Dream beams: Extreme-scale computing enabling new accelerator technologies for the energy and intensity frontiers

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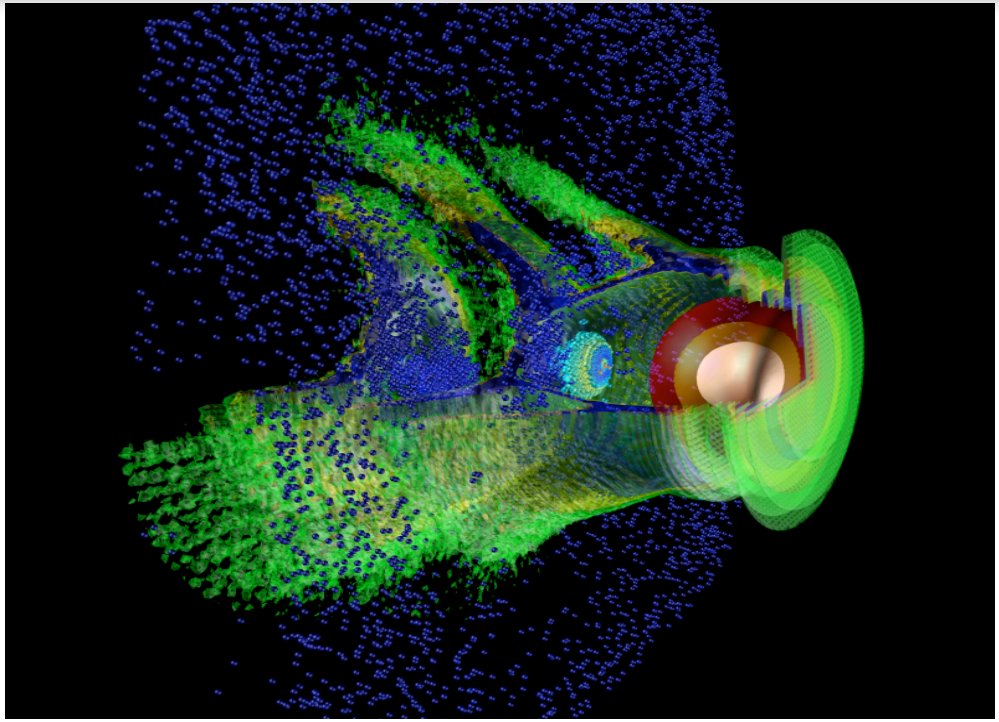
Astronomy and of Electrical Engineering

Institute of Digital Research and Education



Office of Science

SciDAC
Scientific Discovery through Advanced Computing

Collaborators

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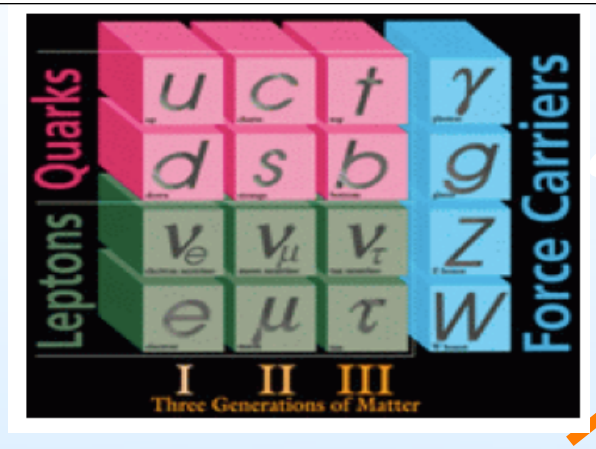
Twentieth Century Revolution in Physics



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S,W,G

Standard Model

Gell-Mann

Quarks (74,77,95)

Chadwick

Neutron (1932)

Rutherford

Proton,Nucleus (1911)

Thomson

Electron (1897)

Particle Accelerators Collide two, tightly focused beams of very high energy charged particles against one another

Circular:
Electron Synchrotrons
Proton Synchrotrons
Linear:
LINACS

ENGINES OF DISCOVERY

A Century of Particle Accelerators
Andrew Sessler·Edmund Wilson

Large Hadron Collider (LHC)at CERN

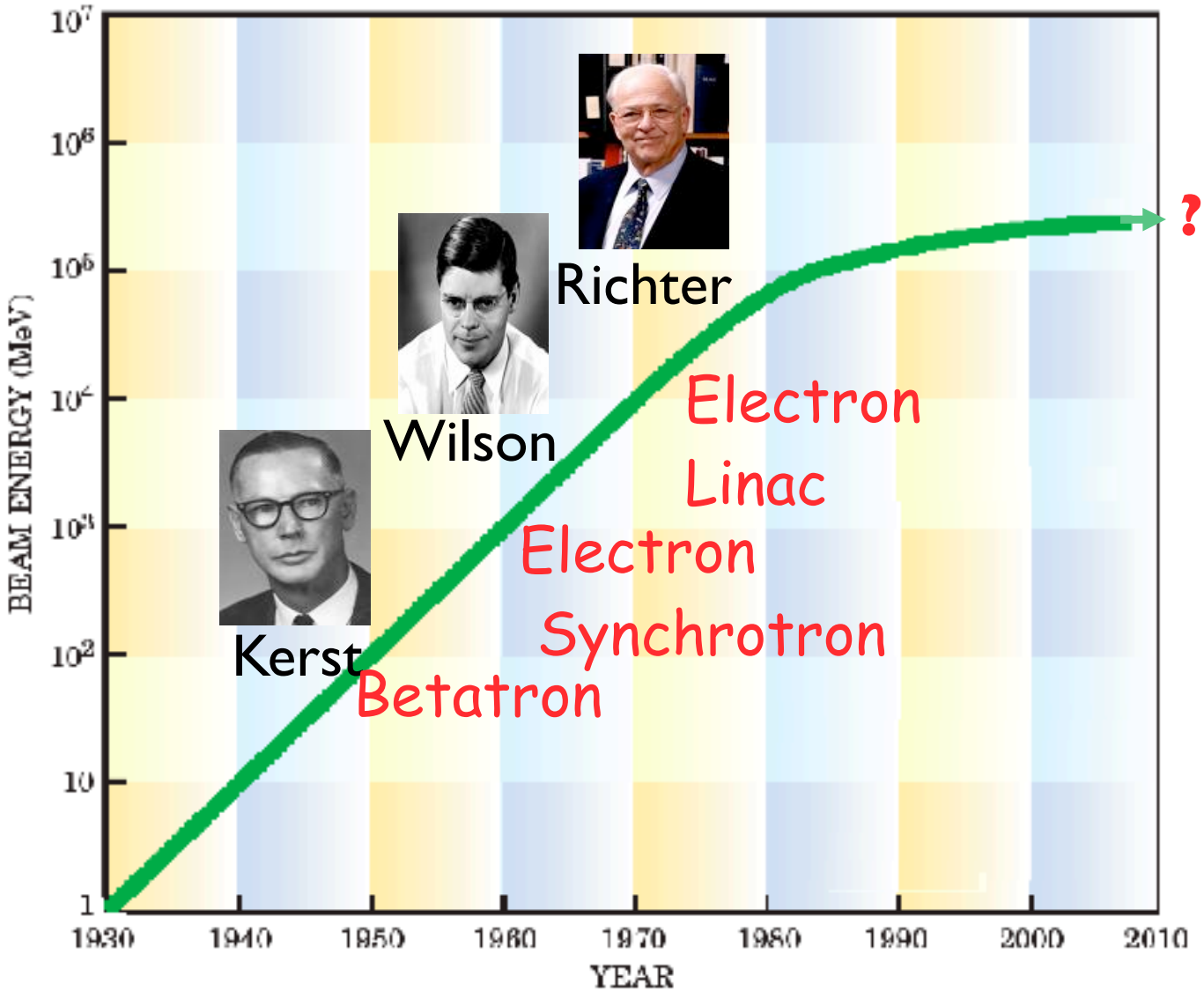
Terascale Physics

14 Trillion Volts *(CM) pp*

27 km circumference

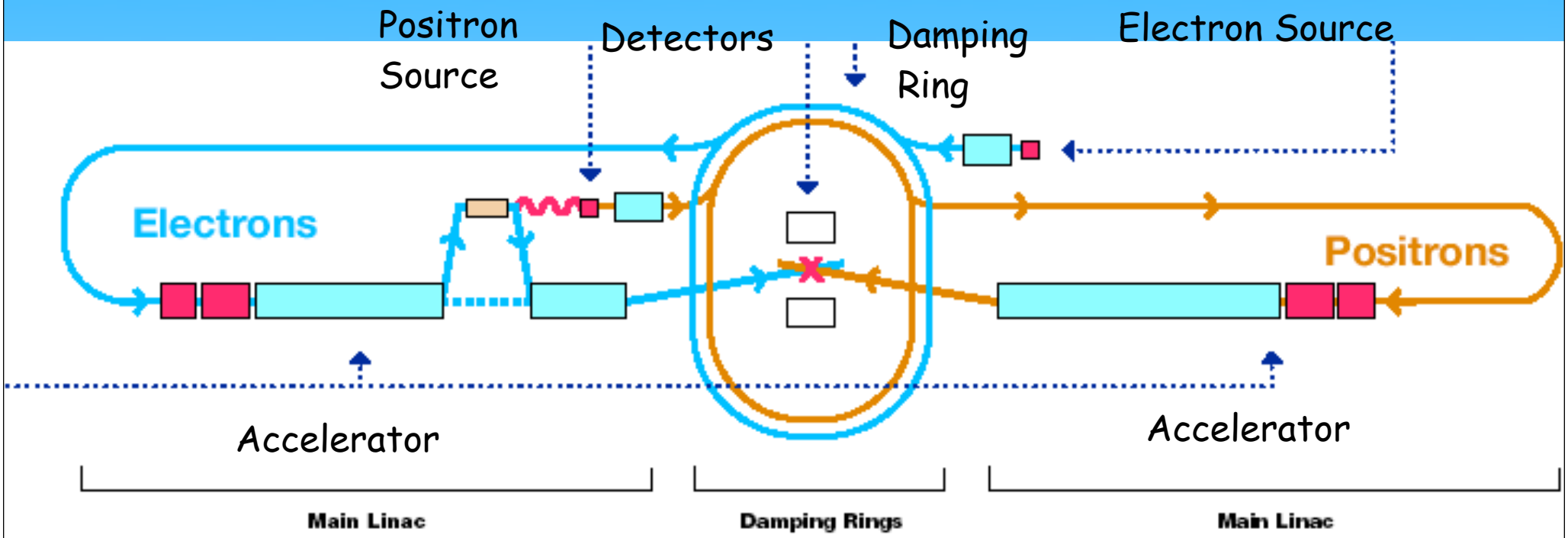
$6 Billion+?

Evolution of Electron Accelerators



All high energy accelerators use microwave fields

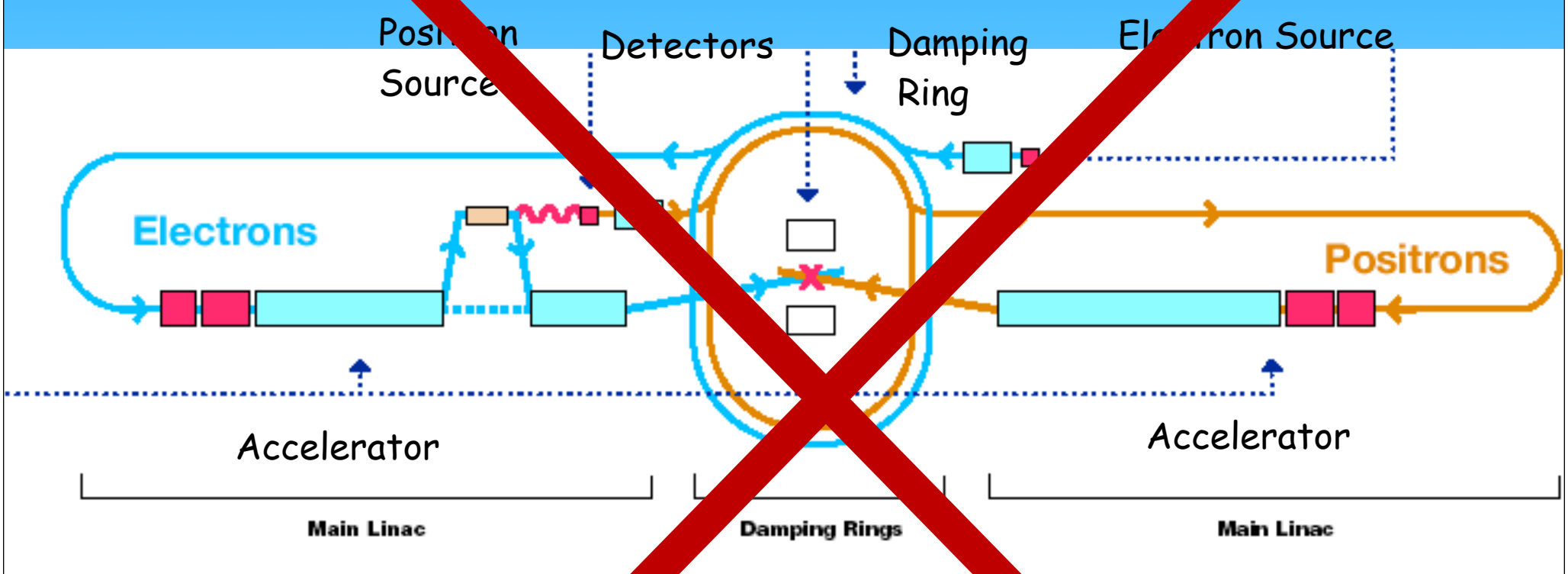
International Linear Collider



Origin of mass
Extra dimensions of space
More fundamental particles

31 km
500 GeV CM
$????

International Linear Collider



Origin of mass
Extra dimensions of space
More fundamental particles

1 km
500 GeV CM
$?

How do we move forward?

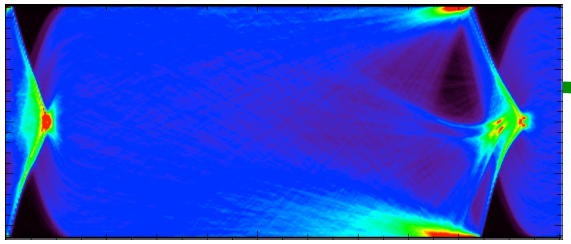
- **Improve and upgrade existing accelerators**
- **New accelerator concepts**
  - **Muon colliders**
  - **CLIC**
- **New acceleration technologies**
  - **Higher gradients**
  - **Cheaper accelerators**

  - **This is primarily a talk about new acceleration technologies, how simulation is advancing discovery and progress in it, and about what the future holds for it.**

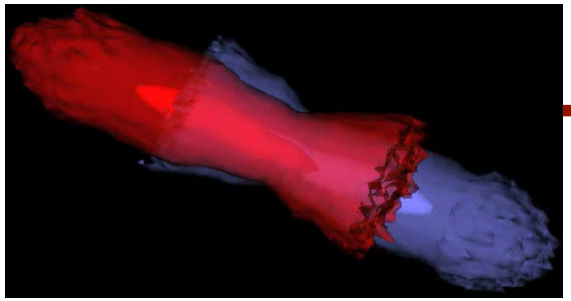
ComPASS HPC accelerator simulations are important for optimization of existing accelerators and plans for new/upgraded accelerators

- Electron cloud simulations in the Main Injector for Project-X
- Beam-beam simulations in the Tevatron for Run II
- Space charge simulations in the Debuncher for Mu2e

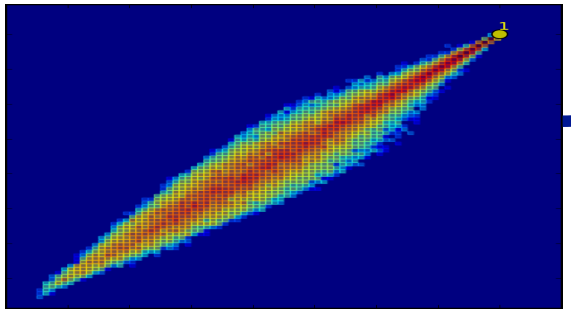
Electron cloud



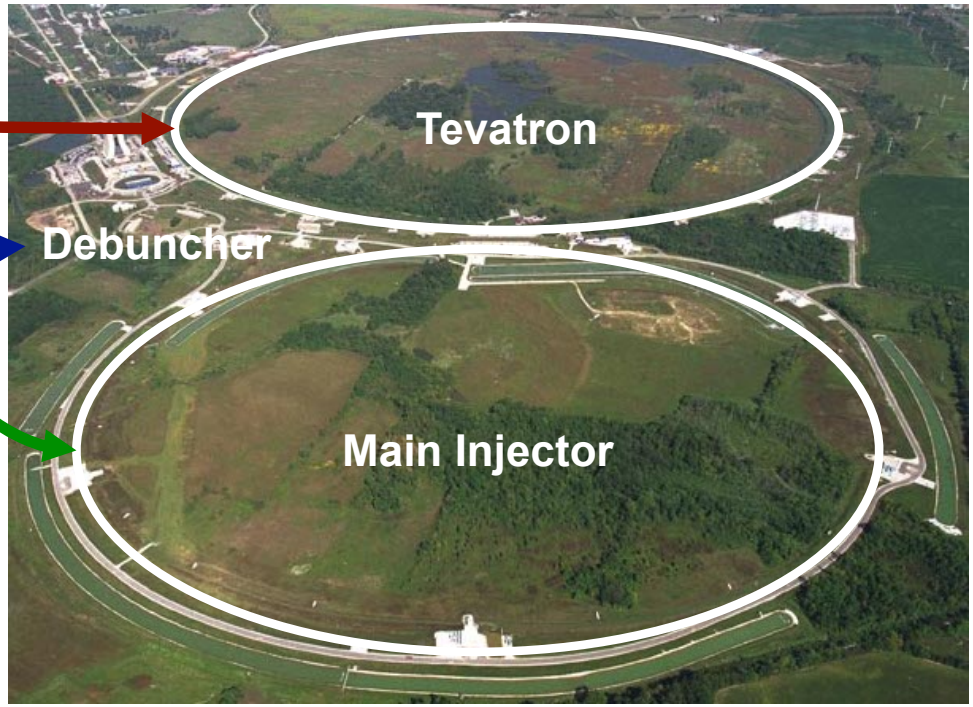
Beam-beam



Space charge

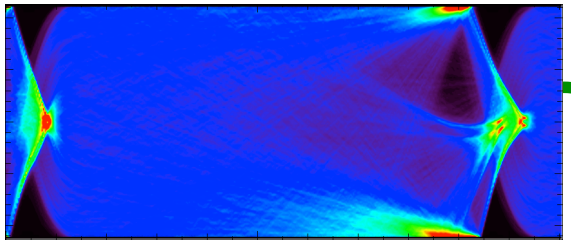


Fermilab

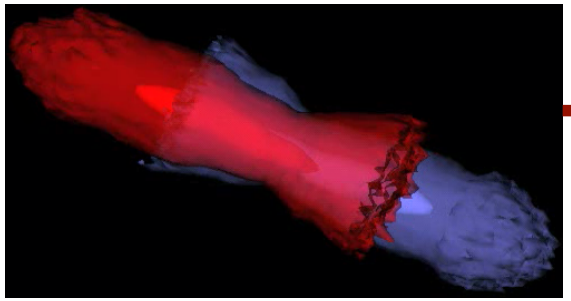


ComPASS HPC accelerator simulations are important for optimization of existing accelerators and plans for new/upgraded accelerators

