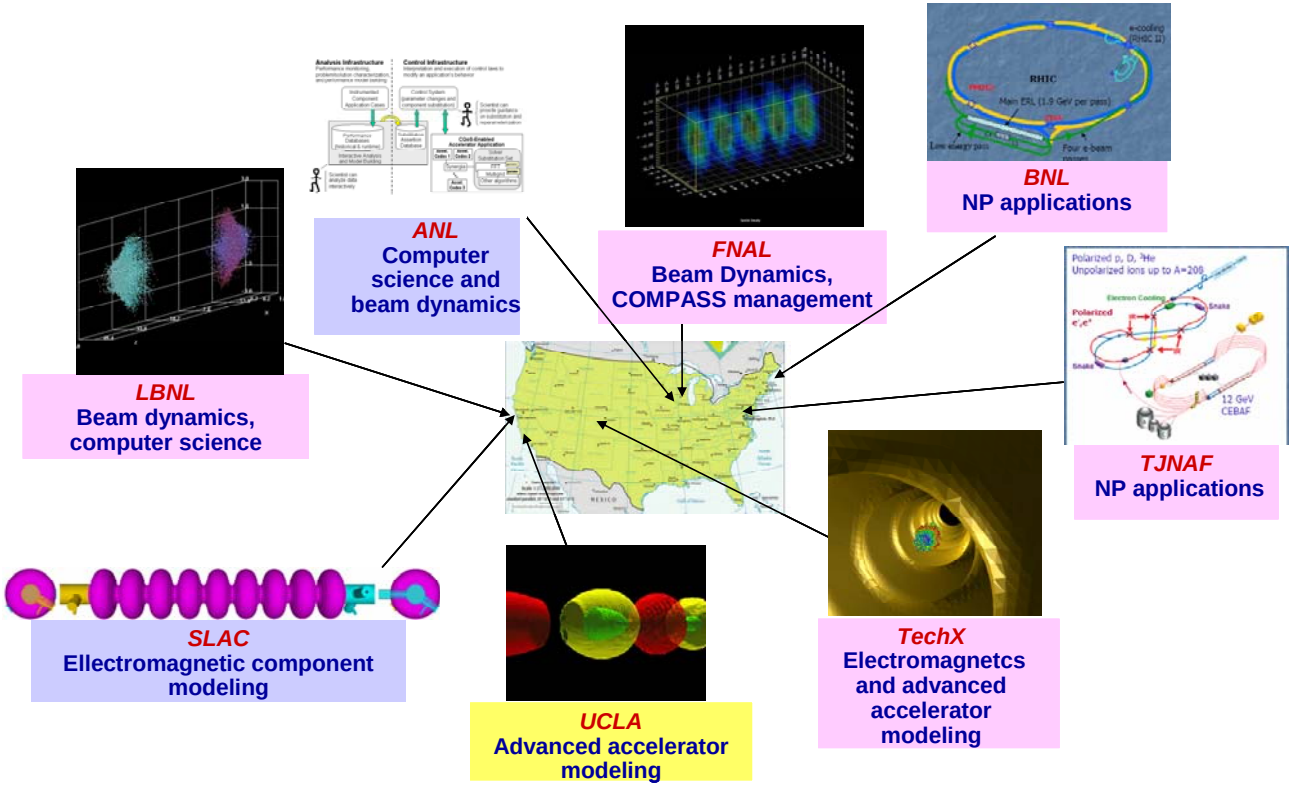
ComPASS: advancing computational science for future accelerators and accelerator technologies

Panagiotis Spentzouris, Fermilab

for the ComPASS team

ComPASS

- Community Petascale Project for Accelerator Science and Simulation (ComPASS)



Project, proposed January 2007, funded August 2007

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ComPASS program motivation

- Accelerators enable many important applications, both in basic research and applied sciences
- Different machine attributes are emphasized for different applications
  - Different particle beams and operation principles
  - Different energies and intensities
- Strong overlap in underlying basic accelerator science concepts

➪ a wide spectrum of requirements for very complex instruments. Assisting their design and operation requires an equally complex set of computational tools.

