Particle simulation of laser wakefield particle acceleration – M558

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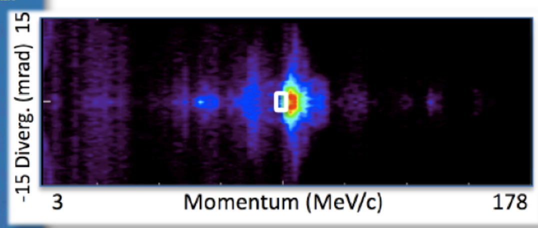
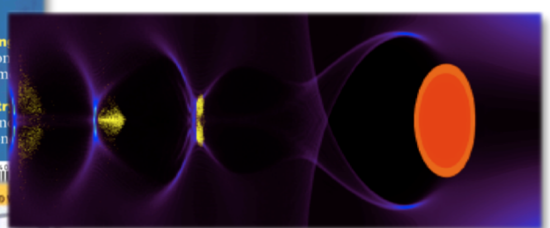
Tech-X, http://www.txcorp.com
D.L. Bruhwiler, J.R. Cary, B.M. Cowan, C. Nieter, K. Paul, V. Ranjabar

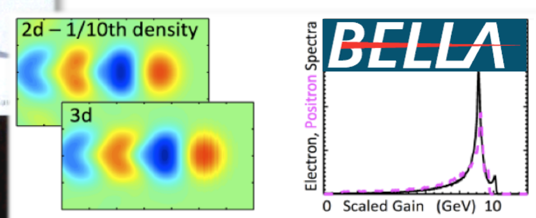
Oxford
W. Andreas, S. Bajlekov, N. Bourgeois, T. Ibbotson, S.M. Hooker

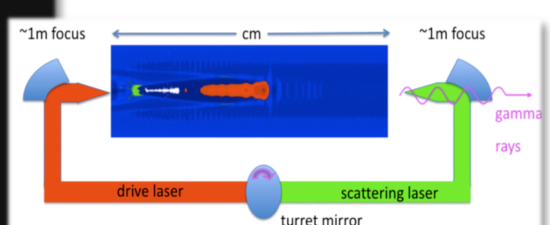
NA-22/Nonproliferation R&D

Simulations support LOASIS experiments and BELLA design









Outline

- BELLA project + collaborators: High gradient laser – plasma accelerators
- Quantitative modeling of self-trapped low ΔE experiments[1] using new numerics[2]
- Physics of controlled trapping for low momentum spread bunches: downramp experiments[3] & colliding pulse injection
- Design of efficient 10 GeV stages for BELLA and laser plasma collider concept & emittance control[4]
- GeV stages - Thomson gamma sources for SNM detectionl[5]
- Compute requirements & outlook

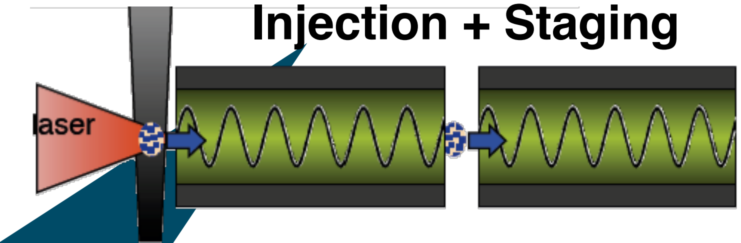
[1] Geddes et al., SciDAC Review 2009 & Nature 2004; [2] Cormier-Michel et al., PRE 2008;
[3] Geddes et al., PRL 2008; [4] Cormier-Michel et al., ICAP 2009; [5] Geddes et al., CAARI 2008

BELLA 40 J PW Laser – Components for a Laser Plasma Collider + Radiation

10 GeV stages

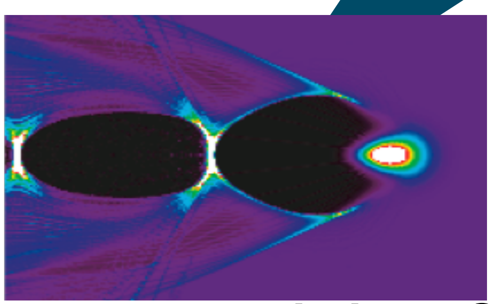
Energy spread &
Emittance preservation

Injection + Staging

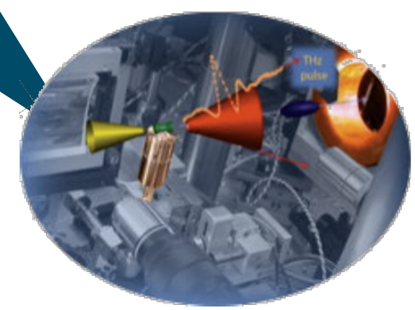


PW laser
40 J / 40 fs

Positron acceleration + PWFA expt.'s



Radiation sources



Will augment existing LOASIS experiments on two existing beam lines

LOASIS team – development of laser plasma accelerators

Staff
E. Esarey (T)
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G. Plateau (PhD)
S. Shiraishi (PhD)
T. Le Corre (M)
H. Vincente

Collaborators include:
LBNL : K. Barat, M. Battaglia, W. Byrne, J. Byrd, R. Duarte, W. Fawley. K. Robinson, D. Rodgers, R. Donahue et al.
Tech-X: J. Cary, D. Bruhwiler, et al.
SciDAC team

Oxford: S. Hooker et al.
MPQ: F. Krausz, F. Gruener et al.
LOA: O. Albert, L. Canova
GSI: T. Stoehlker, D. Thorn

Simulation Collaborators

LOASIS: C.G.R. Geddes, C. Benedetti, M. Chen, E. Cormier-Michel
E. Esarey, C.B. Schroeder, W.P. Leemans

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Tech - X & U. Colorado J. Cary

Oxford W. Andreas, S. Bajlekov, N. Bourgeois, T. Ibbotson, S.M. Hooker

NERSC, visualization: W. Bethel, J. Jacobsen, Prabhat, O. Rubel,
D. Ushizima, G. Weber

NERSC : M. Howison,...