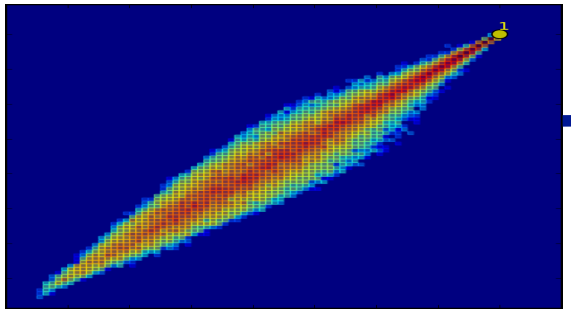
Electron cloud



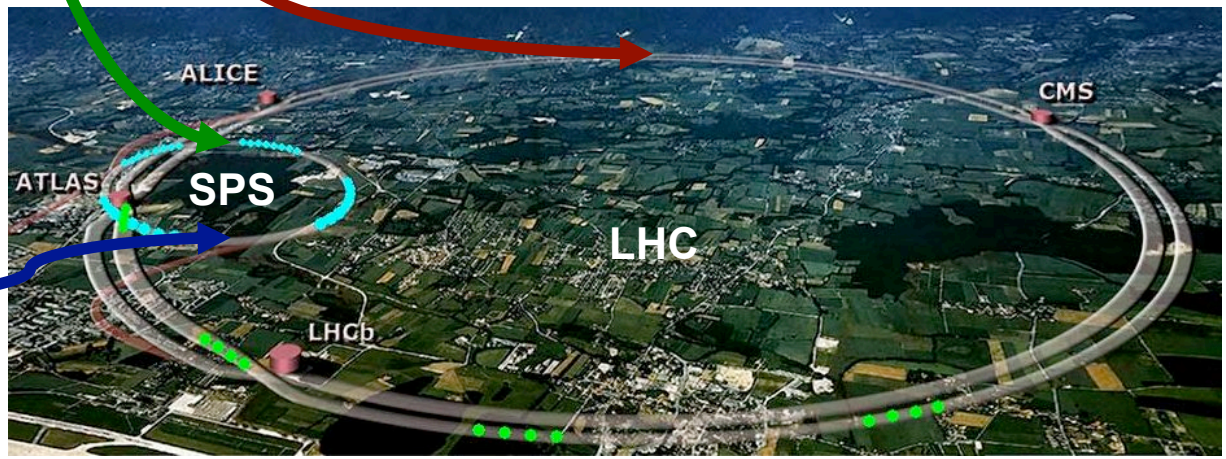
Beam-beam



Space charge

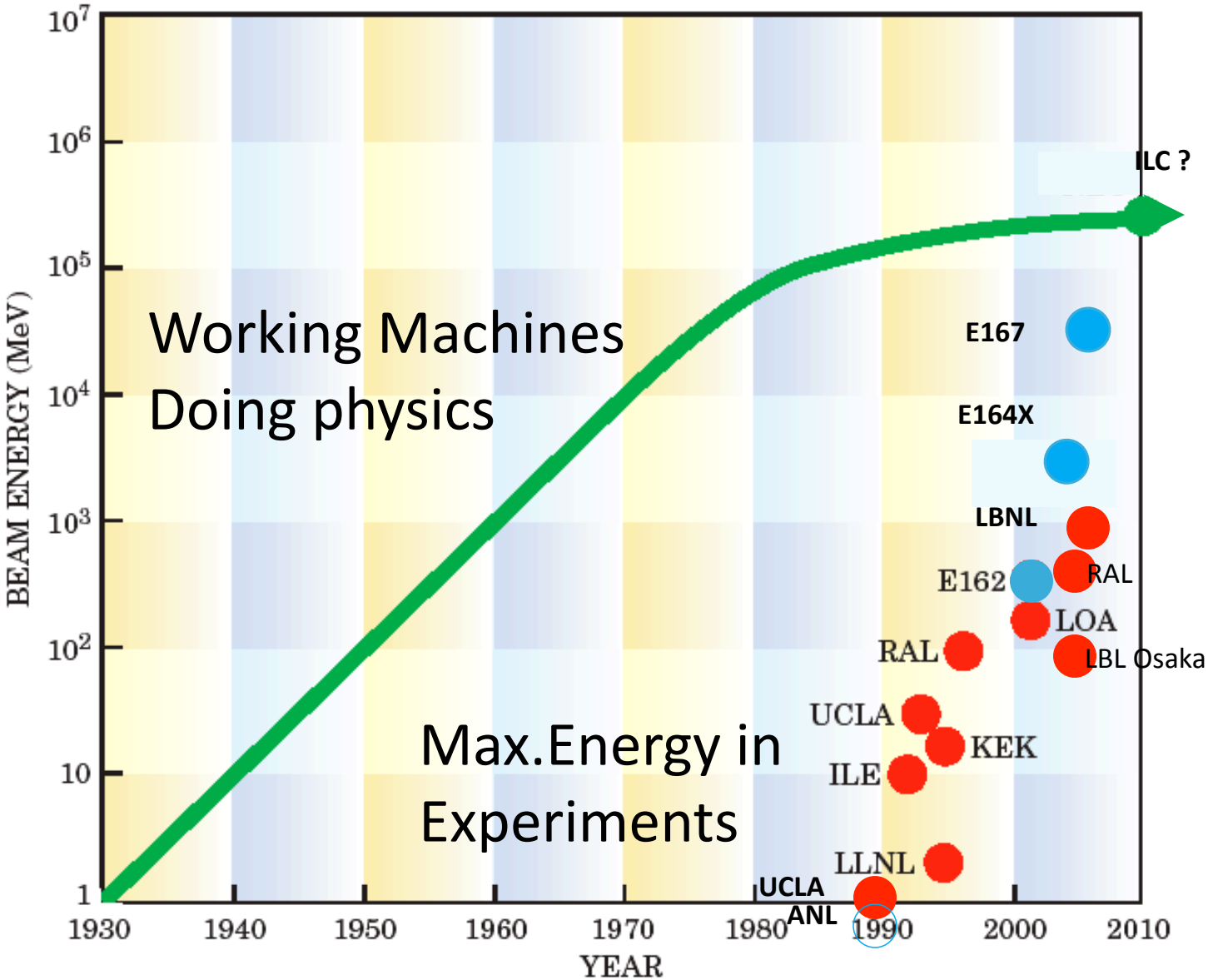


- Electron cloud attenuation and space charge simulations in the SPS
- Beam-beam simulations in the LHC



Plasma Accelerator Progress

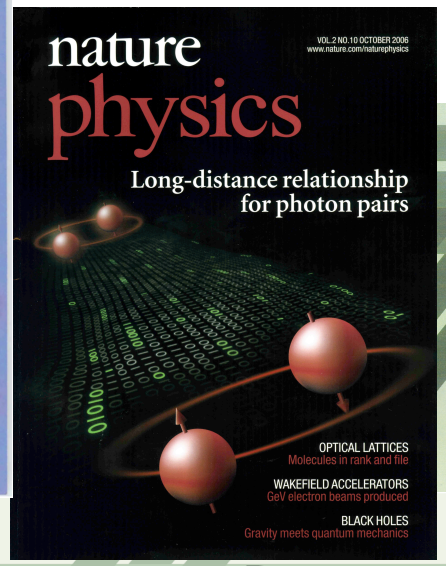
"Accelerator Moore's Law"

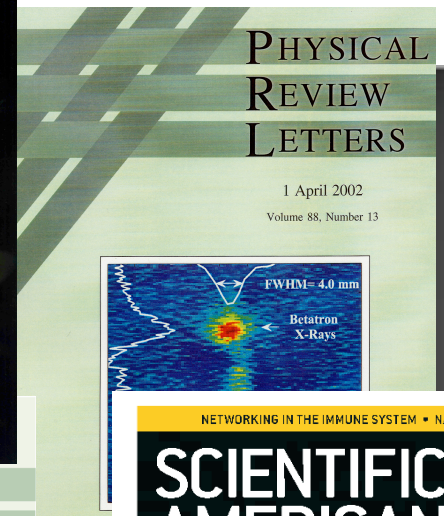


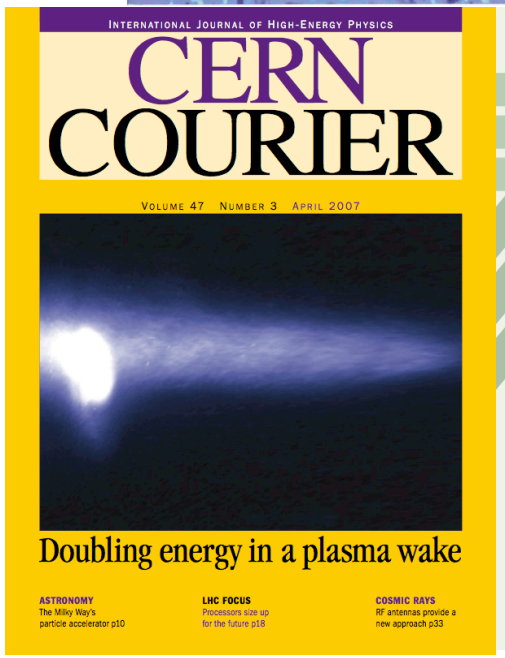
SCIENTIFIC AMERICAN
How to Protect New Orleans from Future Storms
FEBRUARY 2006
WWW.SCIAM.COM
Big Physics Gets Small
Tabletop Accelerators Make Particles Surf on
Plasma Wakes
-Smaller?
-Cheaper?

A story of SciDAC codes leading to SCIENCE DISCOVERY

Simulations were an important part of each of these highlights



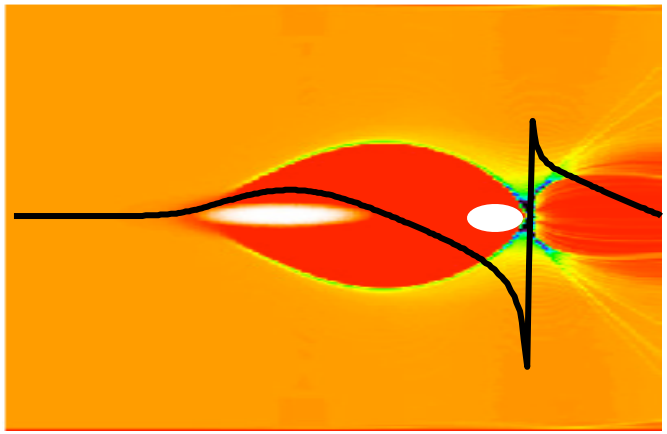




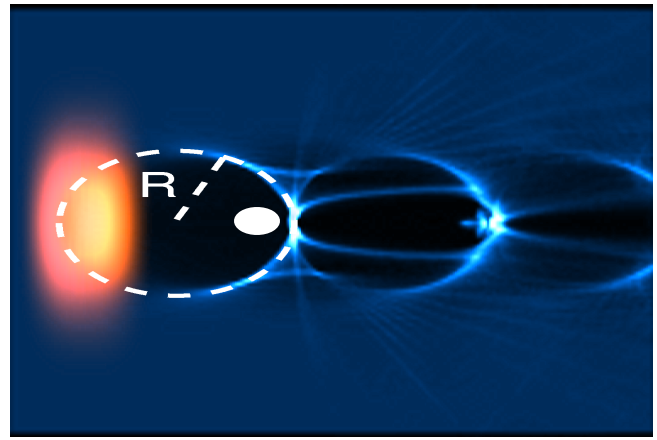
A story of wakes:
Wake Behind a Motor Boat

Wakes in plasmas: >10 GeV/m acceleration gradients

Driven by an electron beam



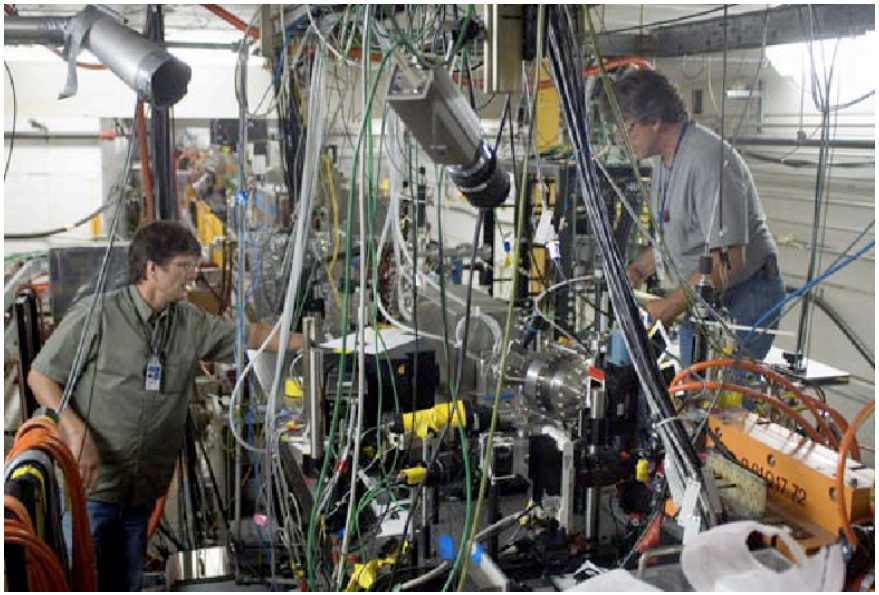
Driven by a laser pulse



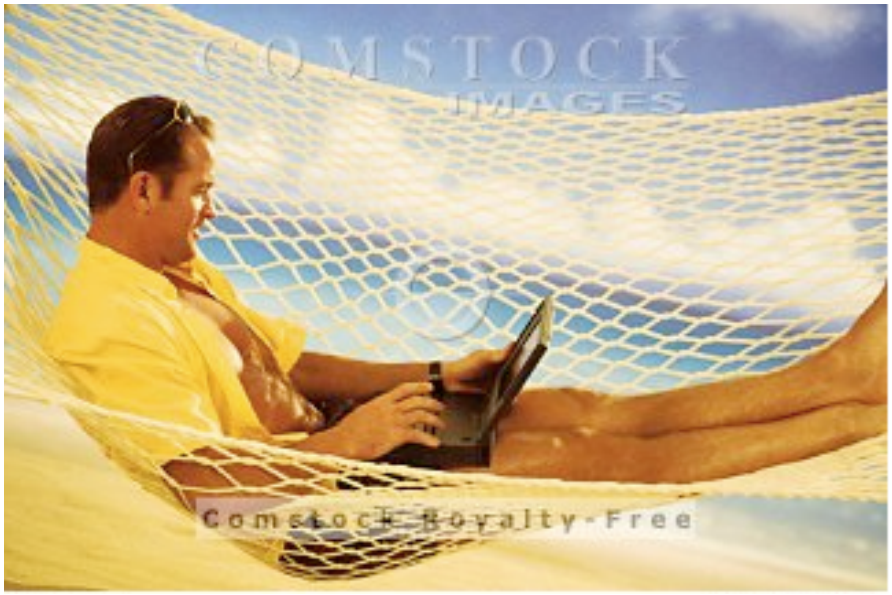
- **Evolution of a laser or particle beam**
- **Plasma response to driver: wake excitation and wake evolution**
- **Evolution of trailing beam**

Need nonlinear and particle based models

A story of the close connection between experiments and simulations



Life of an experimentalist



Life of a simulationist

My experimental colleagues
view of the world

A STORY OF MANY MODELS
HIERARCHY OF APPROACHES / APPROXIMATIONS

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

Disparity of time scales

- **Laser period ~fs**
- **Pulse length ~50fs**
- **Evolution driver ~ps**
- **Acceleration time ~ns**

The PIC algorithm
Deceivingly simple: Challenge to optimize and not all PIC codes are the same

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

Integration of equations of motion, Push particles

$\mathbf{F}_k \rightarrow \mathbf{u}_k \rightarrow \mathbf{x}_k$

Interpolating

$(\mathbf{E}, \mathbf{B})_{ij} \rightarrow \mathbf{F}_k$

Δt

Depositing

$(\mathbf{x},\mathbf{u})_k \rightarrow \mathbf{J}_{ij}$

Integration of Field Equations on the grid

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

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

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

Ponderomotive guiding center

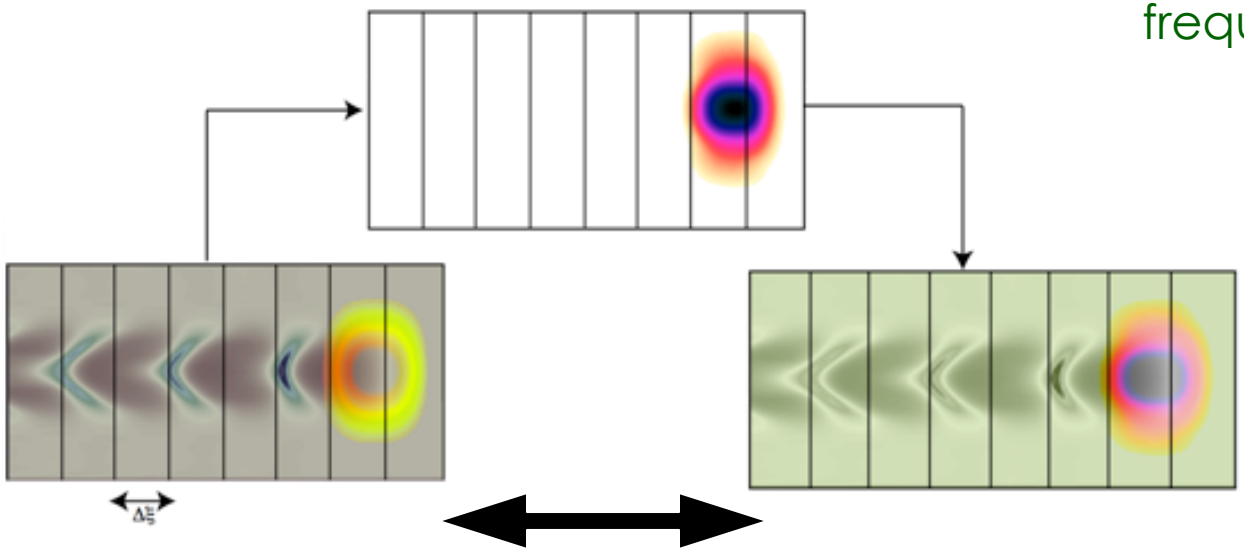
Potential (w_0/w_p)^2 savings

$$\left[2\partial_s\left(-ik_o-\partial_\xi\right)-\nabla_\perp^2\right]\hat{\mathbf{A}}^{\mathbf{laser}}=\frac{4\pi}{c}\mathbf{J}$$

Laser evolution:

Envelope Approximation

Average out laser frequency!