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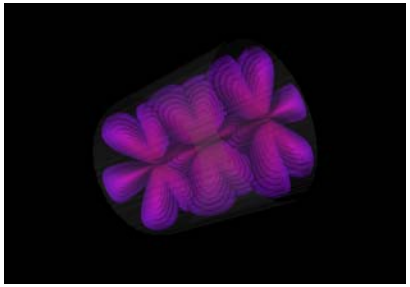
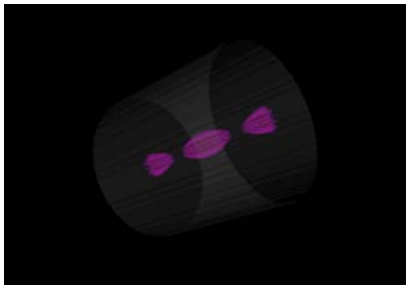
Multi-scale, multi-physics requirements





- Wide range of scales:
  - accelerator complex (10^3m) → EM wavelength (10^2-10 m) → component (10-1 m) → particle bunch (10^{-3} m) → PIC (10^{-12})
  - Need framework to connect scales and allow inclusion of multiple physics effects at each level

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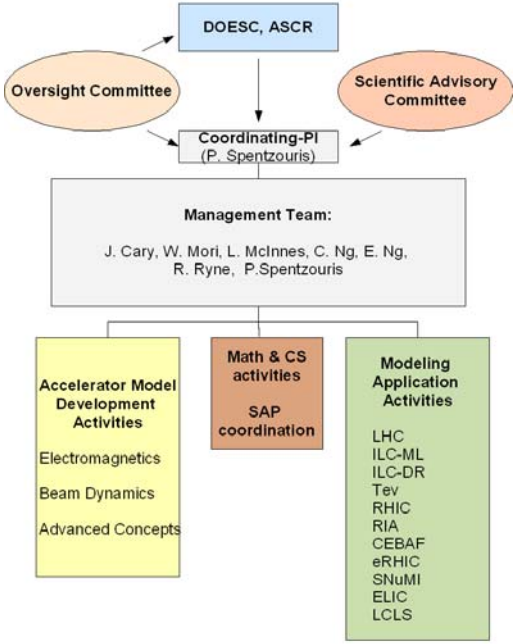
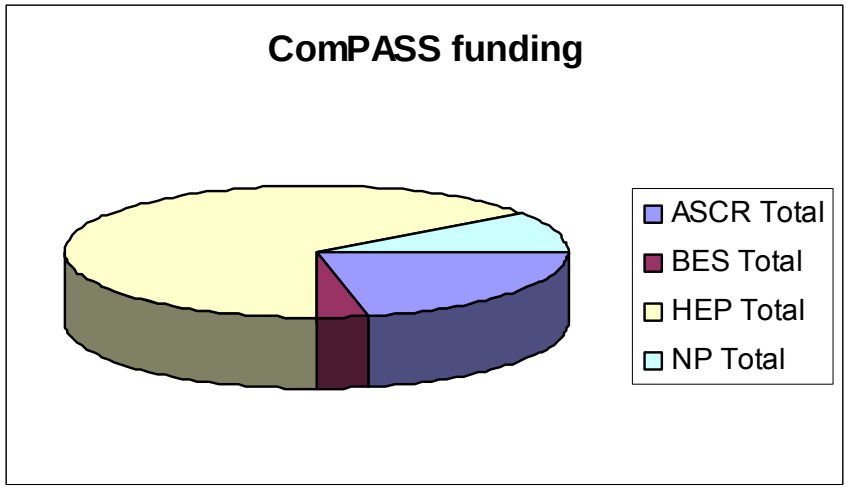
ComPASS vision

- Accelerator science and technology objectives:
  - Achieve higher energy and intensity, faster and cheaper machine design, more reliable operation
- To assist these objectives, ComPASS aims to develop integrated modelling capabilities
  - Multi-physics, multi-scale for beam dynamics; "*virtual accelerator*"
  - Thermal, mechanical, and electromagnetic; "*virtual prototyping*"
- Utilization of such tools requires massive computing resources!

