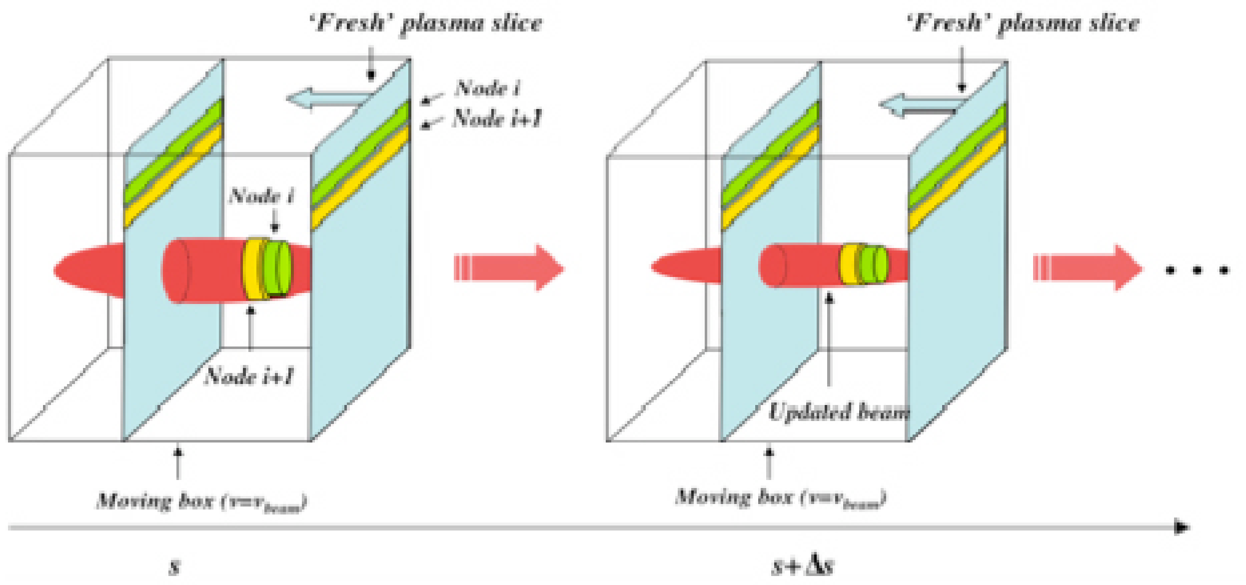
beam quality in the 100GeV run!

- Two electron bunches with initial energy 10GeV are accelerated up to 36GeV (brown line) and 106GeV (purple line) as shown in the plot.

- The energy spread for the 106GeV run is larger than that for the 36GeV run. Some fine-tuning of the acceleration parameters is needed.



Simulation Code: QuickPIC
Ideal for “pipelining”