DOE Scientific Discovery through Advanced Computing:

LBNL AMAC, CBP: R. Ryne, J.L. Vay, W. Fawley

UCLA: W.B. Mori, F.S. Tsung, C. Huang, M. Tzoufras, M. Zhou,
W. Lu, S. Martins, M. Tzoufras, V. Dycek + collaborators at IST

USC/Duke: T. Katsouleas, X. Wang

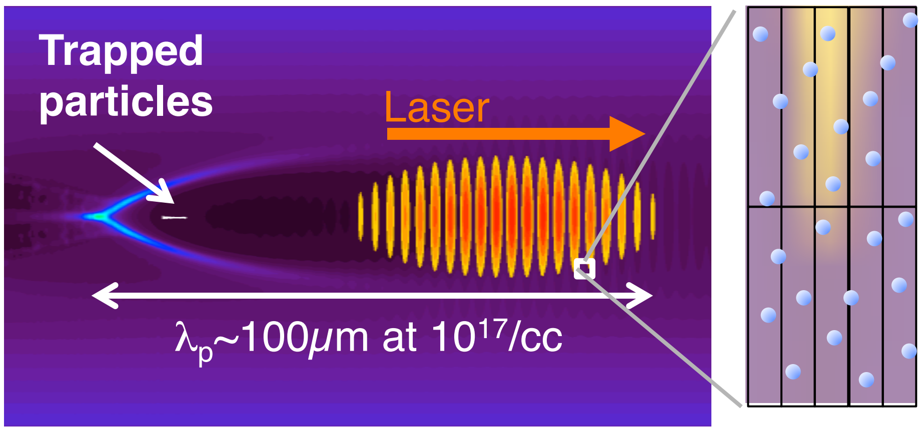
Other collaborations include:

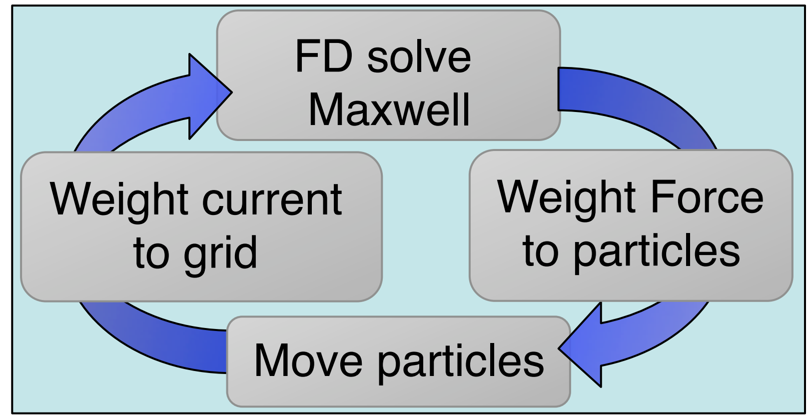
LWFA – Nebraska, B.A. Shadwick et al.;

Gas targets - STI Optronics, W. Kimura *et al*; LBNL APDEC, P. Collela *et al*
Alameda Applied Sciences – M. Krishnan *et al*

Simulation + theory required to model self consistent laser, wake, and bunch

Radiation pressure of intense laser excites space charge plasma wave which accelerates particles with high gradient





Tajima & Dawson PRL 1979; Esarey et al. TPS 1996; Leemans et al., IEEE Trans. Plasma Science (1996); Phys. Plasmas (1998)

- Explicit particle in cell simulates required physics – resolves laser period
  - Mhours CPU for cm-scale GeV (VORPAL*)
  - Domain decomposition parallelization
  - present runs ~ 50cells^3/ processor
- Meter scale of 10 GeV stages – O[Ghours]
  explicit → scaling + new models

Energy gain	$\sim n^{-1}$	(10 GeV at 10^{17}/cc)
Length	$\sim n^{-3/2}$	(1m at 10^{17}/cc)
Gradient	$\sim n^{1/2}$	(10 GV/m at 10^{17}/cc)
Laser w_0&L	$\sim \lambda_p$	(100fs at 10^{17}/cc)
Depletion	~ Dephasing for $a_0 > 1$	

- Require improved accuracy &resolution (compute time) to model collider emittances

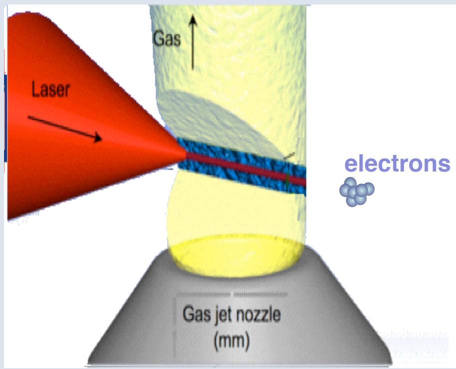
Simulations of past expt.'s : Geddes et al JPCS 2008; ScDAC Review 2009

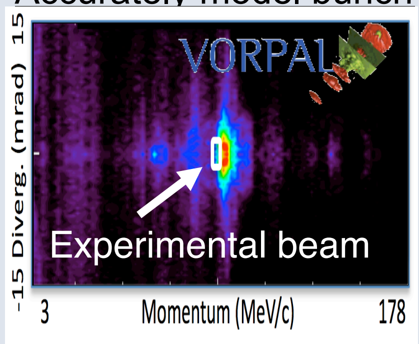
* Vorpal - Nieter & Cary, JCP 2004.