Advance forward resolving wake

dt~.25w_p^-1

The PGC algorithm has been implemented into VORPAL

Mora and Antonsen 1997, Gordon et al. 2000

Quasi-static approximation: QuickPIC

QuickPIC: Huang et al. 2007

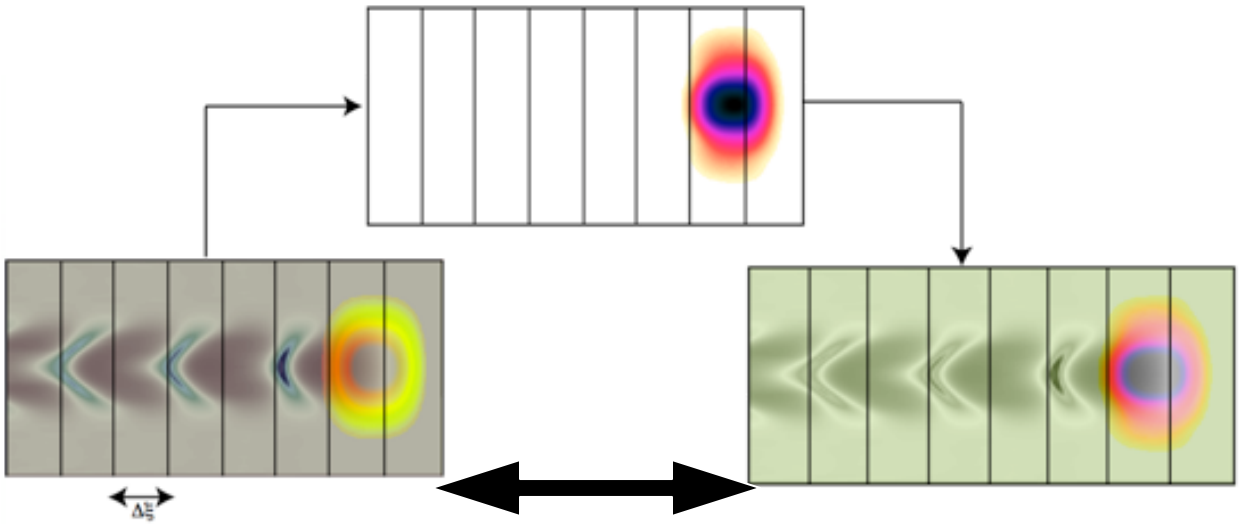
Potential (w_0/w_p)^3 savings

Laser evolution:

Envelope Approximation

(BIG time step)

$$\left[2\partial_s\left(-ik_o-\partial_\xi\right)-\nabla_\perp^2\right]\hat{\mathbf{A}}^{\mathbf{laser}}=\frac{4\pi}{c}\mathbf{J}$$



Advance forward resolving envelope evolution

Plasma evolution:

Quasi-static (frozen field) Approximation

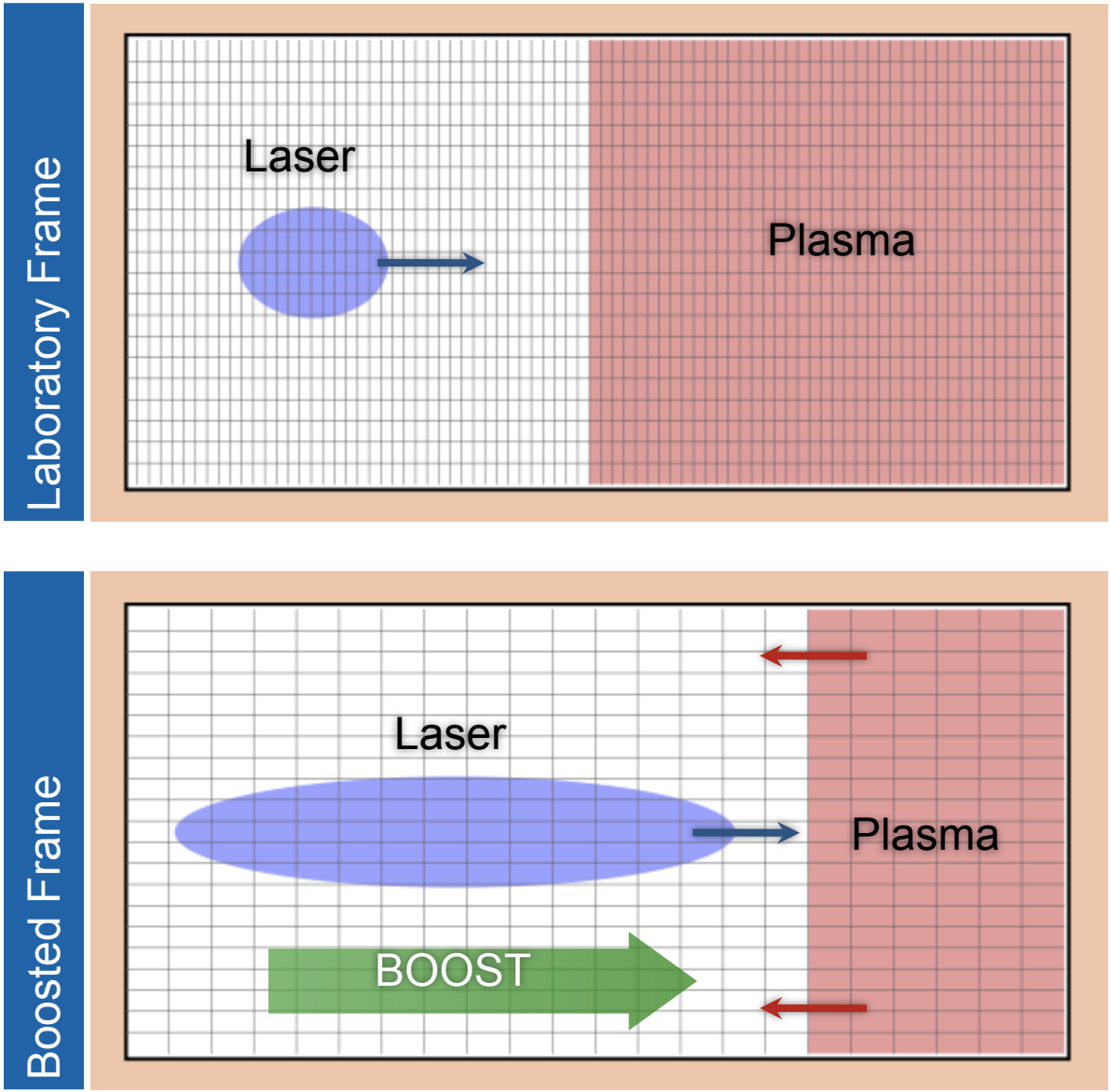
Maxwell's equations Lorentz Gauge

Not susceptible to unphysical Cerenkov radation

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

$$-\nabla_\perp^2\mathbf{A}=4\pi\mathbf{J}$$

Boosted Frames in LWFA simulations



Resolution gains

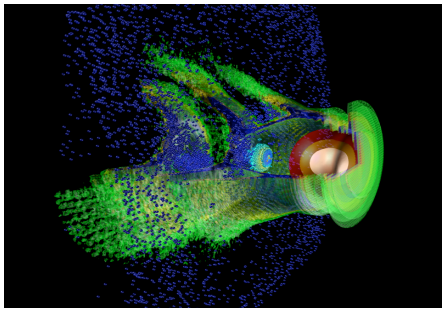
Particles	Resolution	$\beta)$
	Plasma contribution	γ
Time steps	Time step	$\gamma(1+\beta)$
	Total time	$\gamma(1+\beta)$
Total		$\gamma^2(1+\beta)^2$

Moving window in Lab Frame

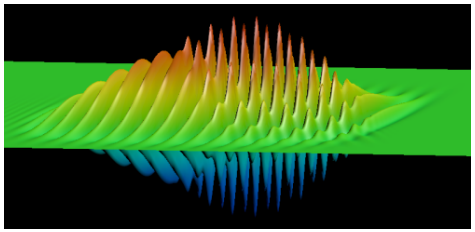
* J.-L. Vay, PRL 98, 130405 (2007).

SciDAC plasma-based accelerator codes

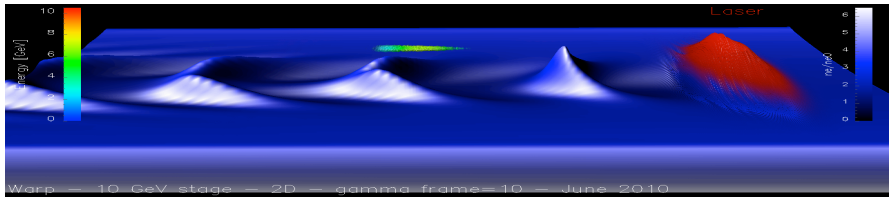
- **OSIRIS**
  - **Full PIC + boosted frame**
  - **part of 4 INCITE awards**



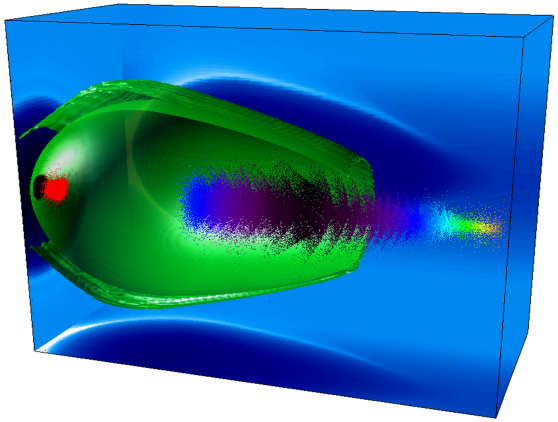
- **VORPAL**
  - **Full PIC + boosted frame + PGC**
  - **Part of a past INCITE award**



- **WARP**
  - **Full PIC + boosted frame**



- **QuickPIC**
  - **Quasi-static +PGC**
  - **Part of 2 INCITE awards**



Optimized and scale well

A Story of Code and Model Verification

UCLA

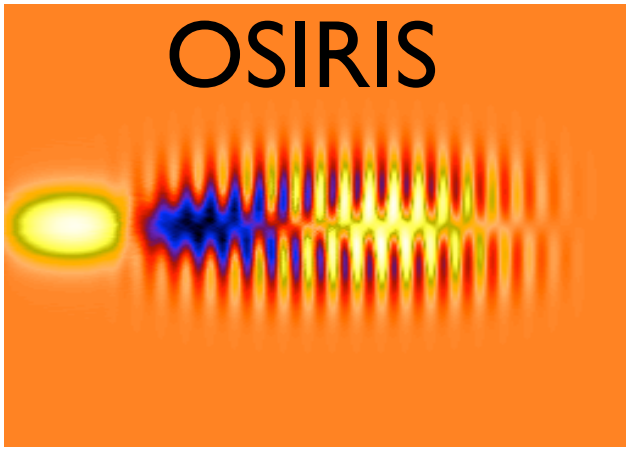
TECH

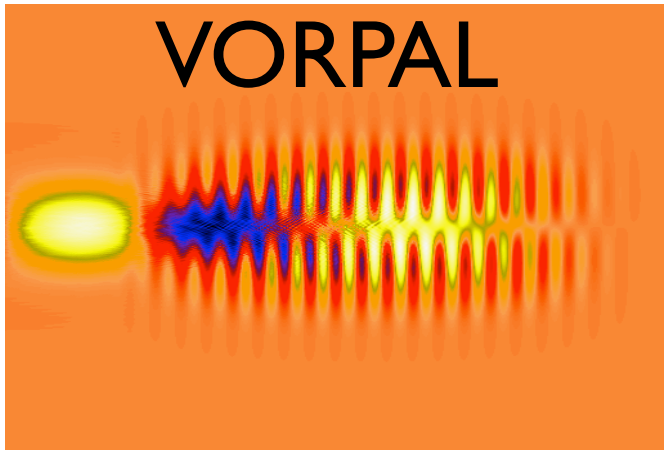
BERKELEY LAB

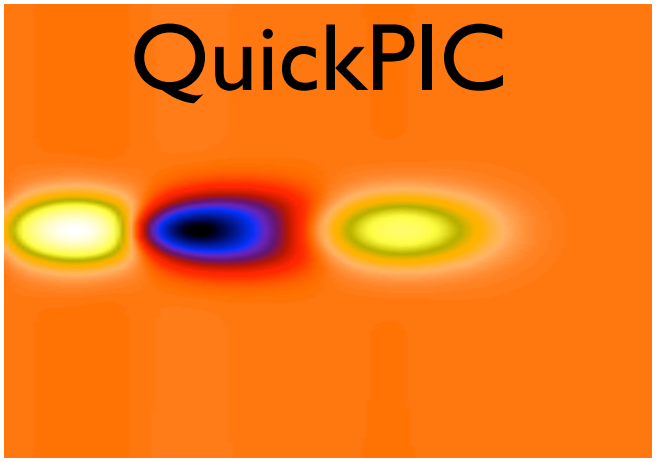
- Code verification is important especially for regime with no analytical results.
- Understanding of different numerical models, algorithms and implementations through benchmarking.

Benchmark Parameters

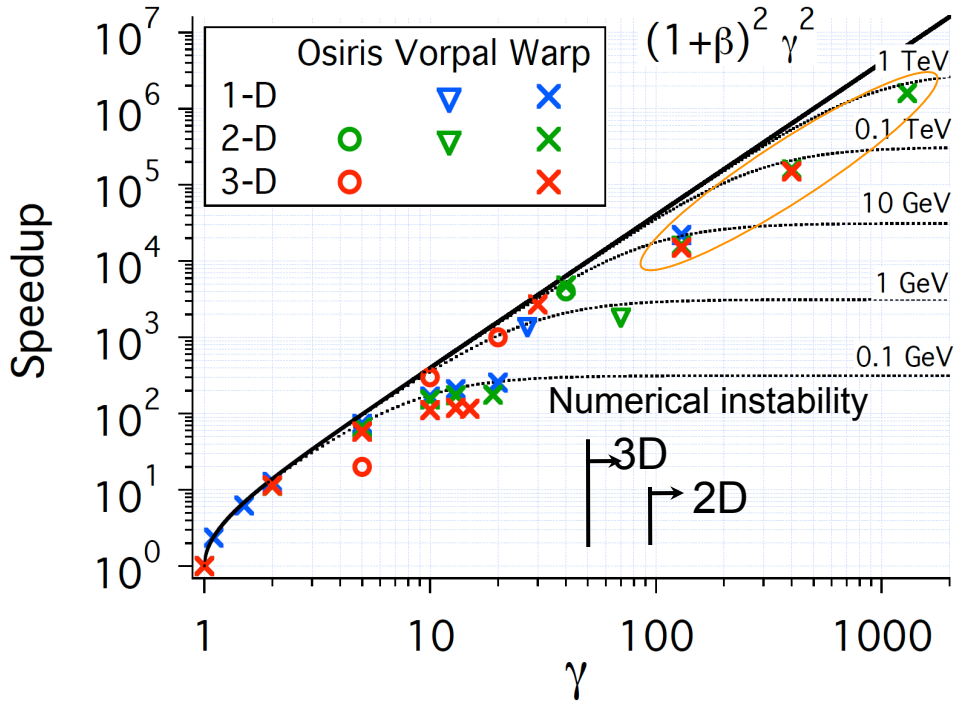
- λ_0=0.8 μm, I_{peak}~10^{18} W cm^{-2}, τ_{fwhm}=30 fs
  n_e=1.38x10^{19} cm^{-3}
- 80x80x20 μm^3 box, rectangular mesh of 512x512x512 cells
- 8 particle/cell for full PIC







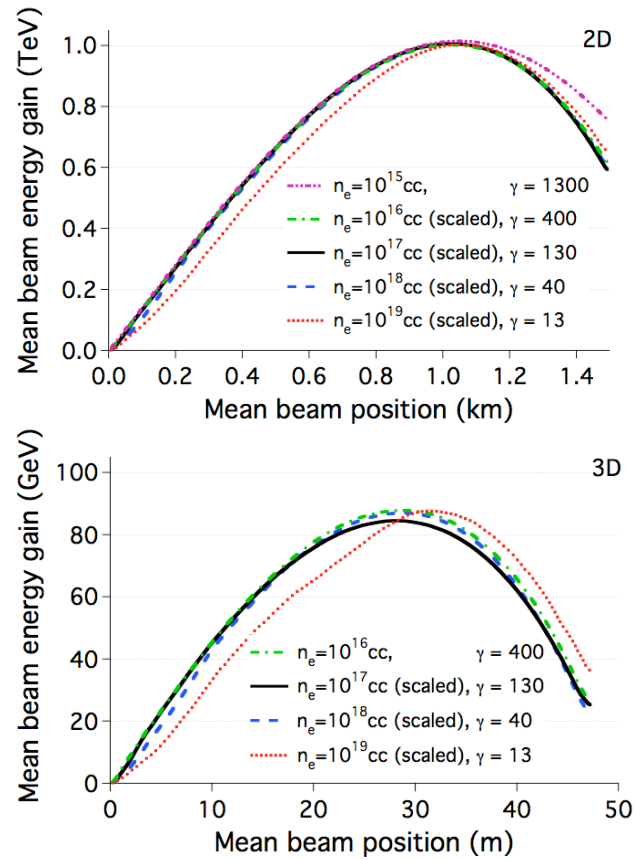
Story of working together to develop new numerical techniques can provide (w0/wp)^2 speed ups