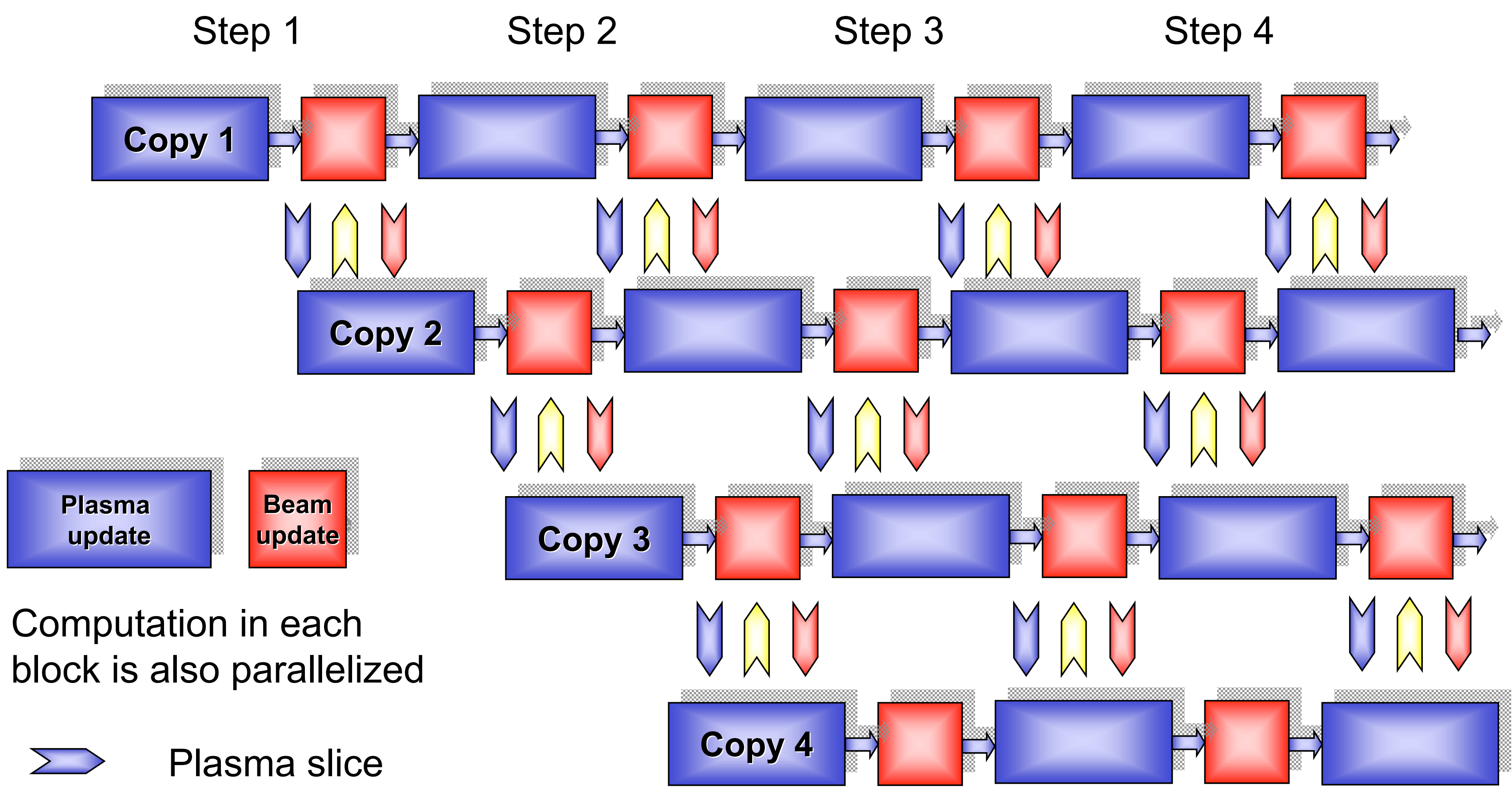


QuckPIC is a quasistatic PIC simulation code that solves the wave equation:

$$2\frac{\partial}{\partial s}\left(-ik_0+\frac{\partial}{\partial \xi}\right)\hat{\mathbf{a}}+\nabla_\perp^2\hat{\mathbf{a}}=\left(\frac{\omega_p^2}{\omega_0^2\gamma_p}\right)\hat{\mathbf{a}}$$

where **a** is the the envelope of the laser vector potential.

Pipelining



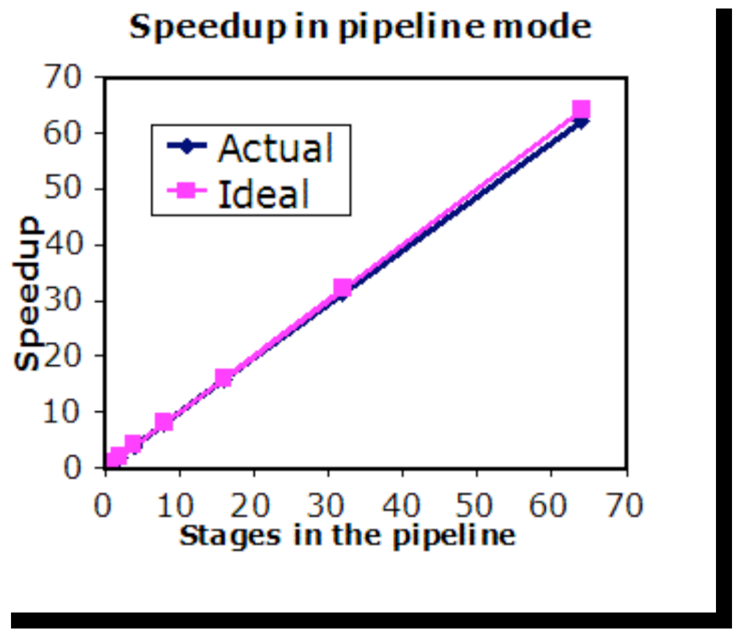
Computation in each block is also parallelized