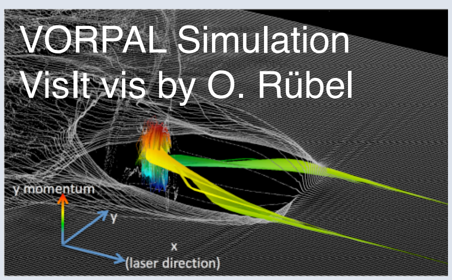
Self trapped experiments: percent energy spread, physics, scaling

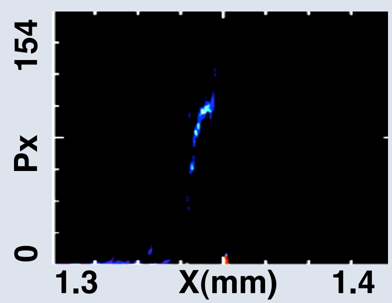
- Laser channeling: first low ΔE/E beams
  - 10 TW laser, 2mm plasma @ 2×10^{19}/cc

Accurately model bunch





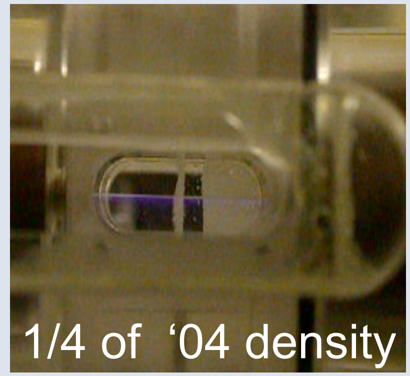


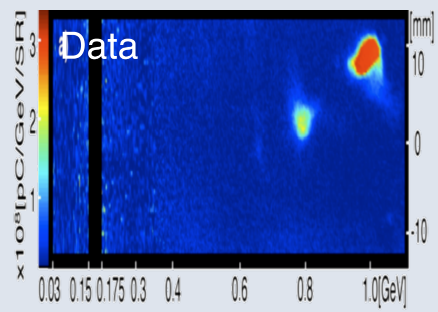


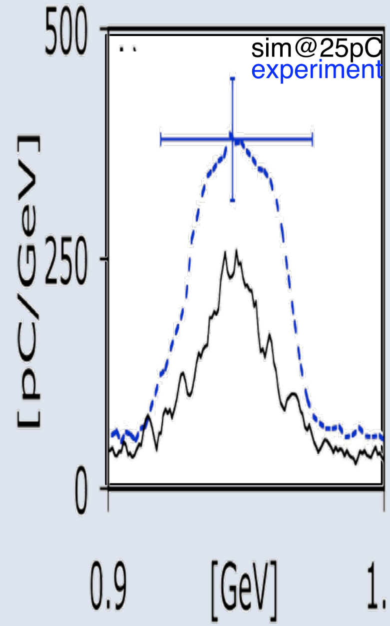
- 3 mrad divergence, ΔE/E 4%, E_{peak}~170MeV

Geddes et al., Nature 2004*

- Capillary channels+low n_e=GeV in 3 cm
  - 40 TW laser, 3cm plasma@4-5x10^{18}/cc







- 1 GeV beams, stable beams at 0.5 GeV

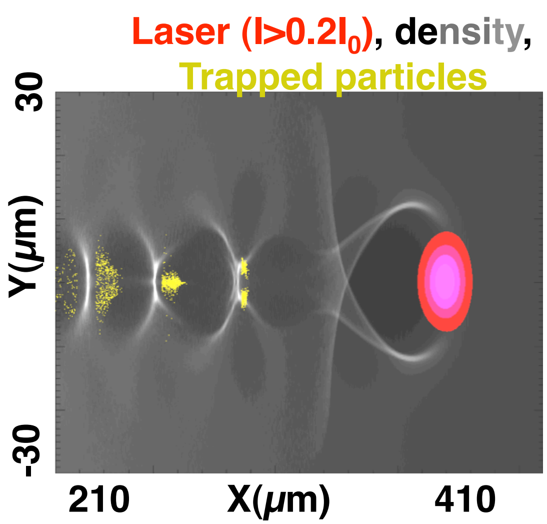
Leemans et al., Nature Phys 2006

- Simulations show physics of self trapping production of narrow ΔE:
- Accurate modeling of phase space with interpolation & smoothing developed**
- 100 MeV 3D production runs at 11kprocessor/36 hr, 2D 256 processor/1 hr

3-5 year outlook: routine 3D modeling at GeV & beyond; parameter scans & auto-analysis

*Also: Faure et al.; Mangles et al. Nature 2004; Tsung et al. PRL 2004, Pukhov APB 2002 VORPAL : Nieter et al., JCP 2004
**E. Cormier-Michel et al., PRE 2008, Geddes et al. AAC 2008 & SciDAC Rev. 2009