ComPASS





- Management structure ensures program execution and priority adaptability.
- ~2.8 ($M)/year (now ~3.0 ($M)/year, thanks Lali!), with planned budget expected to ramp up to 3.3 ($M) for the last (5th) year

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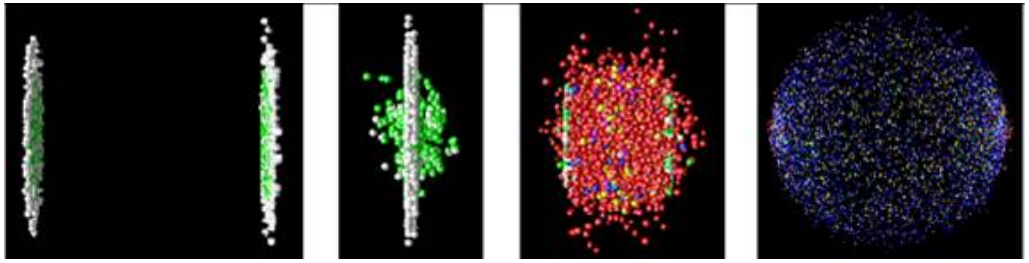
Nuclear Physics Priorities

- Study the properties of nuclear matter and the structure of the nucleus
  - CEBAF (electrons) at JLab and RHIC (heavy ions) at BNL, and future polarized electron-ion collider
- Study nuclei far from stability
  - Future rare isotope accelerator



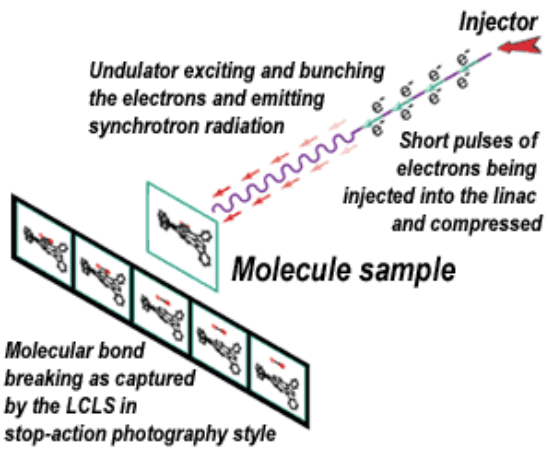
COMPASS Objectives

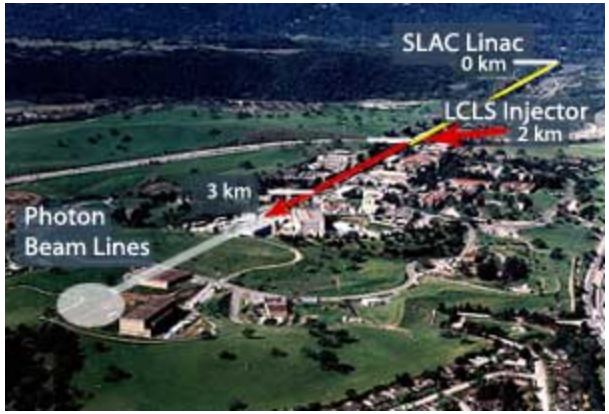
- Develop multi-physics and integrated system modeling capabilities on petascale systems
  - Build on HPC high-fidelity single physics codes developed under SciDAC1
  - Deploy tools under development by SciDAC2 teams in applied mathematics and computer science

- Requirements
  - Algorithm development and optimization on petascale machines
  - Development of framework/component infrastructure for multi-physics, multi-component simulations

Basic Energy Sciences Priorities

- Studies of metals, crystals, and amorphous materials
  - ORNL SNS, LANL LANSCE (spallation neutron sources)
- Studies of arrangement of atoms in organic and inorganic materials
  - LBNL ALS, BNL NSLS, ANL APS, SLAC SSRL (synchrotron light sources), and LCLS (FEL) starting up at SLAC