Osiris: trapped injection, external injection w/beam loading

Vorpal: external injection w/ beam loading

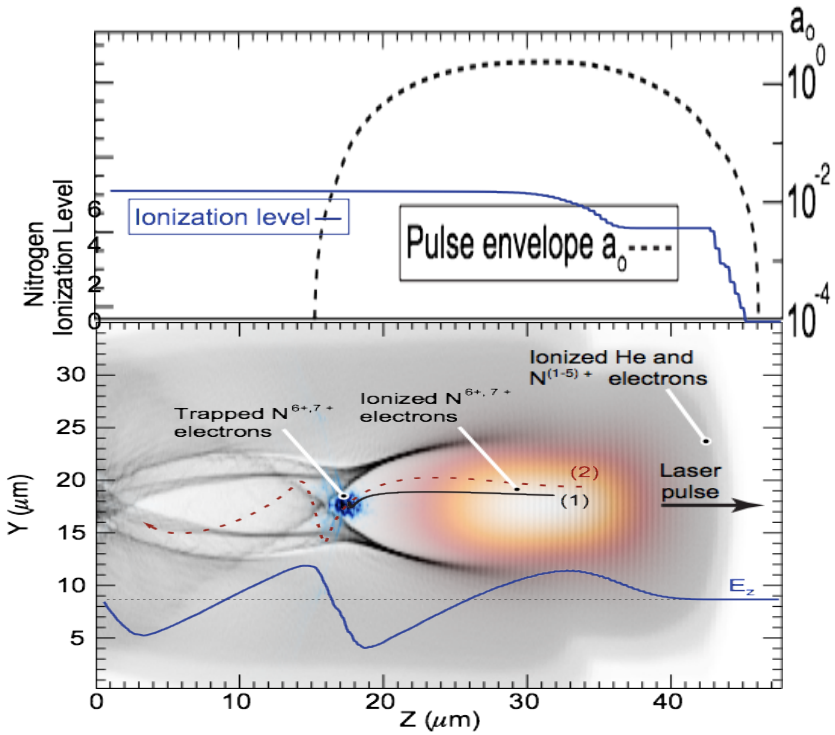
Warp: external injection wo/ beam loading

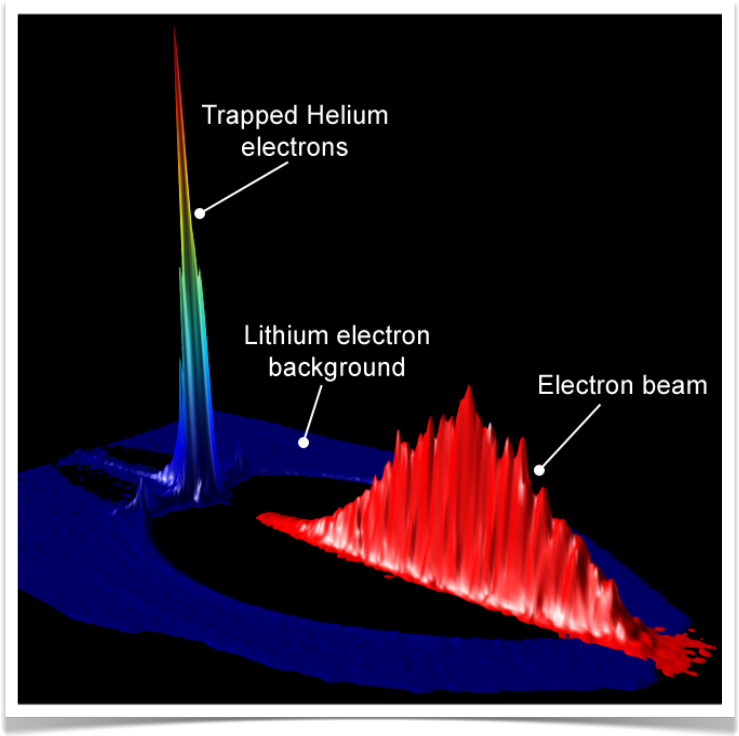


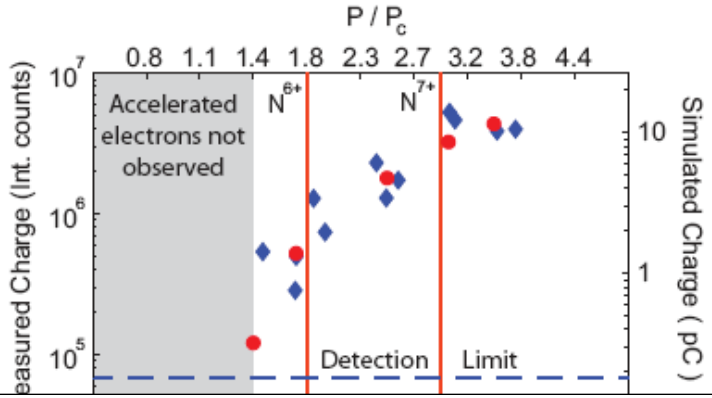
First time verification of scaling of deeply depleted stages up-to 1 TeV.

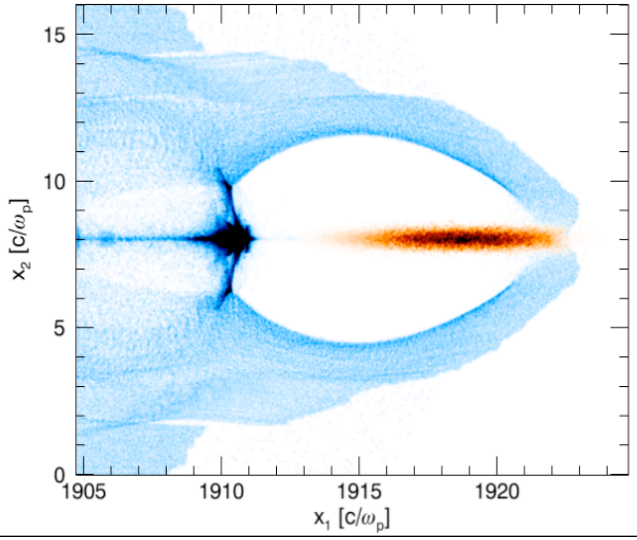
Plasma-based acceleration simulations: Results

Helping to understand physics: ionization trapping in LWFA and PWFA



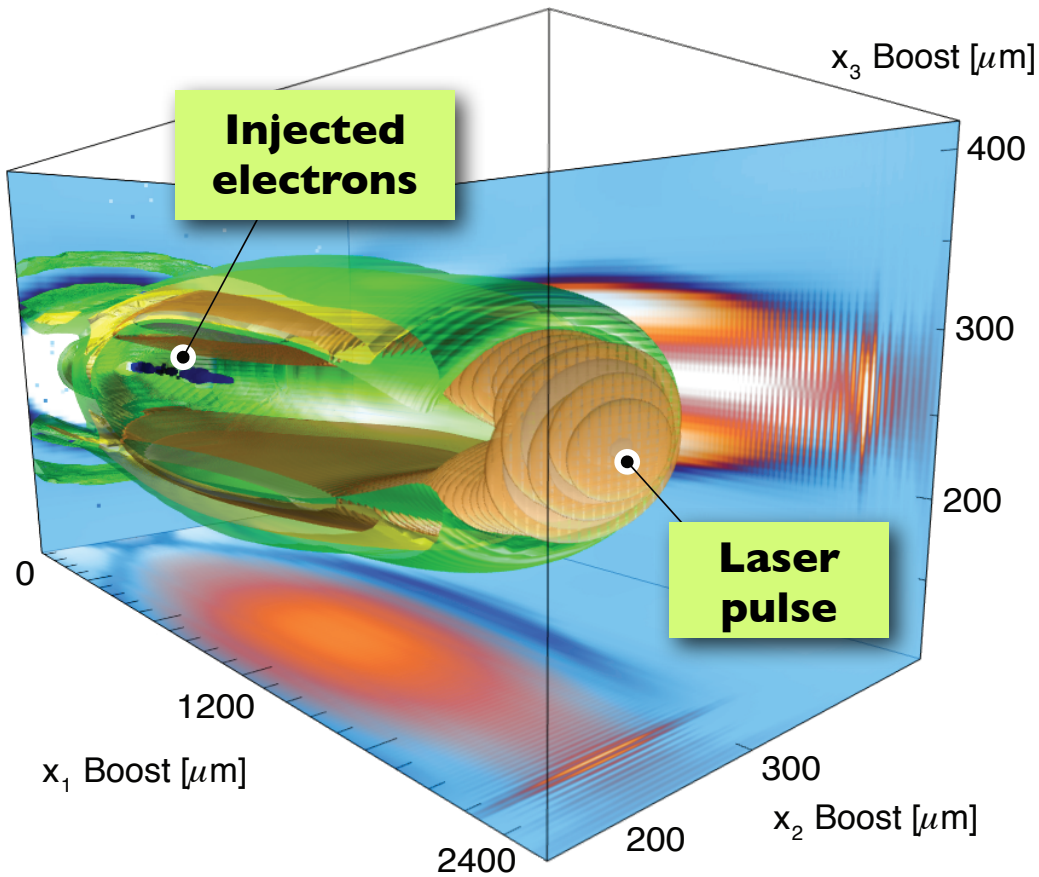


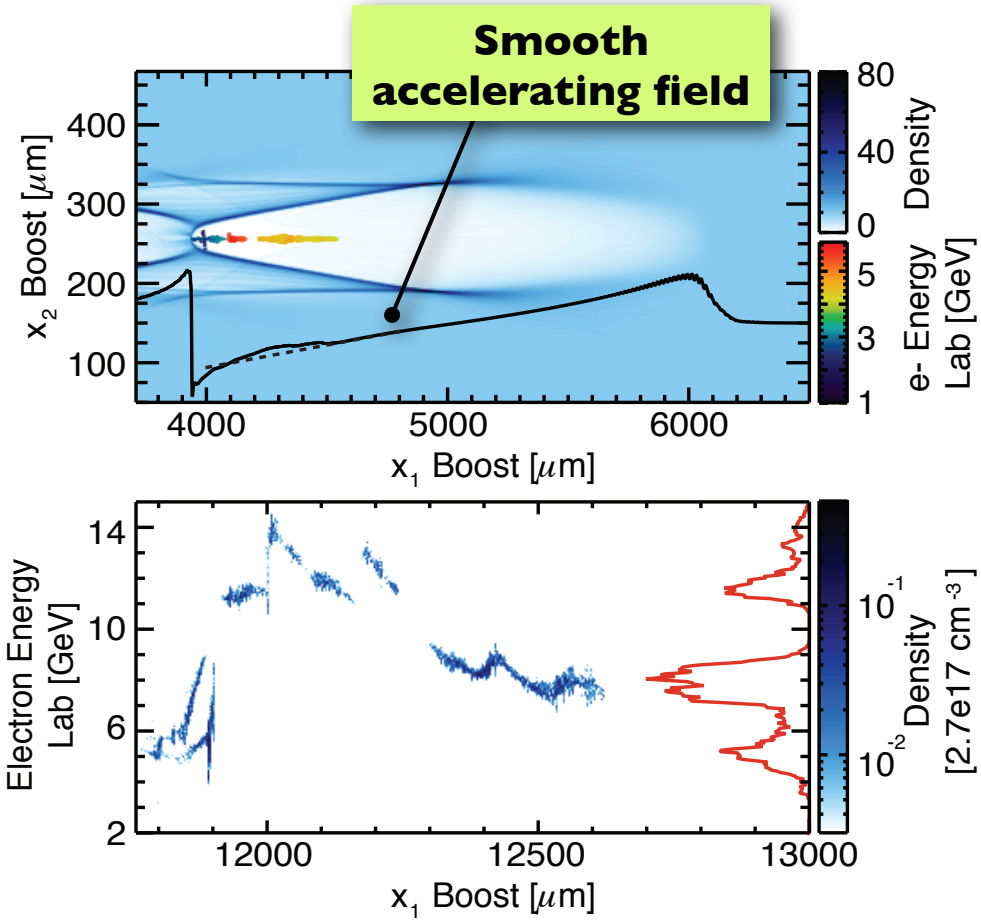




What is possible with future lasers: 250J

10+ GeV electrons in a single stage: self-guiding





Boosted frame
7000x256x256 cells
~10^9 particles
3×10^4 timesteps
$\Upsilon=10$

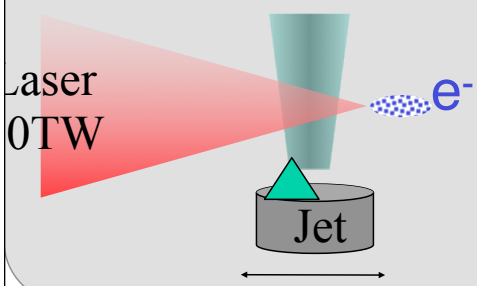
~300x faster
than lab simulation

Martins et al. Nature Physics 2010

7-12 GeV
1-2 nC

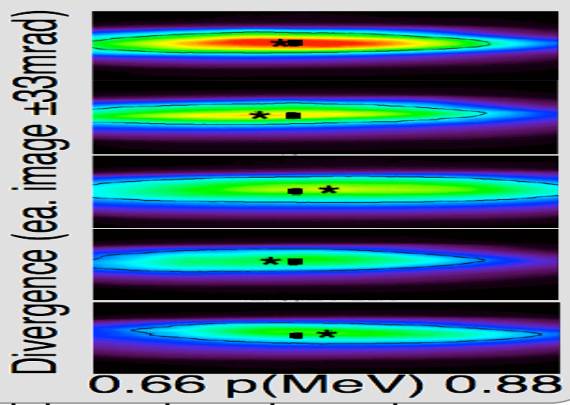
Developing a low emittance injector: plasma downramp trapping & acceleration

Laser focused at end of gas jet

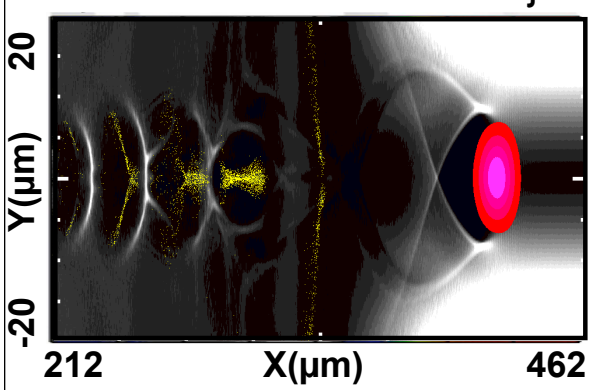


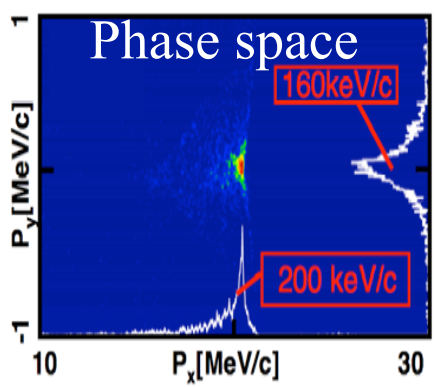
Stable low ε bunches

*centroid, avg



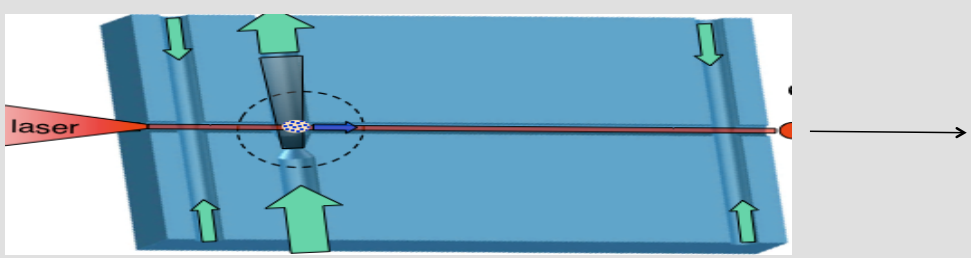
Simulations show injector into channel

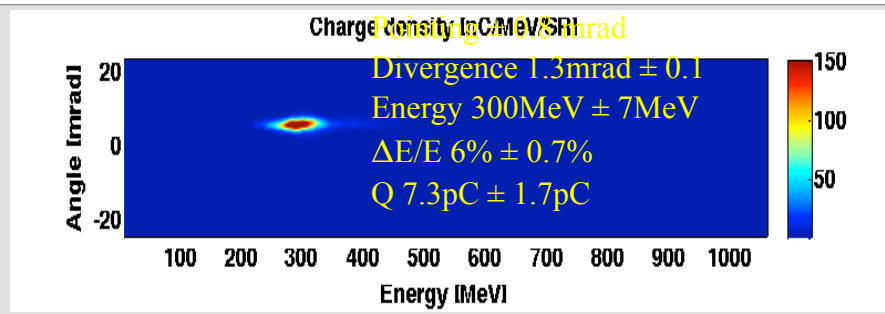




- Plasma density ramp slows wake
- Simulations show ramp creates low-emittance bunches observed in expt
- Validated vs diagnostics of energy spread divergence, laser, THz
- As injector – couple to channel, preserves beam as accelerated
- Experiments -stable, tunable beams
  - Tune for energy spread- in progress