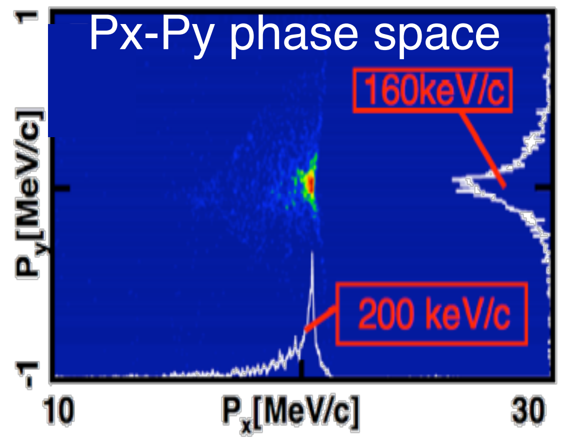
Developing low emittance injectors: plasma downramp & colliding pulse



Process: ramp control of trapping reduces emittance

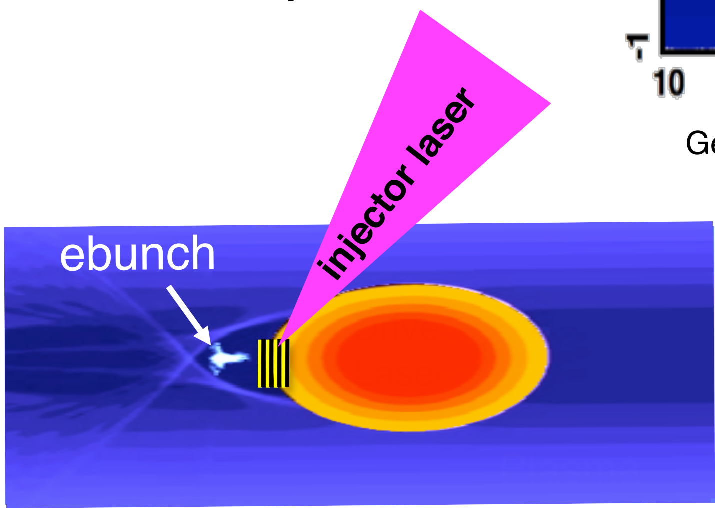
Validate: VORPAL simulations vs. multiple diagnostics

Shows: Bunches ~ 30fs long at formation -> injector



- Narrow energy spread, emittance preserved

Geddes et al, PRL 2008.; G. Plateau, PAC 2007; Related: Bulanov PRE 1998,



Process: beat between two lasers injects particles

Separate: wake excitation, injection

- repeatability
- tunable energy
- reduce emittance by controlling injection

Theory: Esarey PRL 97; Experiments: Faure et al Nature 06, Toth Proc PAC 2007, Kotaki PRL 2009

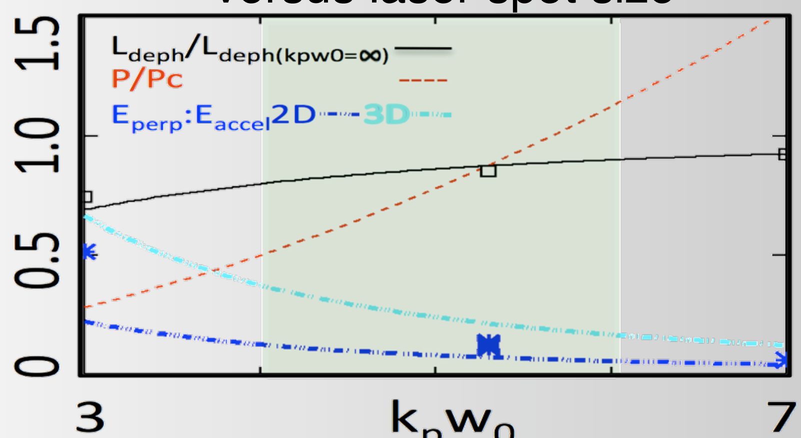
3-5 year outlook: extend resolution and use many runs to design low emittance injector

Develop efficient 10 GeV 40 J, collider-relevant BELLA Stages

- Use and verify linear theory predictions
  - field ~ $1/\lambda_p$ @ const. a0, $k_p L_{laser}$, $k_p w_0$

- Starting to predict10 GeV performance
  - ~1 m at 10^{17}/cc → Ghours (explicit)
  - laser spot size, length, effect of beam loading
  - Lorentz & envelope sim.s → emittance
  - Outlook: loaded emittance, ΔE, shaping

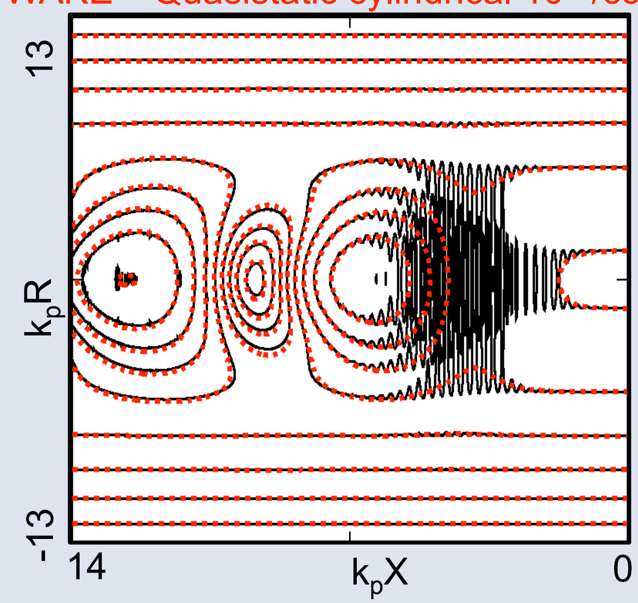
Dephasing, focusing, efficiency versus laser spot size



Leemans & Esarey, Phys. Today 2009; Schroeder et al AAC 08;
Cormier-Michel et al, Proc. AAC 200; Geddes et al PAC & SciiDAC review 2009
Cowan AAC 08; Vay PRL 07