- Plasma slice
- Guard cell
- Particles leaving partition

Scaling to 1,000+ processors

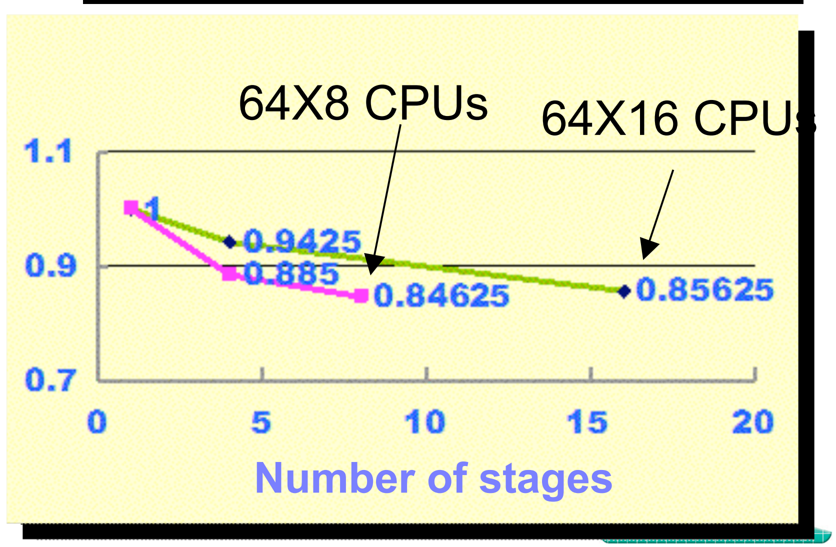
Single stage performance in 2D loop

- Near ideal speed up with number of stages.
- Data transfer between successive stages overlaps with computation.
- Recent performance tuning resulted in 50%(Xeon, Opteron, SP5)~200% (SP3) boost on various platforms.



Overall performance

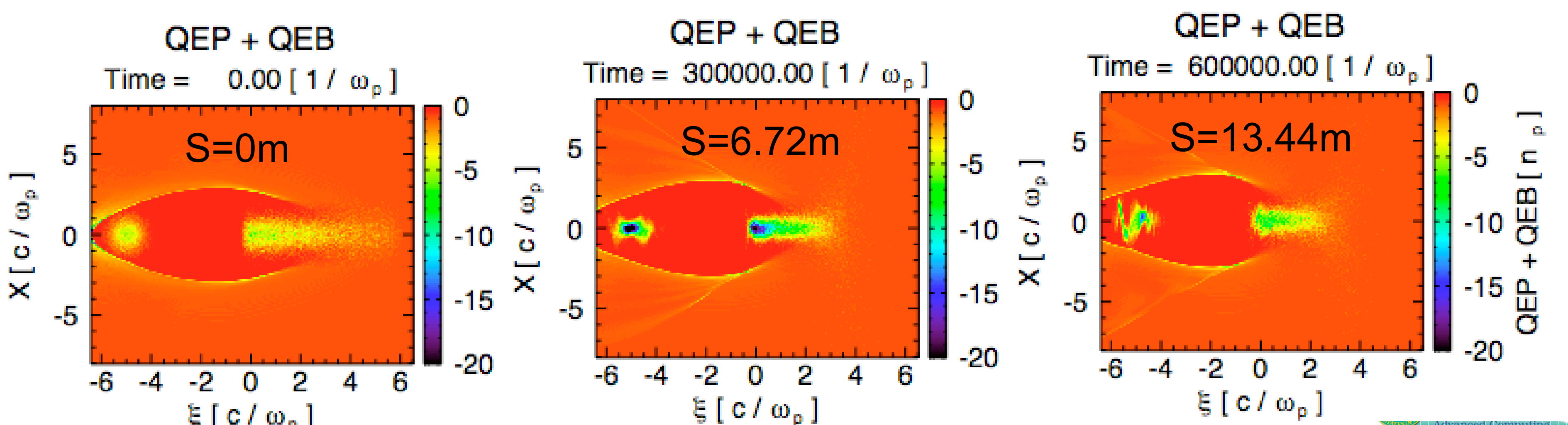
- Achieve good scaling on 1024 cpus on Seaborg. Largest test used 2048 cpus.
- Overhead in communications between successive stages becomes more important for synchronization of shorter stages.
- 3D code (each stage) needs to be load balanced.