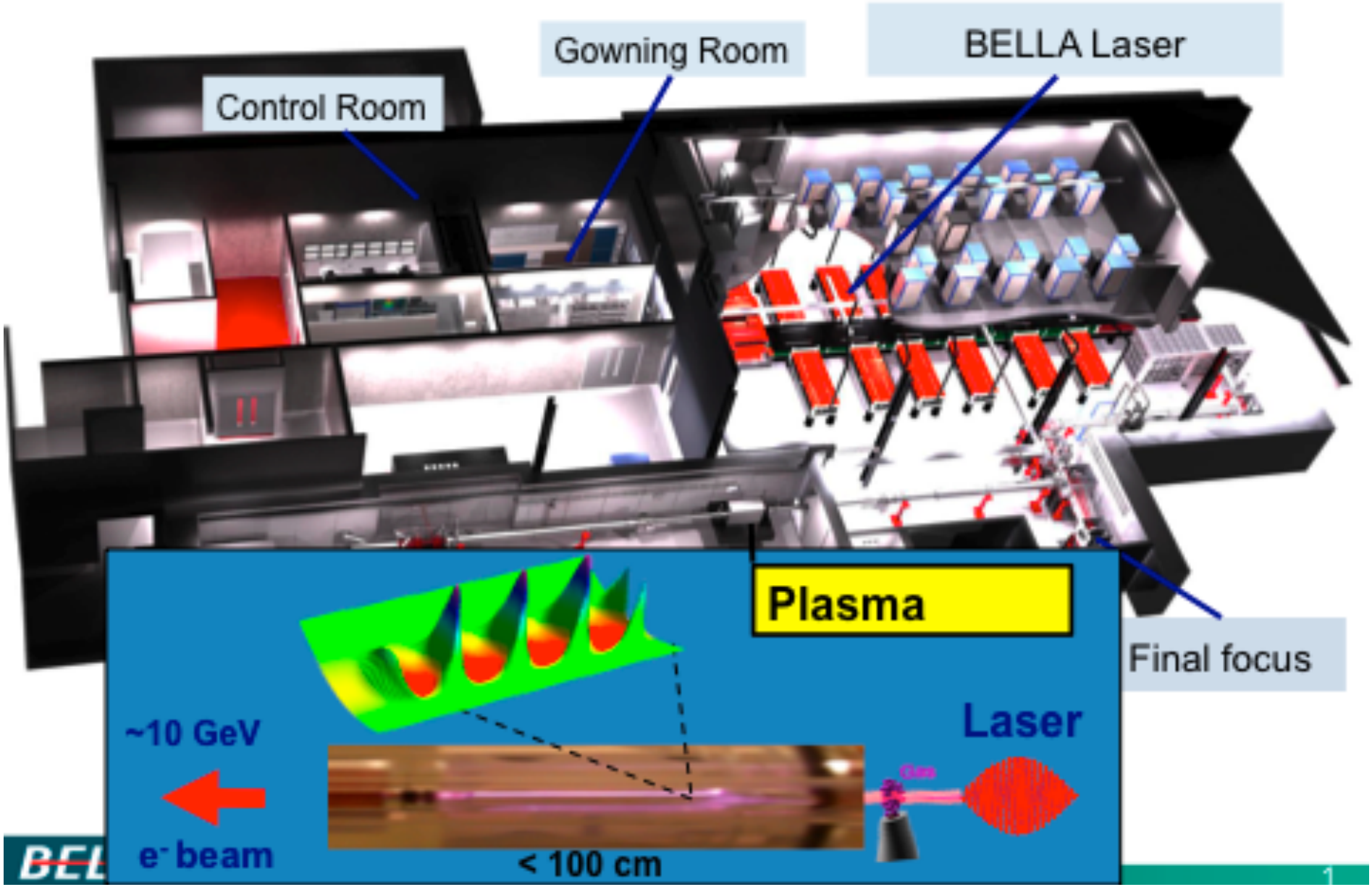
Experiments** showing stable, tunable beams





*Geddes et al, PRL 2008, SciDAC Review 09; G. Plateau, PAC 2007; Related: Bulanov PRE 1998, ** Gonsalves PAC 2009

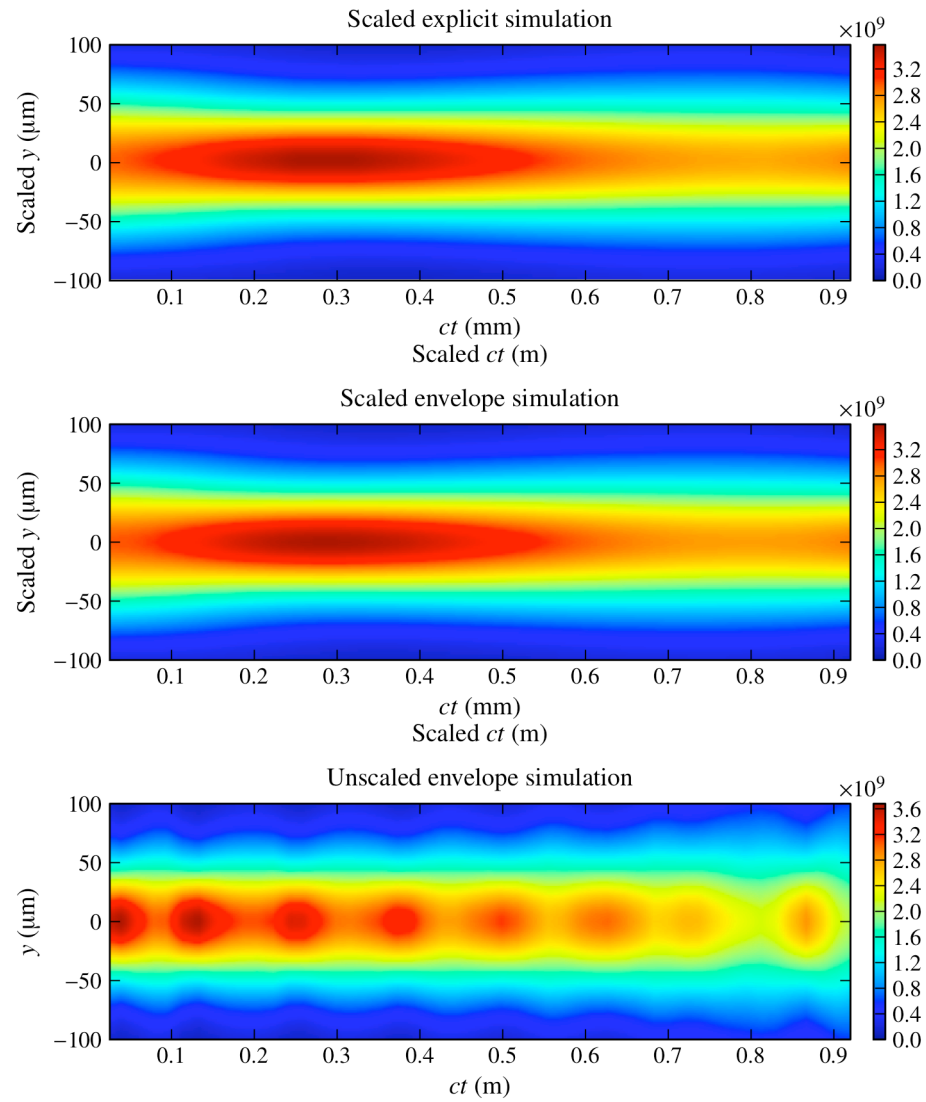
BELLA Project: state-of-the-art PW-facility for laser accelerator science



Ponderomotive guiding center: Full-scale BELLA simulations

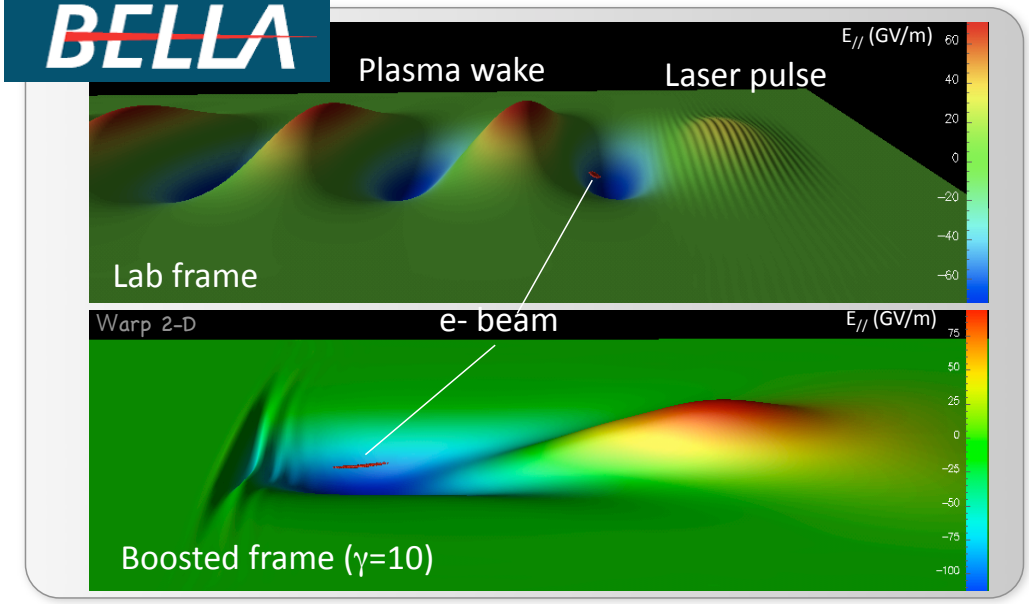
- Compared unscaled envelope and both envelope and explicit scaled to $n_0 = 10^{25}$ m^{-3}
- Unscaled 2D run required 183 CPU hours: (wo/wp)^2 speedup
- Improving envelope solver for longer propagation distances (Cowan et al.)

Gordon also has (3D and 2D r-z PGC)



Envelope model captures self-focusing oscillations

Lorentz boosted simulations of 10 GeV stage for full-scale depletion & stage physics

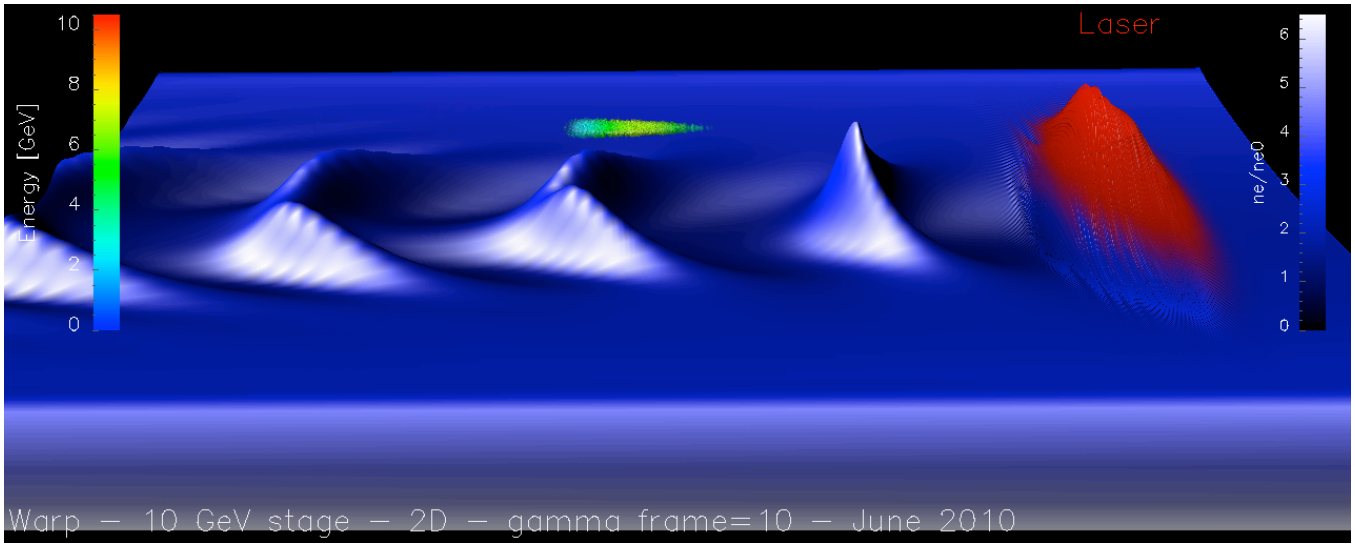


- Calculation in boosted frame
- Minimizes difference of scale from

  λ_{laser} to λ_{wake} to $L_{acceleration}$
- Speedup of >10,000 for 10 GeV
- Directly simulates 10 GeV stages w/ strong depletion
- Noise control techniques developed

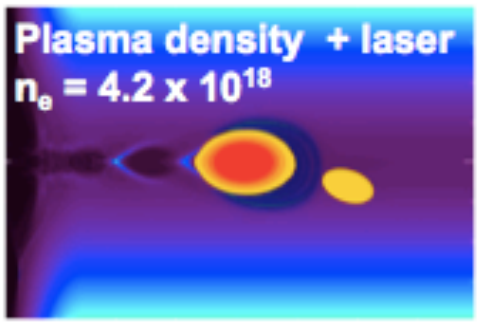
Scaled (10^{19} cc)
Run time:
Sec. in 2D
Min. in 3D

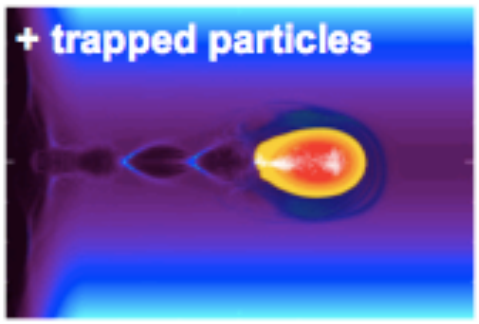
Full scale (10^{17} cc)
Run time:
Min. in 2D
Hours in 3D

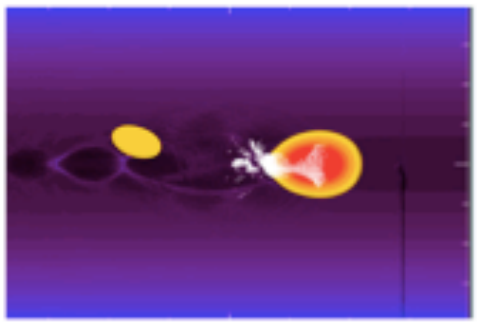


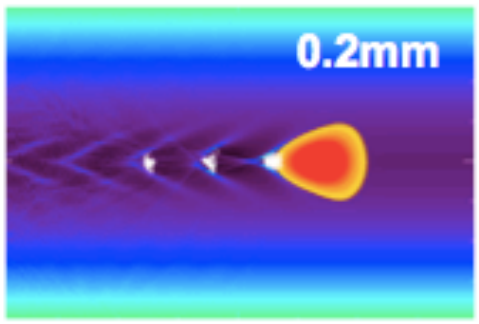
Predictive design of colliding pulse injected laser plasma accelerator experiments

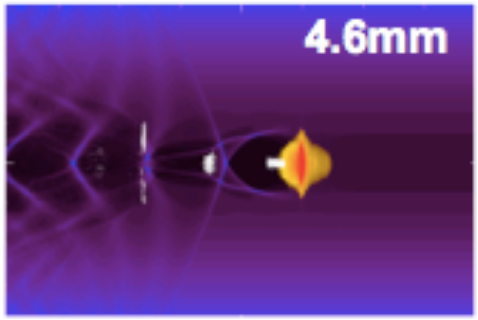
Cormier-Michel

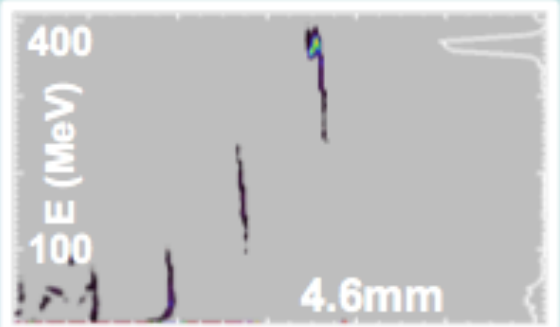






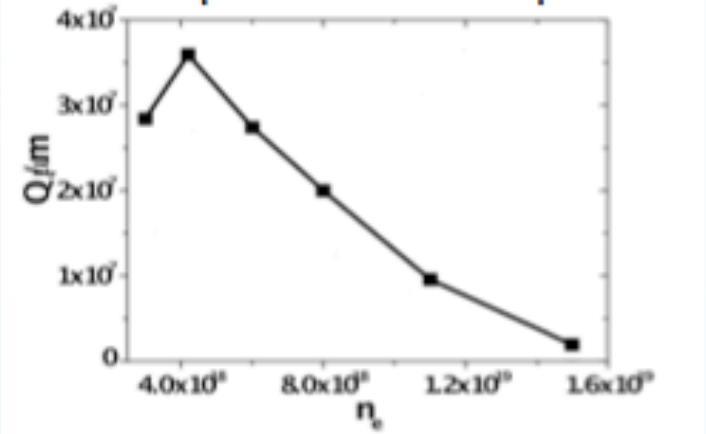




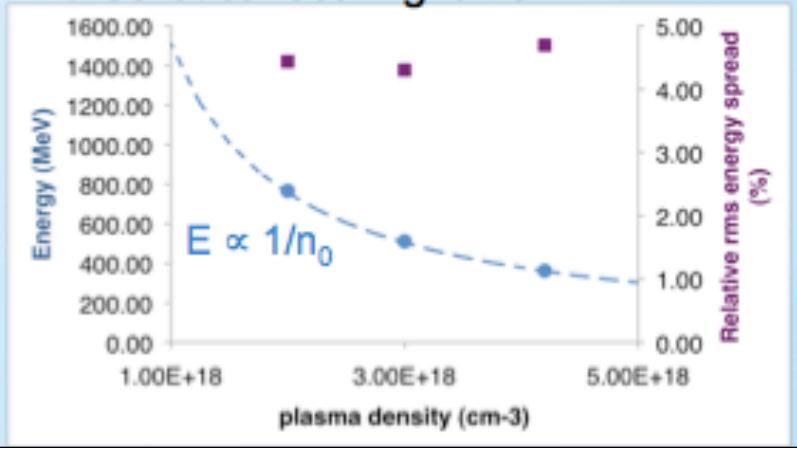


- Colliding pulse injection produce high quality electron beams
- Simulations allow parameter scan to predict best experimental setup