Wake scales with density
Scaled simulations at a=1

Wake contours
VORPAL slab 10^{19}/cc
WAKE** Quasistatic cylindrical 10^{17}/cc



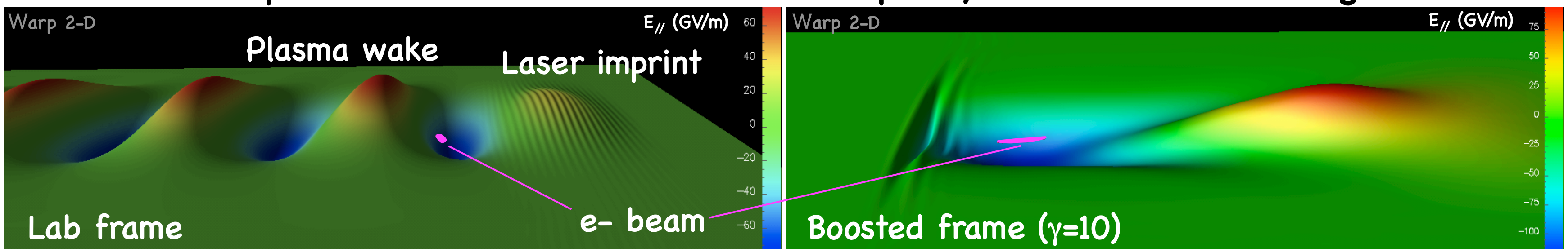
Field ~ $1/\lambda_p$

10^{19} cm^{-3} =	120 GV/m
10^{18} cm^{-3} =	40 GV/m

**Antonsen and Mora 1996

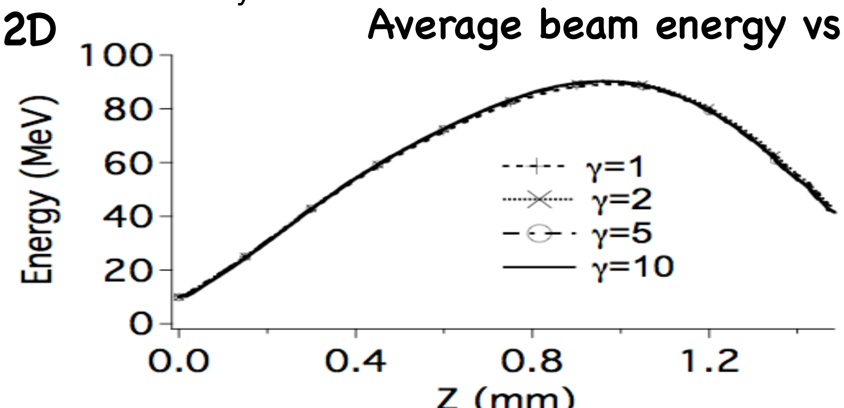
New models - full scale 10 GeV simulation
Increased capacity needed for accuracy

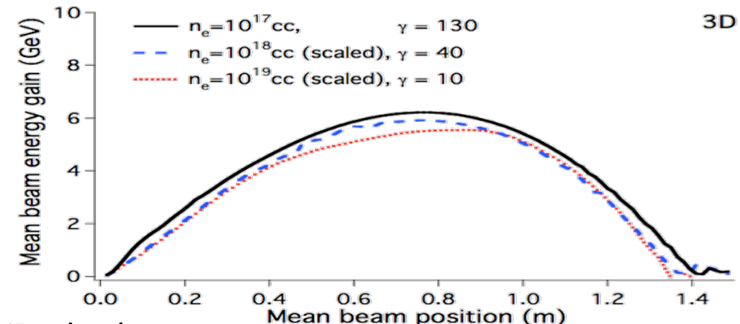
Boosted computational frame* reduces scale disparity – allows 10 GeV stage simulations



*J.L. Vay et al. PRL 2007

Average beam energy vs position in lab frame

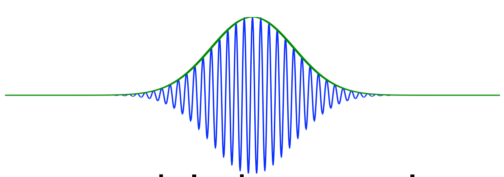




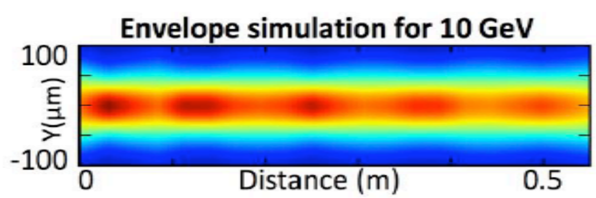
10^{17}cc/3D/256 CPUs: 3h γ_{frame} = 130 ≡ > 1 year in lab frame!