TeV PWFA simulation

TeV PWFA parameter		Numerical parameter	
Initial Energy (GeV)	500/500	Number of grids	1024 × 1024 × 1024
Beam charges (1E10)	3.0/1.0	Beam particles	4M
Emittance (mm.mrad)	2230/2230 (30/30*)	Plasma particles	2048 × 2048
Spot size (μm)	15/15 (1/1*)	Simulation box size (μm^{-3})	760 × 760 × 288
Drive beam length (μm)	145	Number of processors	1024
Witness beam spot size (μm)	10	Total time step	3256
Separation (μm)	100	Number of processors	1024
Plasma density (cm^{-3})	5.66E16	Wallclock time (hour)	~ 200 (ongoing)
Plasma length (cm)	2188		

* if scaled to a narrow beam



VORPAL Simulations of LWFA Experiments at LBNL – Status, Future Plans & Needs

- 2D/3D runs ongoing at NERSC and LLNL/Atlas
  - 100 MeV / gas jet & 1 GeV / capillary
  - down ramp injection of particles vs self-trapping
  - exploring benefits of smoothing / high-order particles
  - using 256 to 1,928 processors
- Developing PGC/Envelope model for laser pulse
  - orders of magnitude faster than explicit PIC
  - benchmarking 1D/2D/3D light-frame implementations
- Pushing toward petascale
  - using 10,000 processors by end of Year 1
    - roadblocks may require assistance?
    - additional computer resources?

VORPAL

Scientific Discovery through Advanced Computing

OSIRIS/QuickPIC Simulations of Single stage LWFA Including experiments at LBNL

Status, Future Plans & Needs

- 3D (2D) runs continue at NERSC, DAWSON, and HPC
  - 100 MeV to 100 GeV
  - OSIRIS (full PIC) can handle self-injection
  - OSIRIS and QuickPIC are tested against each other
  - QuickPIC is already modeling 100 GeV stages!
- Exploring key physics for LWFA at the energy frontier
  - Single stages: self and external guiding
  - Developing nonlinear beam loading theory
  - Testing new scaling laws (Lu et al.)
- Pushing toward petascale
  - The goal is to show scalability to 10,000 processors for OSIRIS by end of Year 1
  - The goal is to add pipelining to laser solver in QuickPIC (scale to over 1000 processors by the end of Year 1)
  - What will “petascale” and beyond machines look like?