- Optimal density for trapped charge found for experimental laser parameters

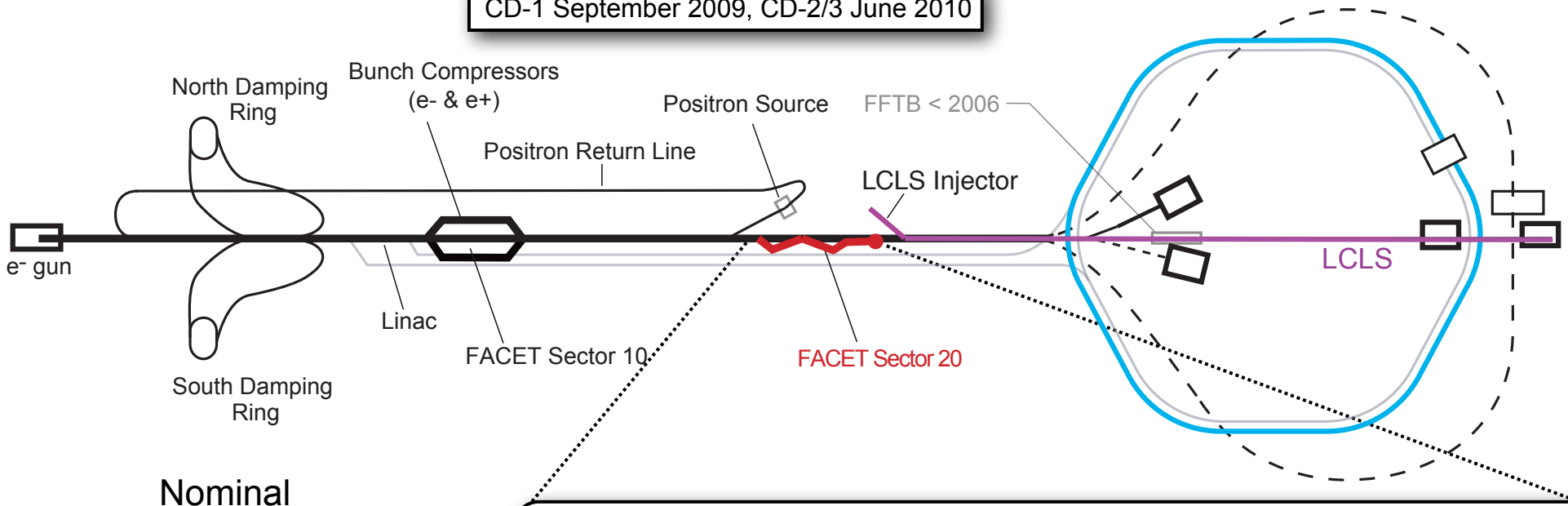


- Scaled laser parameters show theoretical scaling laws



The FACET Facility

CD-1 September 2009, CD-2/3 June 2010



Nominal
FACET Beam Parameters

Energy	23 GeV
Charge	3 nC
Sigma z	14 μm
Sigma r	10 μm
Peak Current	22 kAmps
Species	e^- & e^+

Beam Parameters Driven by Science Needs

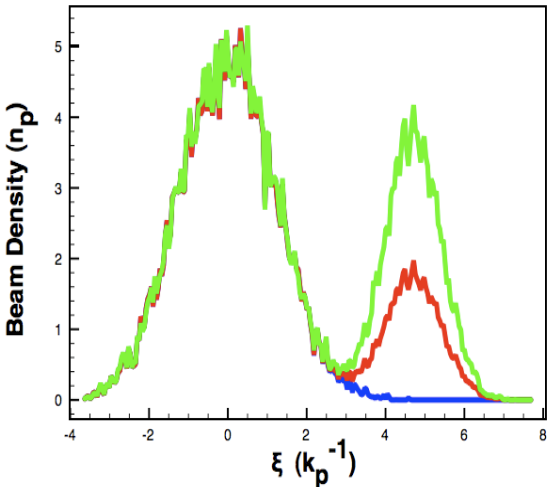
Delivered to 100m area with three distinct functions:

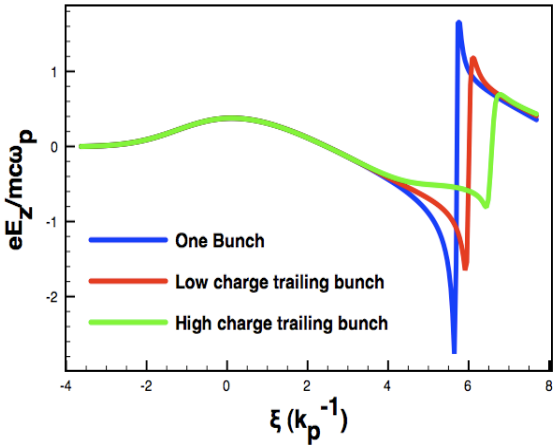
1. Chicane for final stage of bunch compression
2. Final Focus for small spots at the IP
3. Experimental Area(s)

Advantageous location:

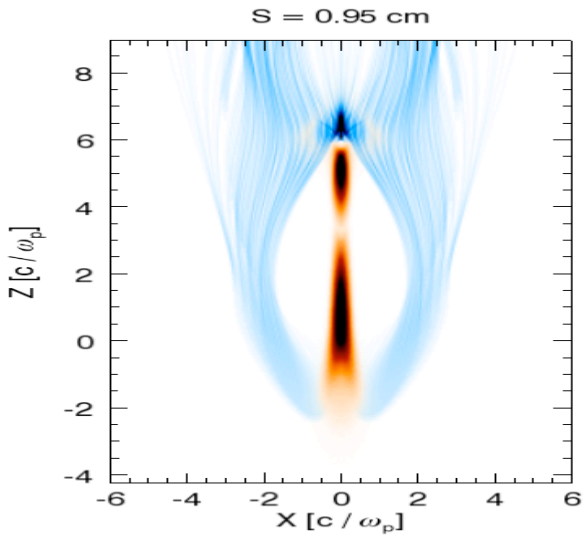
- Preserves e+ capability
- No bypass lines or interference with LCLS
- Linac setup virtually identical to SPPS/FFTB

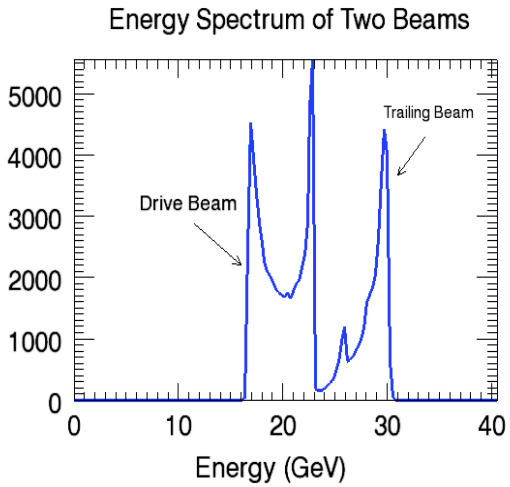
Simulations of Plasma Wake Field Accelerator (PWFA) Experiments at FACET (An et al. using QuickPIC)





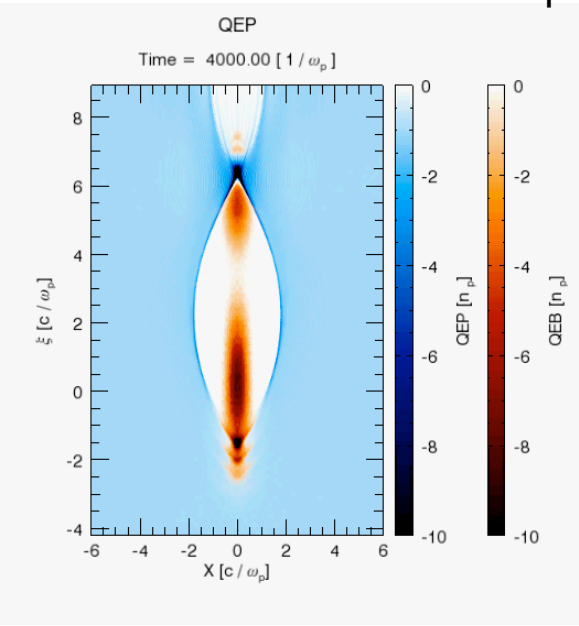
Two buches beam loading

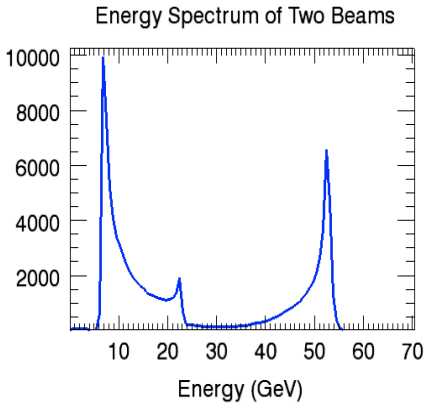




Simulation in a field ionized plasma using Cs

Simulation in a pre-ionized plasma





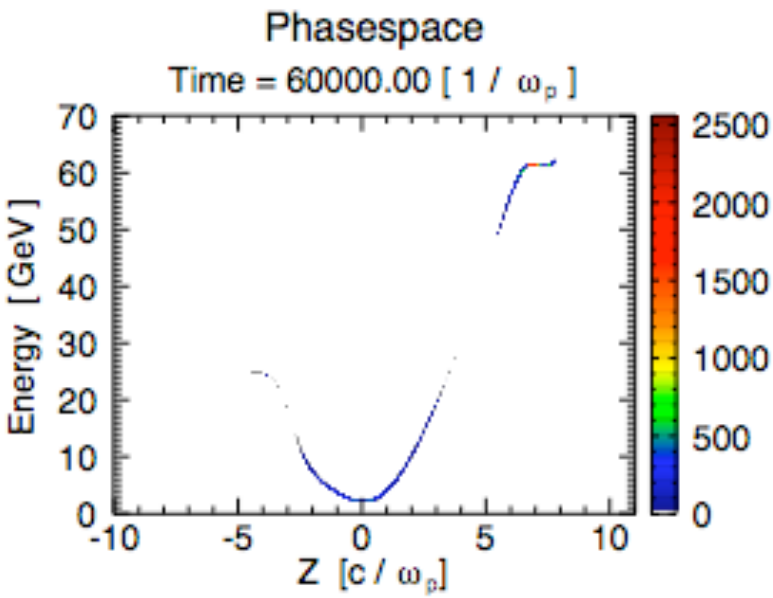
UCLA

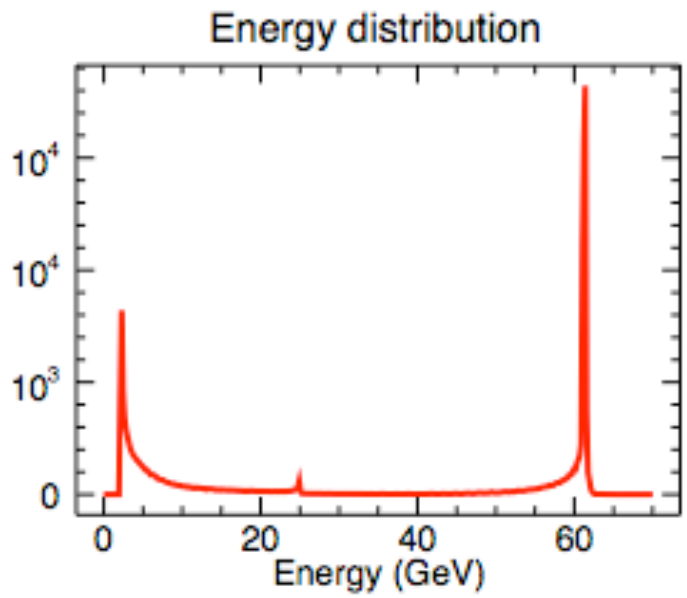
FACET

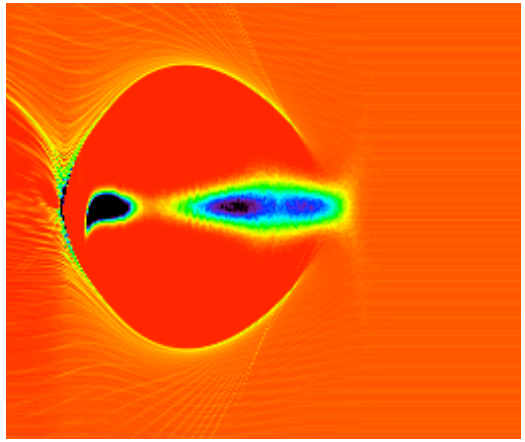
2010

Nominal 25 GeV stage

Preionized







n_p= 1×10^{17}cm^{-3}

N_{driver} = 2.9×10^{10}, σ_r= 3 μ, σ_z = 30 μ, Energy = 25 GeV

$N_{trailing}$ = 1.0×10^{10} , σ_r= 3 μ , σ_z = 10 μ, Energy = 25 GeV

Spacing= 110 μ

R_{trans} = $-E_{acc}/E_{dec}$ > 1 (Energy gain exceeds 25 GeV per stage)

1% Energy spread

Efficiency from drive to trailing bunch ~48%!

Extreme computing is enabling realistic 3D simulations of PWFA-LC

Nominal PWFA-LC stage

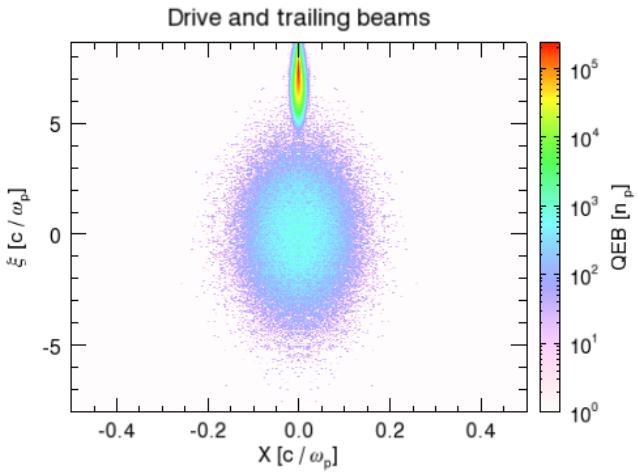
- **Drive beam: 3×10^{10} electrons, 25 GeV**
- **Main beam: 1×10^{10} electrons, 25 GeV**

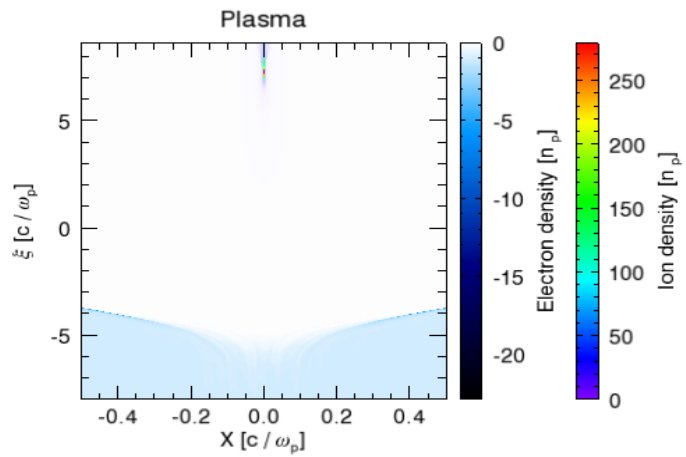
High resoluton required for modeling TeV collider beams

- **Drive beam emittance: 10 mm·mrad, matched spot size is 1 μm.**
- **Main beam emittance: 0.093 mm·mrad, matched spot sizes is 100 nm for $n_e=1\times10^{17}$ cm^{-3}, requires < 100nm resolution.**

High resolution required for modeling ion dynamics

- **Resolve real atom separation of ~20 nm at 1×10^{17} cm^{-3}.**
- **Simulation resolution: 49nm×49nm×152nm, 1.37×10^{11} (8192×8192×2048) grid points, 4 particles/cell (for plasma).**
- **16384 cores, ~ 6TB memory on ORNL Jaguar machine.**





Emittance growth from ions is slower than expected!

Efforts for using advanced architectures

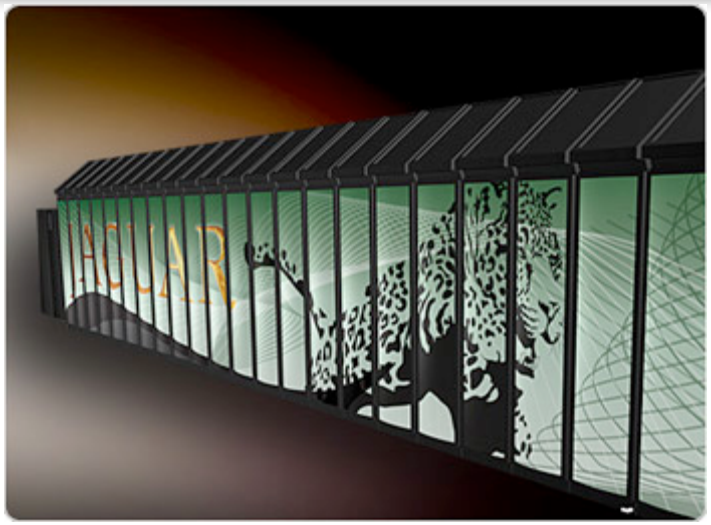
SIMD units

VM SSE/

GPGPUs

CUD STREA

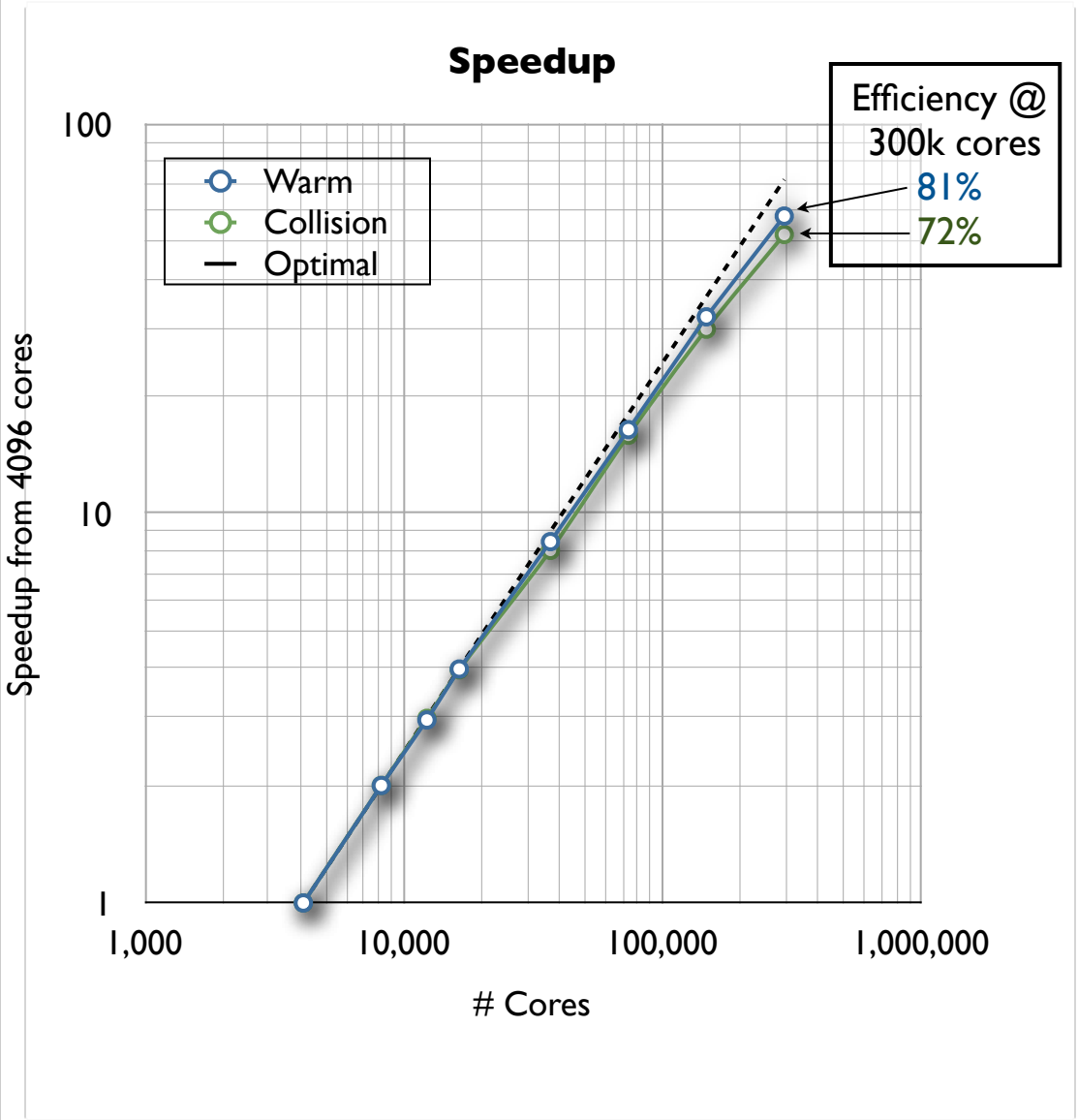
FZ Jülich Jugene
IBM BlueGene/P
#5 - TOP500 Jul/10
294912 cores
R_{max} 825 TFlop/s