*Courtesy J.L. Vay – similar work by Bruhwiler et al (Tech X), Martins et al (UCLA/IST) ⇒ speedup > 10,000

Envelope model – reduced resolution requirement – allows 10 GeV stage simulations



Laser modeled as envelope + phase reduces required resolution

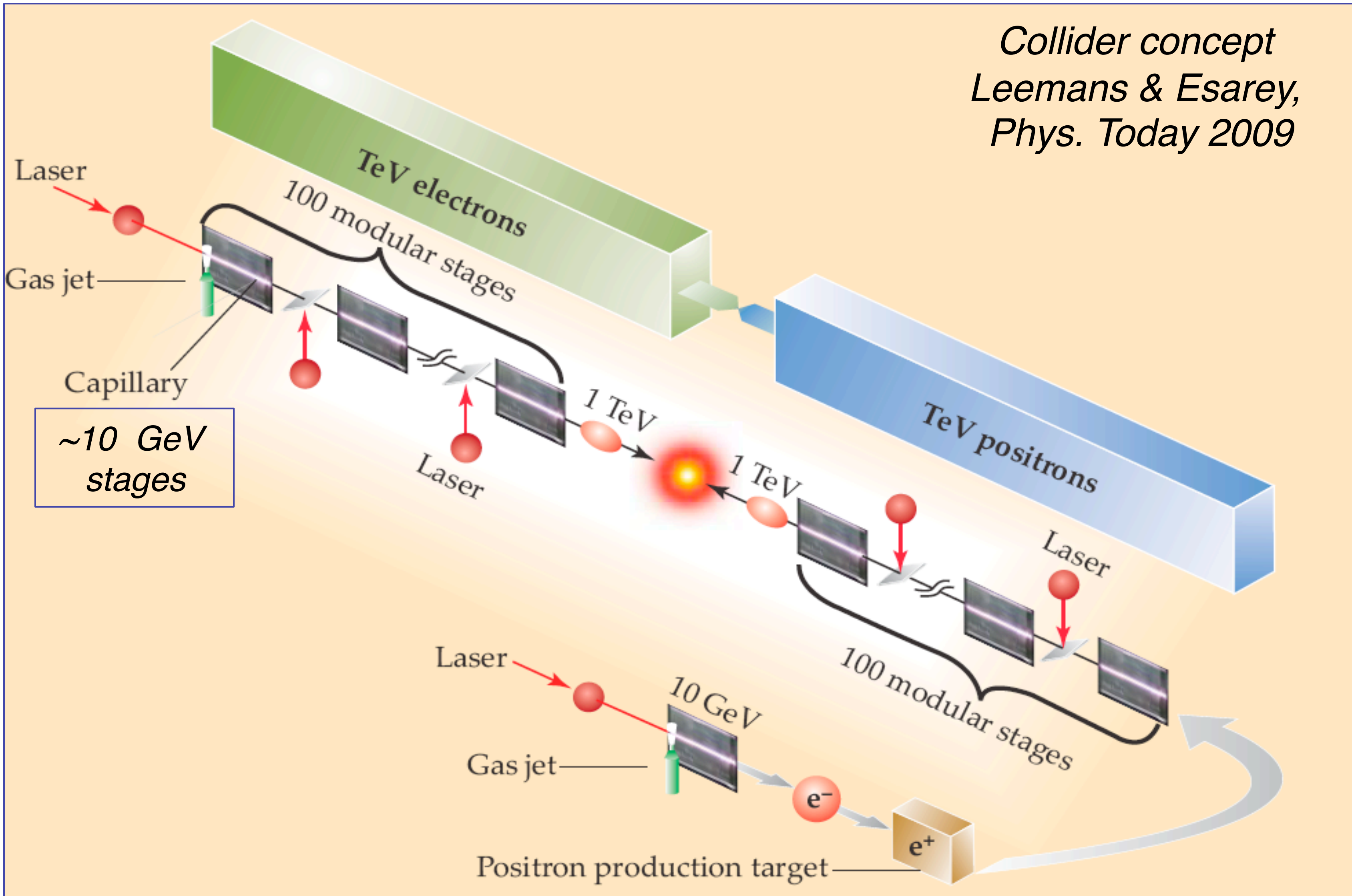


correct betatron period

VORPAL –Cowan AAC 08; also in turboWAVE, & at NRL; WAKE, QuickPIC+quasistatic

3-5 year outlook: fast codes + new comp. capacity to accurately model collider stages for e-/e+ including very low emittance, radiation, scattering contributions, and staging

Compact plasma accelerators – BELLA PW laser and towards conceptual future LPLC & sources



Current HPC Requirements

- Architectures : Cray XT
- Compute/memory load
  - 3.5 Mhours in 2009
  - production simulations up to 11k-processors – typical 4k (scheduling convenience)
  - 24hours/run
  - Memory 100GB (<1GB/core)
  - processors communicate edge cells each time step to neighbors – order 30k-cells
  - Run startup often requires python scripts for set up
  - Analysis most efficient on fewer nodes with large memory – 4GB
- Data read/written
  - 2TB written per run – sets disk requirements
  - 50 Gb/checkpoint (approx every 30 minutes)
  - restart involves read of one checkpoint
  - 5 TB/year moved out of NERSC
  - Off line storage 20 TB

Current HPC Requirements

- Codes: VORPAL (WARP, other finite difference time domain)
  - Fields and fluids are represented on a structured Cartesian mes
  - Plasma usually represented by particlesby using 2nd-order leap-frog algorithm via PIC (particle-in- cell), or fluid
  - Laser and EM fields:
    - Explicit FDTD advance in lab or boosted frame OR
    - Envelope representation of laser field with Trilinos library suite (Aztec)
  - WARP and VORPAL also used for RF accelerators – relevant to staging
- Necessary software, services or infrastructure
  - HDF5 and assistance in tuning and working with it for large jobs
  - Tuning assistance – particularly file system
  - VisIt, IDL, perl, python
  - Visualization work and assistance in visualizing and analyzing large datasets, and in extracting physics data from them.
- Known limitations/obstacles/bottlenecks
  - Operators are all local, which enables local communication via MPI
  - Production simulations up to 11k-processors – limited by capacity/allocation
  - Scaling of parallel I/O (e.g. H5) needed especially for non-constant domain sizes
  - For production parameter exploration, tools for batch executing, checking and relaunching, and automated analysis