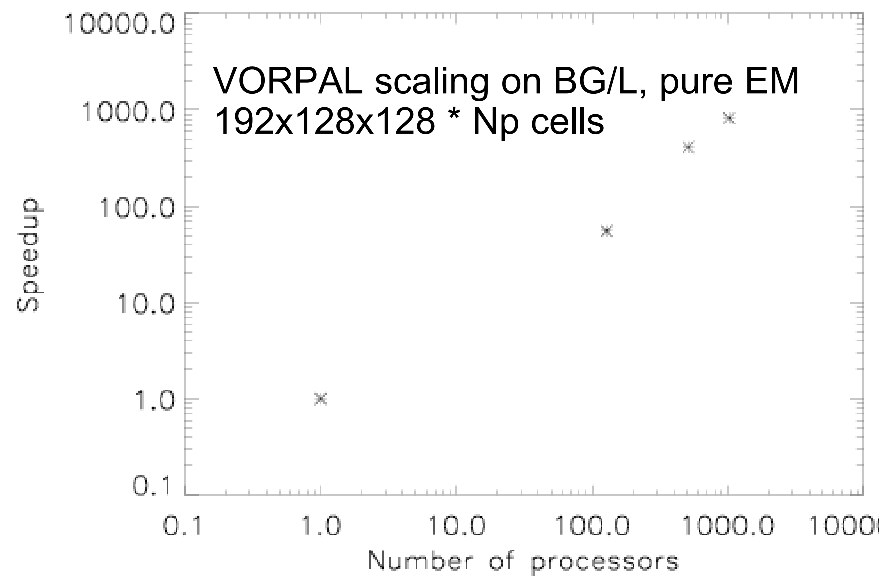
QuickPIC Simulations of 250 -500 GeV PWFA Afterburner stages

Status, Future Plans & Needs

- 3D runs with pipelining ongoing at NERSC and DAWSON
- Exploring key physics
  - Hosing
  - Beam loading
  - Transformer ratios
  - Head erosion
  - Ion motion
  - Help design and model SABER experiments
- Pushing toward petascale
  - Pipelining was added
  - Need to optimize single processor performance
  - Need mesh refinement
    - Will use HPC libraries developed in CETs
  - Will utilize the highly optimized routines in UPIC (Decyk tomorrow)

Are HPC libraries the answer to optimization of LWFA simulation codes on petascale systems? Perspective of VORPAL.: Useful for discussion for all codes

- **Goal: VORPAL should take full advantage of petascale systems**
  - avoid manual optimization of core algorithms on every new system
  - use highly-tuned numerical libraries for the core algorithms in VORPAL?
- **Utilizing HPC libraries has strong advantages:**
  - Benefit from long-time efforts like PETSc, Trilinos
  - Optimization effort for these libraries benefits VORPAL
  - Provide feedback to library developer
  - Reduction of code base
- **Ongoing DoE/ASCR Phase I SBIR project ('VORPALite')**
  - Planned collaboration with PERI for advanced performance analysis
- Petascale analysis of VORPAL
  - Provide baseline for optimization work/performance comparison
  - Scaling of core algorithms
    - FDTD, particle push, I/O
  - Application performance in core domains (ILC cavities, LWFA)
- Now addressing FDTD algorithm
  - Modification of data layout, communication pattern
  - Library based vs. hand-crafted implementation



Needs?

- Full PIC codes scale to 10,000+ processors
- Quasi-static PIC scale to 10,000+ processors
- Single processor optimization
  - Particle push and deposition
- Poisson solvers on block structured meshes with complicated boundaries
- Optimization on iterative solvers with particles
- Mesh refinement (needed for both PWFA and LWFA)
  - Poisson solvers (quasi-static PIC)
  - EM solvers (full and PGC PIC)
- Visualization and data analysis for large field and particle data sets

- Some will be covered by UPIC (Decyk tomorrow)

Need to work together

- Compare OSIRIS and VORPAL
  - Both are full PIC but there are differences
  - Having two independent codes is beneficial and important
  - Convergence and parameter choices
- Compare Full PIC against Reduced PIC
  - OSIRIS and QuickPIC have been compared
  - Effort should be broadened
- Spectral and higher order field solvers might be useful
  - Comparison between FDTD with Spectral PIC will be done
- Exploring key physics
  - VORPAL, OSIRIS, and QuickPIC are all being used to study LWFA
    - Single stage vs. staging
    - Self-injection
    - Ion motion (important for both LWFA and PWFA)
    - Laser evolution and ph
- Pushing toward petascale
  - Many common issues will be encountered
  - There are no HPC libraries for particle push and deposition (UPIC?)