Jaguar
#1 - TOP500 Jul/10
224,256 cores
R_{max} 1.7 PFlop/s

- SIMD
  - Vector co-processor
  - Available in most common CPUs
- GPGPU
  - Graphics Processing Units
  - Up to ~ 1 TFlop/s per board
  - “Add-on” co-processor
- Ultra-Massively Parallel
  - Scalability to over 10^5 cores

Strong Scaling to 295k cores:OSIRIS



Strong Scaling Results

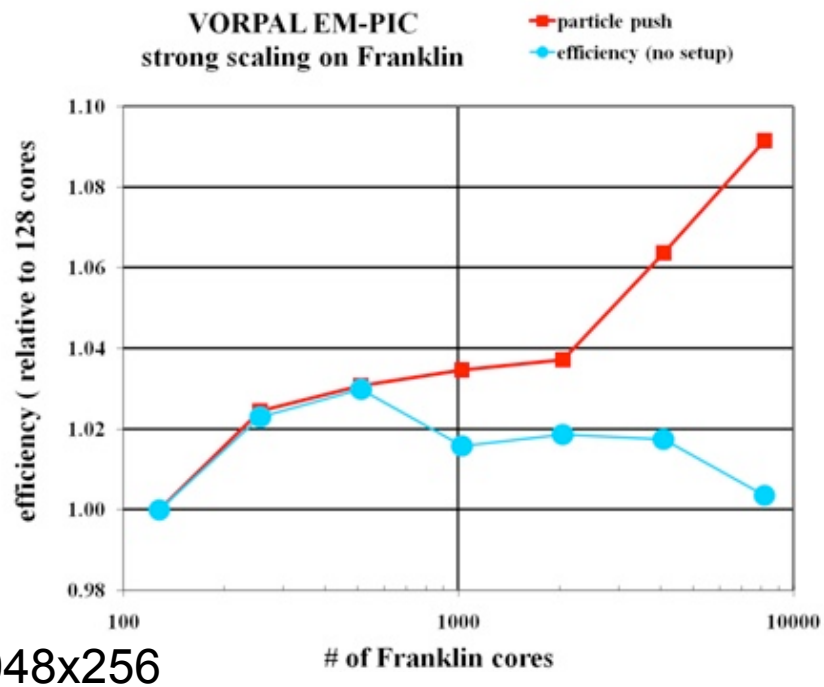
- Excellent scalability to 294912 cores
- Parallel Efficiency
  - Warm: 81%
  - Collision: 72%
- Final problem size very small
  - 1820 grid points
  - 58k particles (warm)
  - 29k particles (collision)

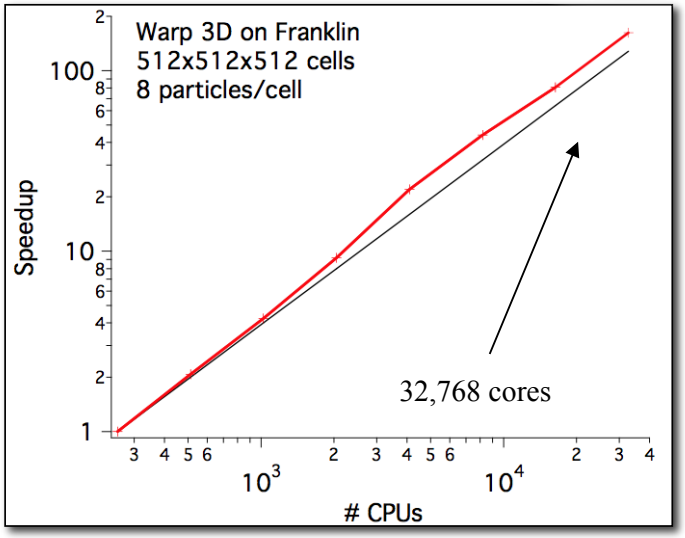
- Above 16k cores choice of parallel topology critical
  - BG network only connects neighbors
  - Use BG MPI extensions to get hardware topology

Additional strong scaling: Vorpal, Warp, QuickPIC, and OSIRIS

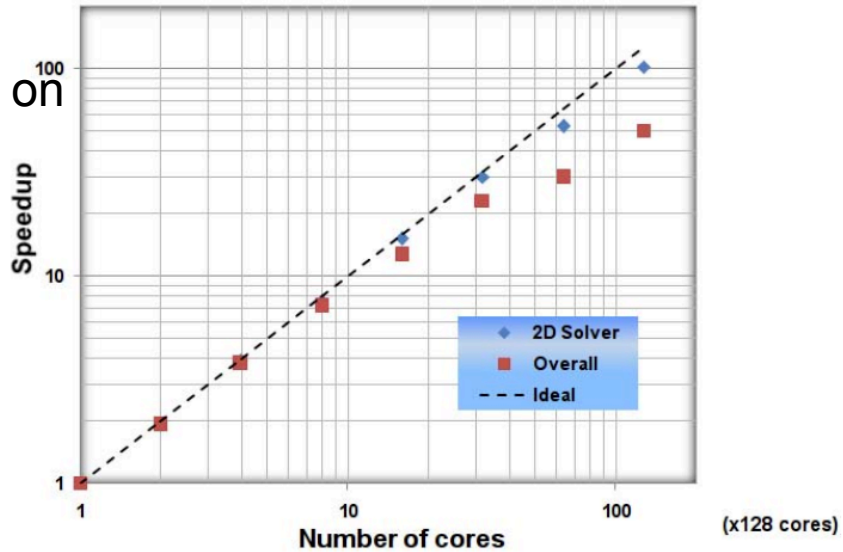
The problem sizes are much smaller than typical production runs

512x512x256 16 ppc

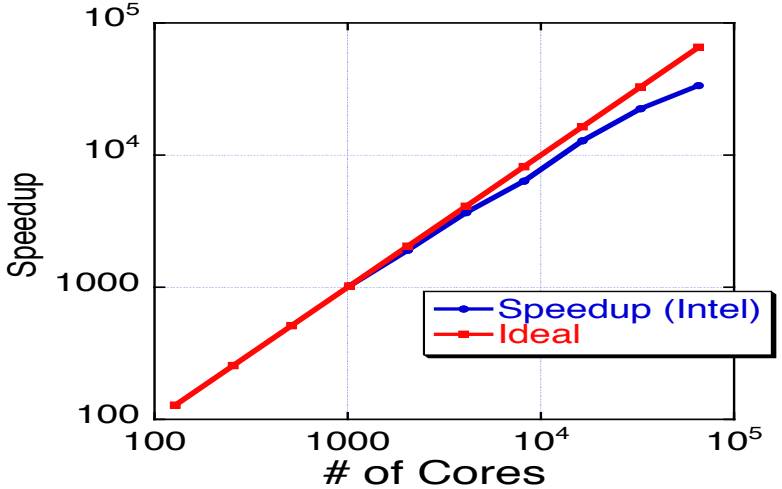




2048x2048x256
4ppc
QuickPIC on
Franklin



OSIRIS on Jaguar:
1024x1024x512 16ppc



GPU acceleration for PIC codes using a rigorous particle sorting routine that is extendable to any many core architecture

	Intel i7	GTX 280	Speedup
Deposit [ns]	8.2	0.21	40×
Push [ns]	19.9	0.43	46×
Sort [ns]	-	0.44	-
Total [ns]	30.0	1.08	**28×**

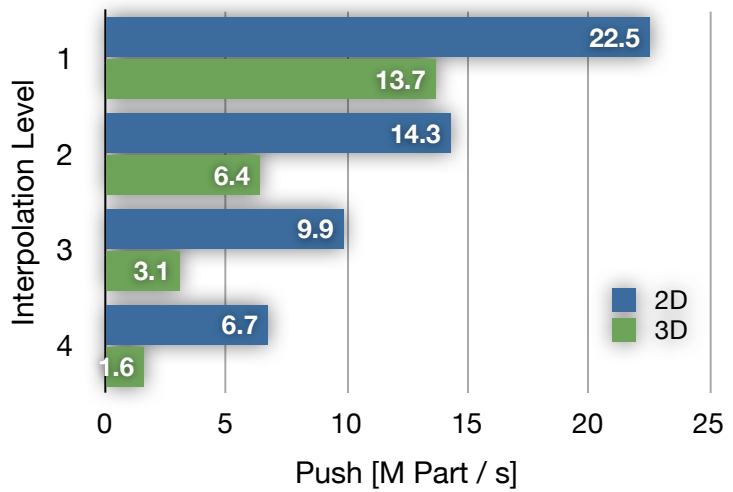
- Overall speedup of about 28 on a 2D Electrostatic code in single precision (Decyk et al. ICAP 2009 proceedings).
- Extrapolating to EM codes (<3ns/particle/step is possible—>100 time speed up!!)
- Implementation of a EM algorithm using a different sorting routine and thread size. Speed ups of 87- 27 depending on the plasma temperature (X. Kong et al. submitted).
- A variety of approaches are being investigated: UCLA and Tech-X

SSE Code Performance: OSIRIS

Frozen Plasma

Peak code performance

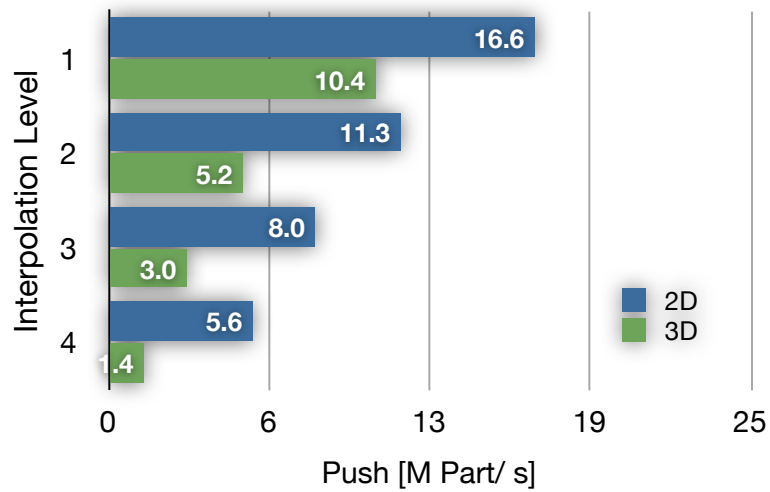
	Push [ns]		Push [M Part/s]	
Level	2D	3D	2D	3D
1	44	73	22.5	13.7
2	70	156	14.3	6.4
3	101	324	9.9	3.1
4	149	625	6.7	1.6



e^+ - e^- Weibel Instability

Typical Simulation

	Push [ns]		Push [M Part/s]	
Level	2D	3D	2D	3D
1	60	96	16.6	10.4
2	88	193	11.3	5.2
3	125	332	8.0	3.0
4	179	739	5.6	1.4



System: Intel i7 965 @ 3.20GHz
Compiler: Intel 11.0 (-Ofast)

Typical simulation performance
~25% below optimal

Summary

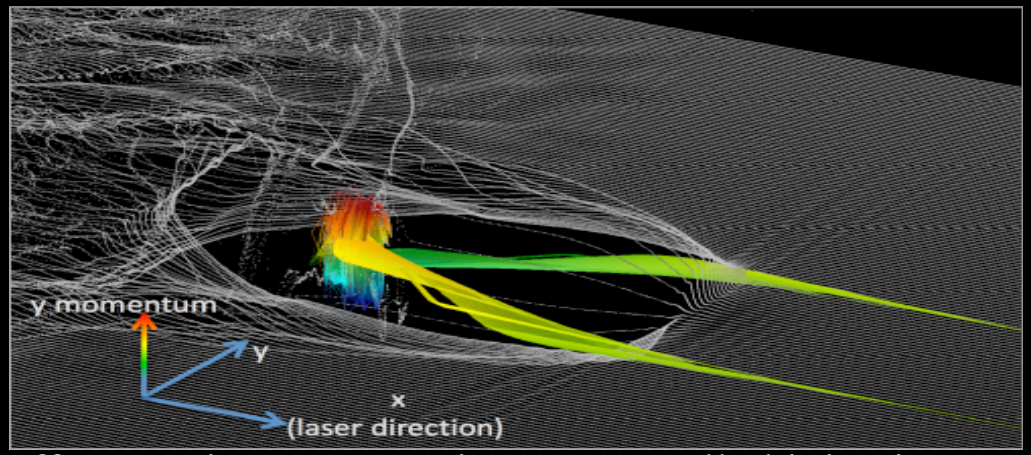
- Need to support more than one code! Benchmarking and algorithm comparison.
- SciDAC AA codes have led to discovery
- SciDAC AA codes helped to make the science case for two new facilities: BELLA and FACET
- SciDAC AA codes are being used to study possible parameters beyond BELLA and FACET: Studying issues of relevance to a future collider
- Within the COMPASS team there are ongoing efforts for developing kernels and production codes for advanced architectures: results are exciting--100 times speed up on GPUs is possible.
- The future is exciting: A combination of algorithmic development and new kernels for new hardware could lead to additional speed ups of >10000

  Real-time steering of experiments (turn around time of minutes)

  Rapid parameter scans to determine how changes in inputs effects outputs (experimental observables and physical processes)

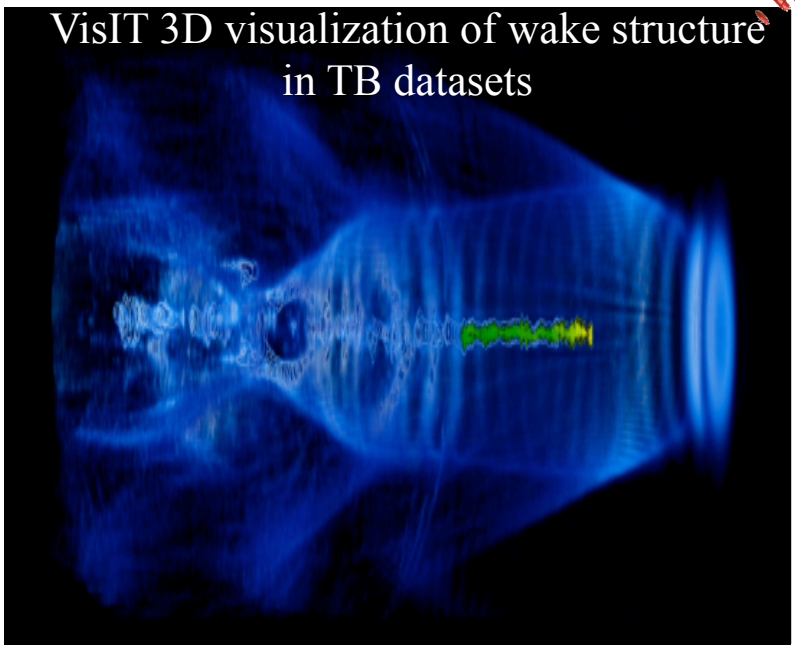
Visualization and analysis of TB data show wake and injection structure

Transverse injection into wake visualized with FastBit indexing and query, particle tracking

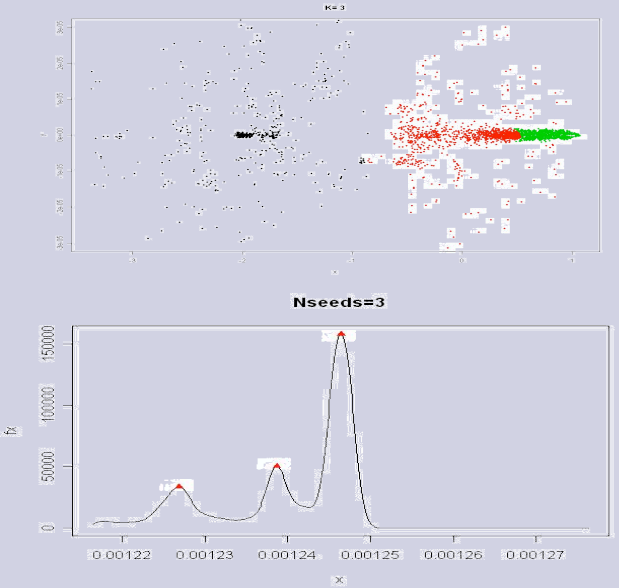


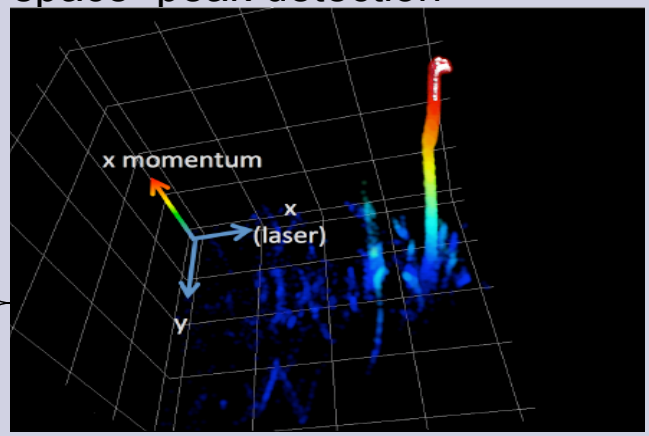
Affects emittance – motivates controlled injection