HPC Usage and Methods Next 3-5 Years

- Upcoming changes to codes/methods/approaches
  - Computational approach anticipated to scale to >100k-core
  - Radiation and scattering models will become increasingly important
  - GPU development in progress – VORPAL, OSIRIS, others
  - PIC codes (e.g. VPIC) also perform well on cell

- Changes to Compute/memory load
  - 50x scaling in resources anticipated to accurately design collider scale stages
  - New models in conjunction with new computers: laser envelope, Lorentz
  - This will be used to:
    - Simulate 10 GeV stages at high resolution to model collider/light source emittances
    - Simulate staging of mulitple modules for high energies
    - Run multiple 3D simullatios to explore parameter space to improve beam quality
      - important to allow simulations to predictively explore parameter space to guide experiments
    - Simulate particle injector at high resolution to determine combination of techniques to produce the required beam quality
  - 150Mhours/year
  - 500kcores @ 12-24hours for large runs + many at 5-50kcores
  - 100 TB memory (< 1 Gb/core)

HPC Usage and Methods Next 3-5 Years

- Anticipated limitations/obstacles/bottlenecks on 10K-1000K PE system.
  - Parallel file I/O such as H5 must be scaled to 10's - 100's of thousands of processors, and must be made robust to varying mesh sizes on different processors.
  - Communication of the edge information from each processor to processors handling neighboring domains is required each step- may need to be multi-layered on many-core or GPU systems
- Strategy for dealing with multi-core/many-core architectures
  - Algorithm scales to 100's of k-cores at this time
  - Different communication can be used between cores and nodes

HPC Usage and Methods Next 3-5 Years

- Changes to Data read/written
  - 50+ TB for large runs – determines on line storage
  - 1 TB/dump (assumes some data subsetting developed – else ~ 50TB)
  - Off line storage 200TB

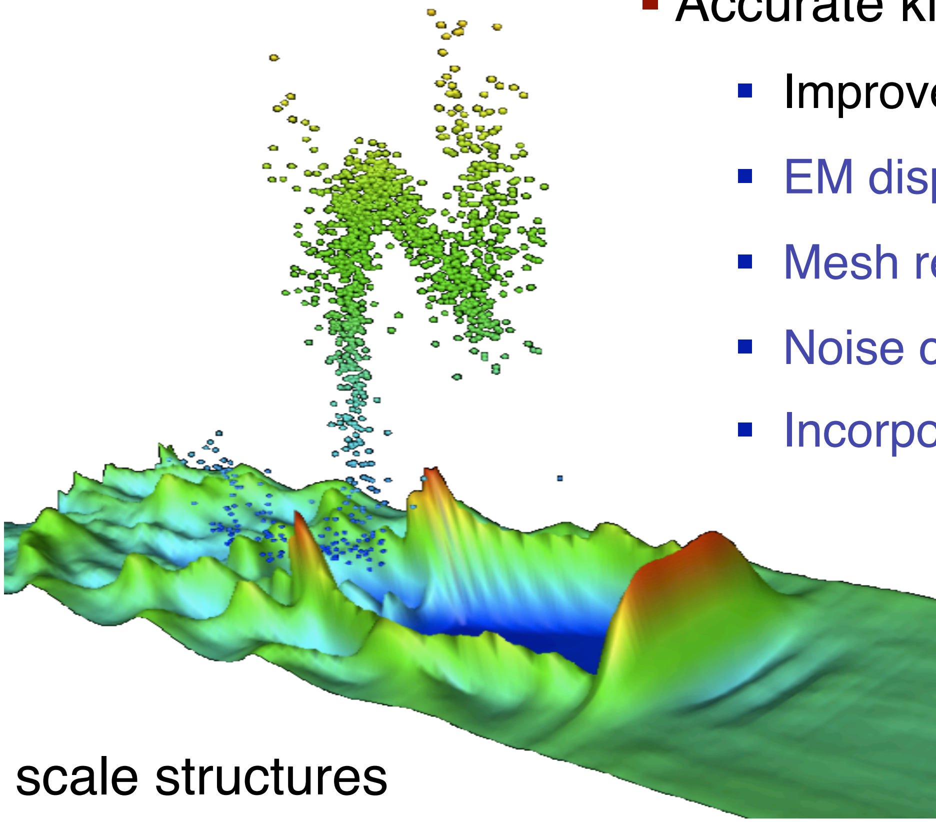
- Changes to necessary software, services or infrastructure
  - Parallel file I/O such as H5 must be scaled to 10's - 100's of thousands of processors, and be made robust to varying mesh sizes on different processors.
  - Data subsetting must be developed in line to reduce dump file size
  - Error checking and job-relaunch services that detect if a job has terminated partway through and automatically restart
  - Scans of parameter space are needed requiring automation to generate and run sequentially large numbers of jobs, and to extract the data from them.
  - Parallel visualization and analytics tools must be further developed, to provide similar functionality to well-known serial tools

Summary

- NERSC architecture, configuration and service requirements :
  - Parallel I/O scalability + access to data for analytics
  - Failure detection and ability to restart jobs
- With access to ~50X NERSC resources:
  - Design of collider relevant laser plasma accelerator stages & emittance
  - Many 3D simulations allowing exploration of parameter space to predictively design experiments
  - Simulate controlled injection and beam conditioning with high fidelity
- “Expanded HPC resources” important for project:
  - availability of 500+ kcores for large runs
  - batch execution of many runs at the 5-50kcore level
  - job error detection and restart services
- Any other special needs or NERSC wish lists?
  - Parallel analytics tools matching functionality of serial solutions
  - Development of H5 and other parallel file architectures & flexible domains

end

Simulation challenges



- Accurate kinetics and bunch emittance
  - Improve accuracy in momentum advance
  - EM dispersion (cerenkov and particle noise)
  - Mesh refinement at particle bunch
  - Noise control – fluids
  - Incorporate radiation & scattering