VisIT 3D visualization of wake structure in TB datasets



Fuzzy clustering in 6D phase space+peak detection





Automated beam detection for optimization

Rübel et al., Procedia Computer Science (2010).
Bethel et al., J. Phys.: Conf. Series (2009).
Wu et al., J. Phys.: Conf. Series (2009).
Rübel et al., Comp. Science & Discover (2009).
Ushizima et al ICMLA 2008
Geddes et al, SciDAC Review 09
Wu et al, SciDAC Review 09

Particle tracking

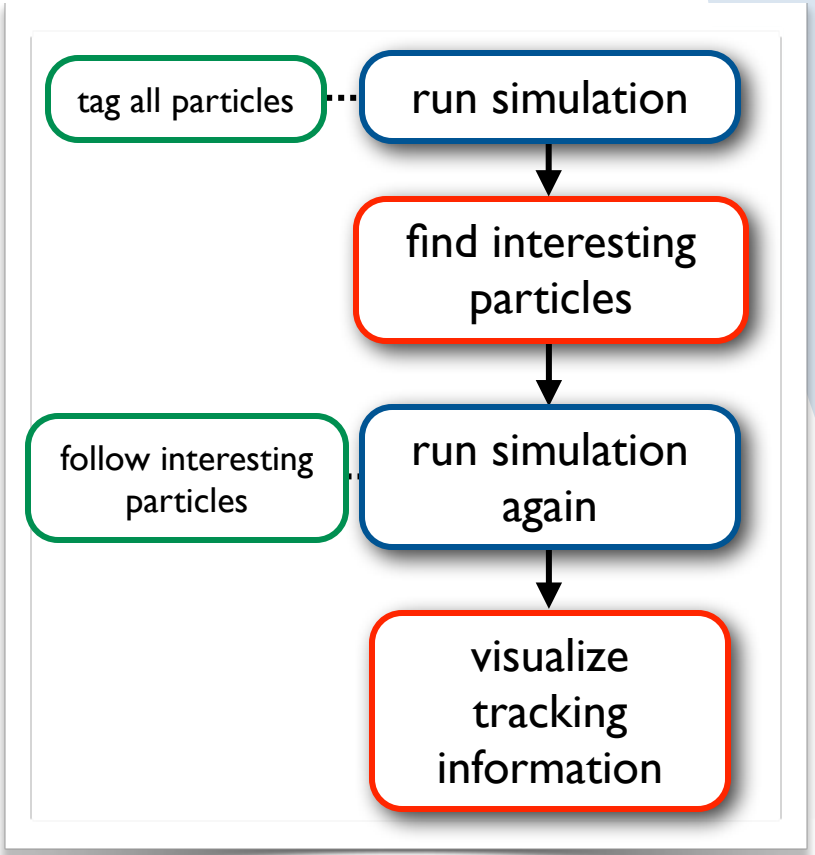
UCLA

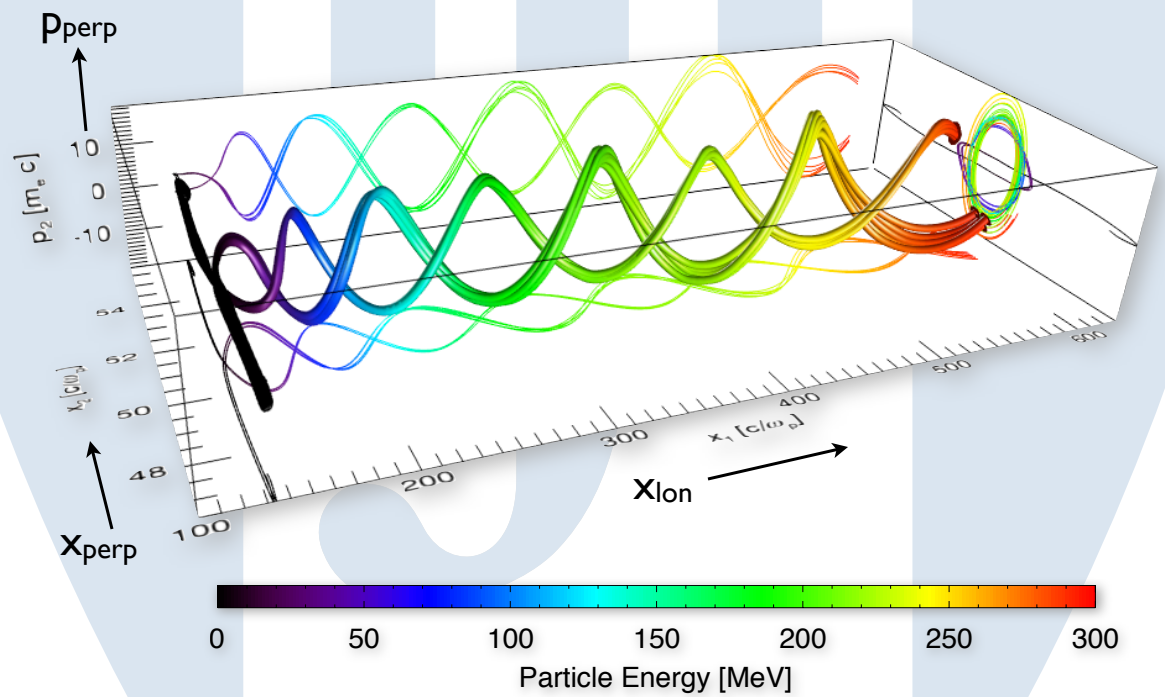
Relevant physics associated with small subset of particles

- Record detailed 7D phase-space of "interesting" particles

Technically challenging

- Subset of ~10^3 particles in ~10^9
- Storing information for every particle not feasible
  - 10^4 iter. × 10^9 part. ⇒ ~ 0.5 PB

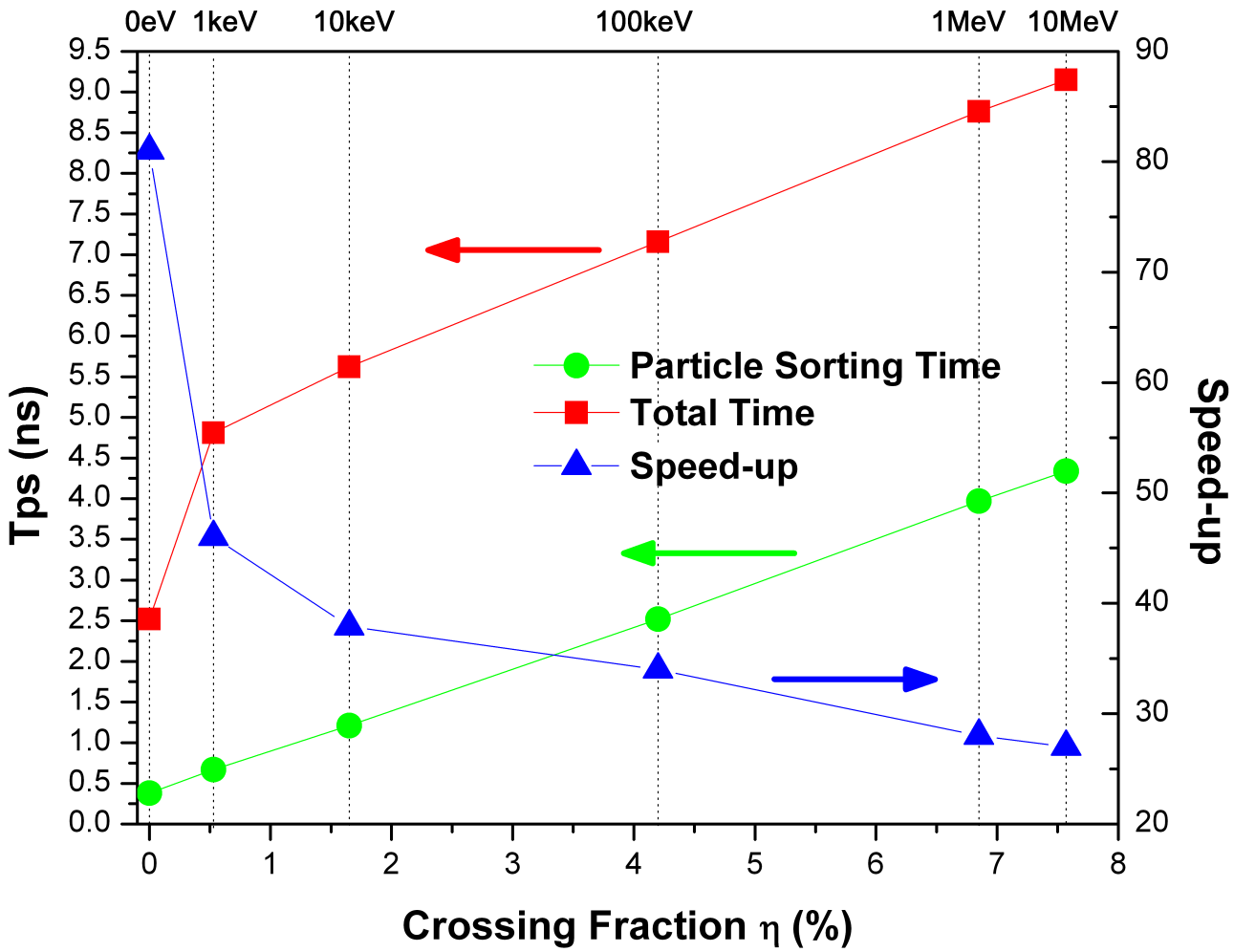




see J L Martins et al., P4.148

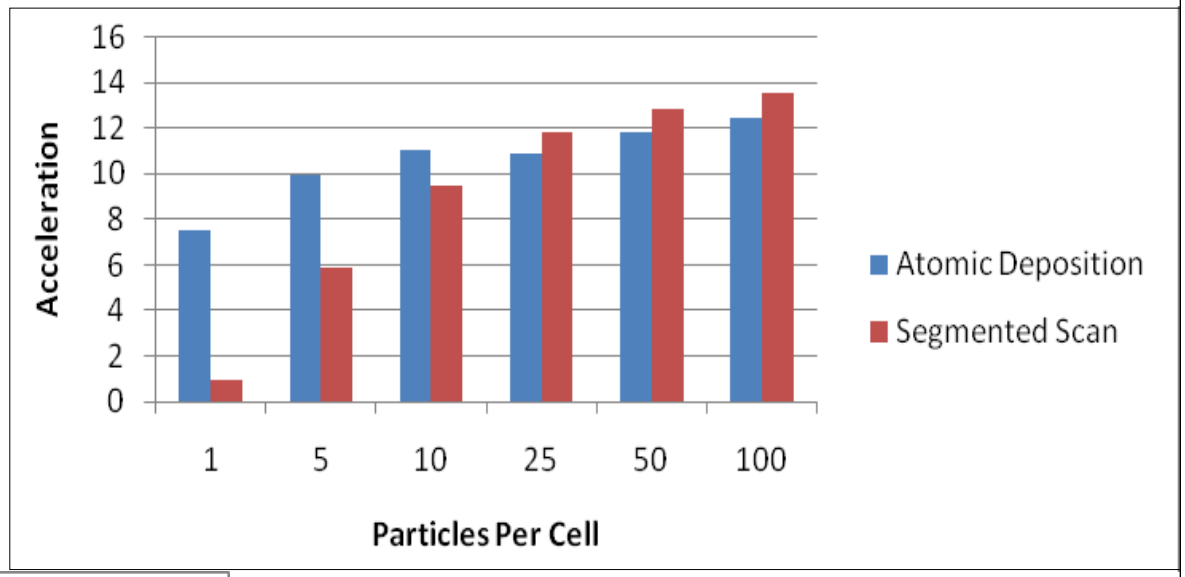
The GPU code achieved 27-81x speed-up over the CPU code OSIRIS

Kong et al. submitted

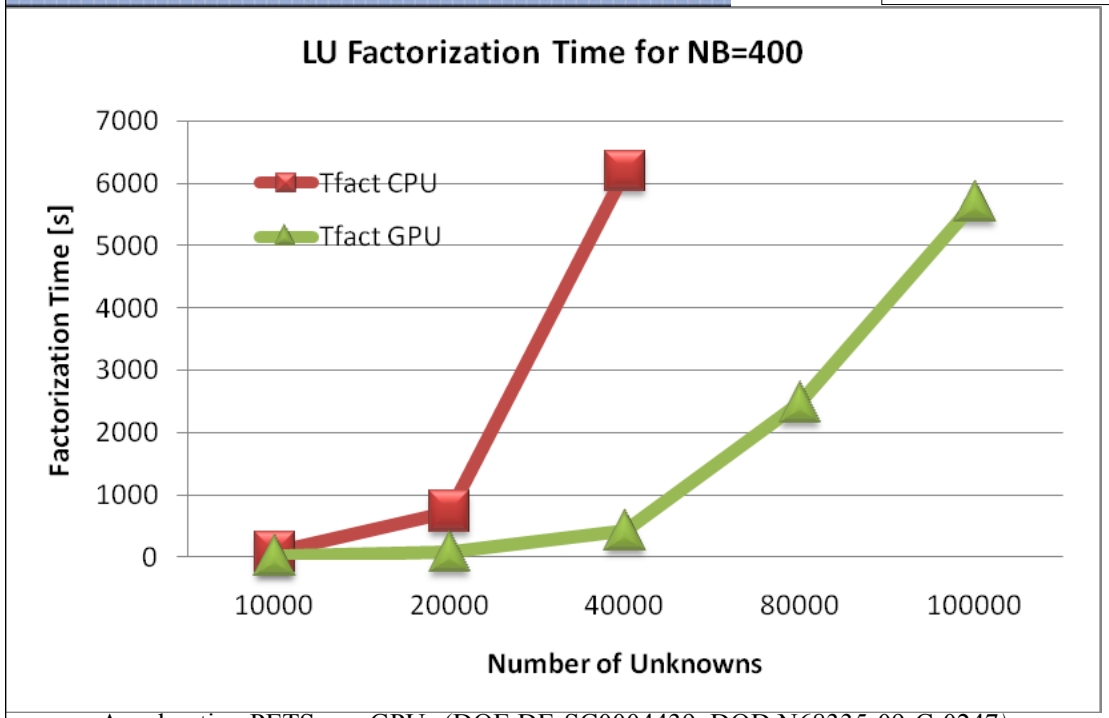


Preparation for Exascale: GPU acceleration of PIC & Linear Solvers is underway

- 3D particle push on GPU
  - interpolation, move, charge deposition
- deposition via segmented scan or atomics
  - atomics on NVIDIA Fermi is competitive for few particles per cell
  - segmented scan attractive for many particles
  - O(10x) acceleration for full push
- Hardware and software-based interpolation

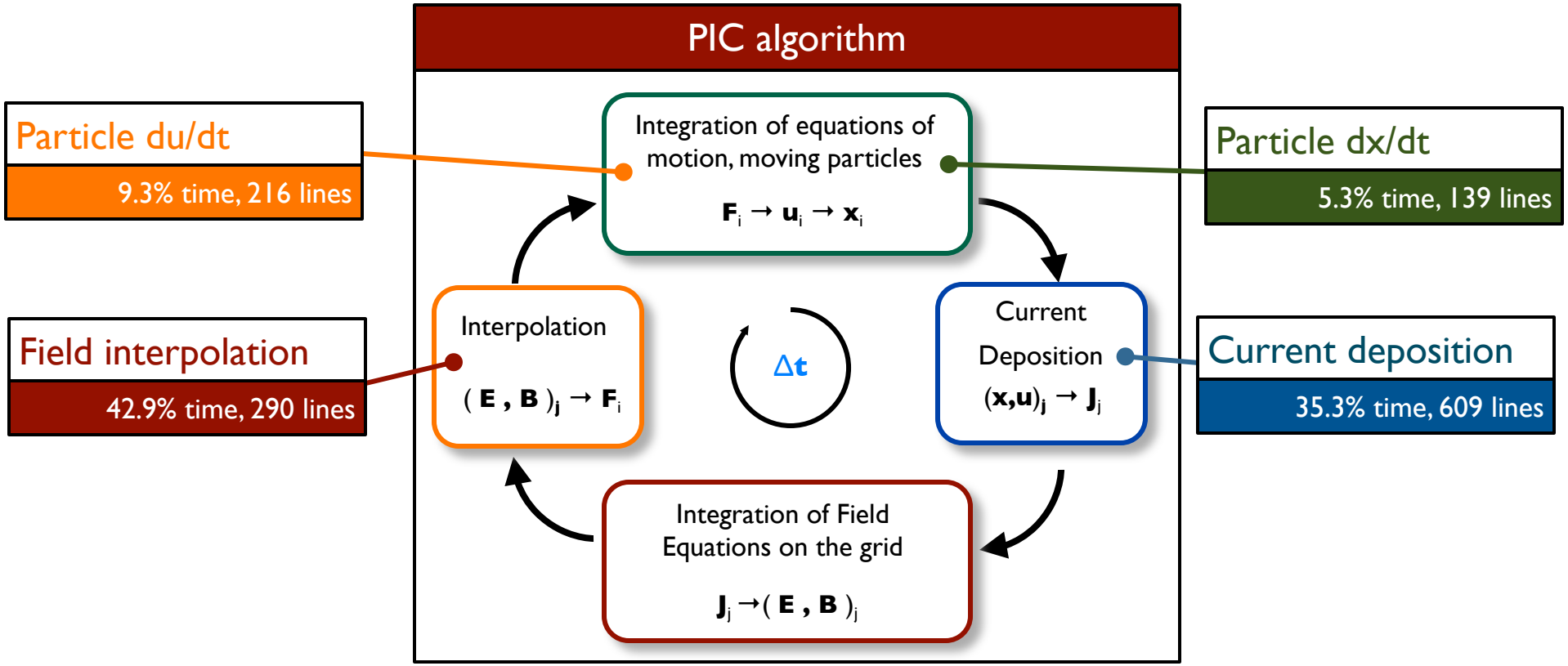


Speedup of electrostatic PIC on GPUs (DOE DE-SC0004585)
K. Amyx, P. Messmer, P.Mullowney and I. Pogorelov



Accelerating PETSc on GPUs (DOE DE-SC0004439, DOD N68335-09-C-0247)
P. Mullowney, K. Amyx, T. Austin, C. Ahrens and P. Messmer

- Goal: PETSc functionality on GPUs
- Implementation via GPULib
  http://gpulib.txcorp.com
- Multi-GPU support via MPI
- > 10x speedup for iterative solver (BiCG-Stab) and out-of-core LU factorization
  (Tesla C1060 vs 2.6 GHz Core2Duo)

TECH-X CORPORATION

Where to use SIMD code