- Meter scale structures
  - Accurate reduced models
  - EM dispersion (laser propagation)
  - Error accumulation
  - Scaling

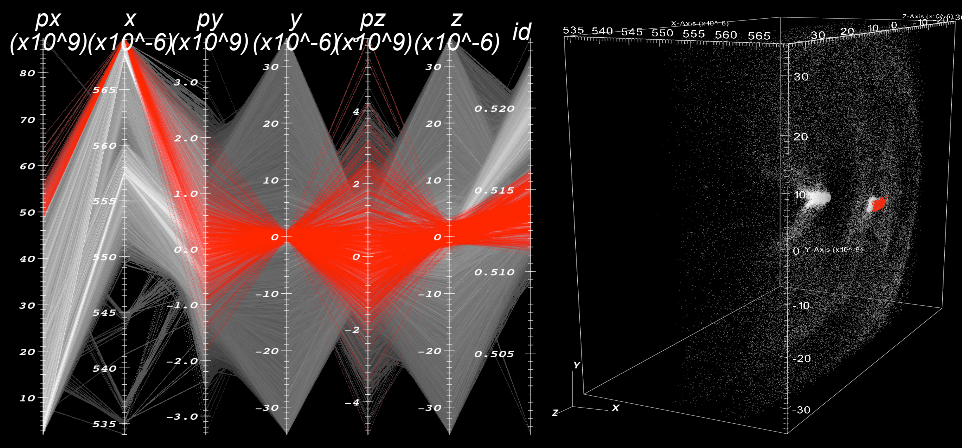
Others:

Automation & data mining

Detailed validation

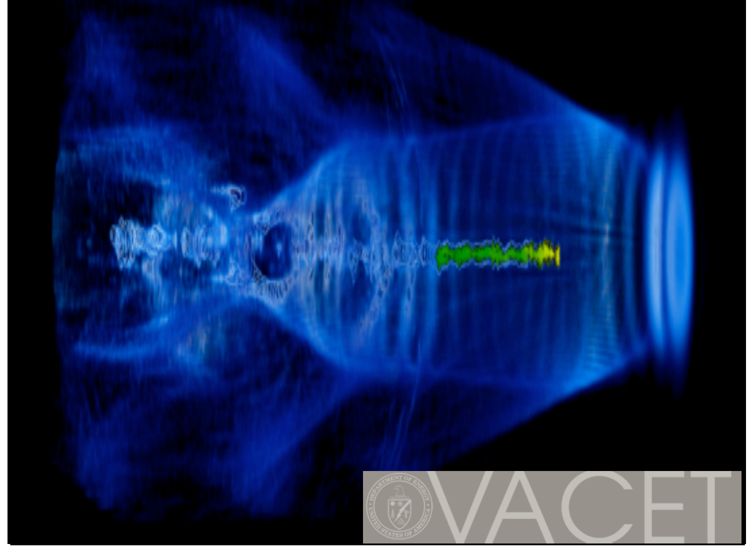
Developed visualization and analysis
Two student projects + VACET

FastBit indexing and query, parallel coordinates*

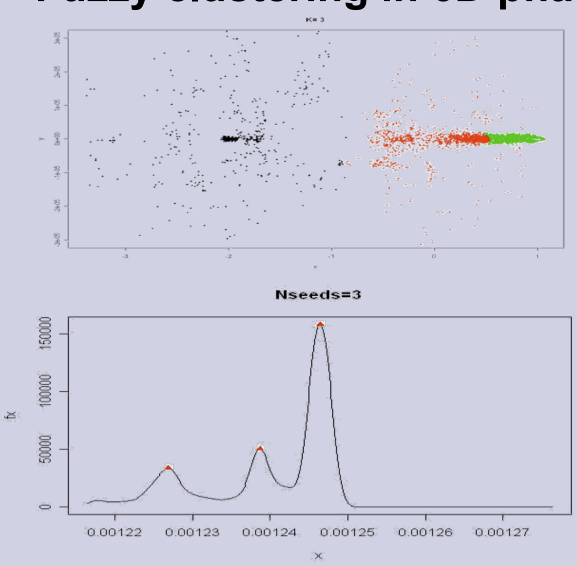


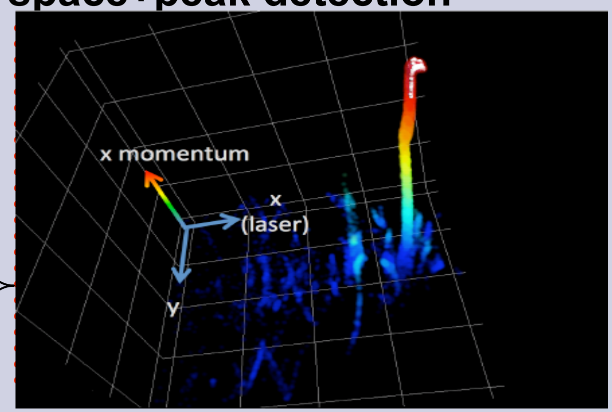
Interactive exploration of TB datasets

VisIT 3D visualization



Fuzzy clustering in 6D phase space+peak detection**





Automated beam detection

*O. Rubel et al., .accepted SC08
** D. Ushizima et al., sub ICMLA08