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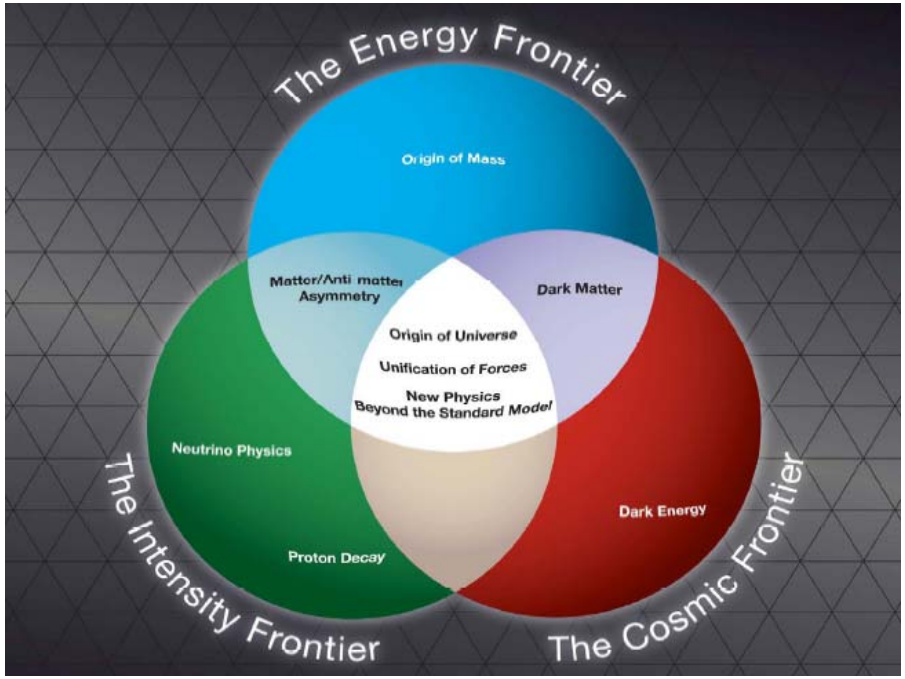
High Energy Physics Priorities

- High energy frontier
  - Use high-energy colliders to discover new particles and directly probe the properties of nature.
    - FNAL Tevatron, CERN LHC, future lepton collider
- High intensity frontier
  - Use intense beams to uncover the elusive properties of neutrinos and observe rare processes that probe physics beyond the Standard Model.
    - Future high-intensity proton source at Fermilab



http://www.er.doe.gov/hep/HEPAP/reports/P5_Report%2006022008.pdf

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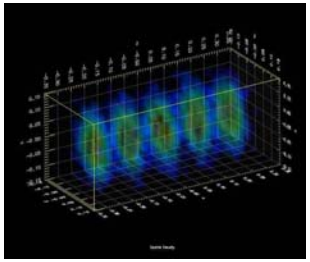
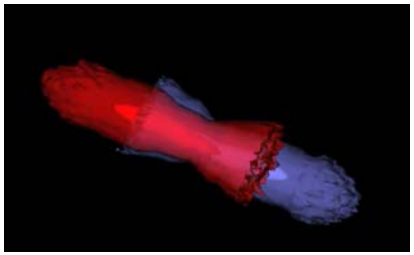
HEP priorities change: first test of ComPASS program flexibility

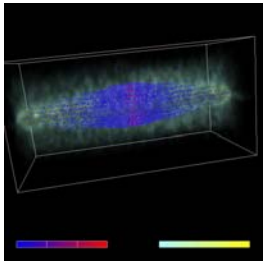
- When the project was proposed, the design of the ILC was the highest HEP priority, thus ILC dominated our application planning.
- Change of HEP priorities triggered
  - **Changes** in application development plan
    - More emphasis on finalizing Tevatron Run-II applications
    - Increased LARP involvement
      - LHC, PS2
    - Plan major participation in Project-X design studies
    - Shift future linear collider design application development to
      - concept design studies
      - generic SRF (Project-X linac)
  - **No changes** in capabilities development plan
    - Justifies original planning

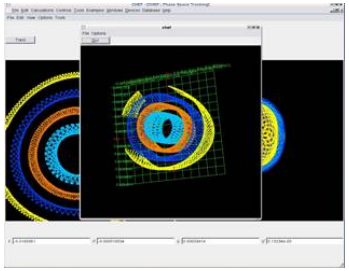
Computationally challenging physics, common to most applications

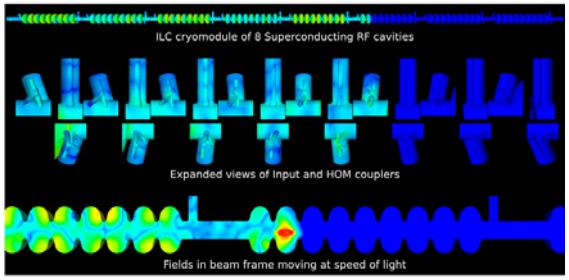
- Machine design: particles affected by machine components, other beam particles, or other beams
  - Space charge
  - Beam-beam
  - Electron cloud
  - Electron cooling
  - Intrabeam scattering
  - Accurate description (optics, position, feedback, etc)
- Component design
  - Impedance
  - Wakefields
  - multipacting
  - Thermal, mechanical
- New acceleration techniques
  - Laser and plasma wakefields

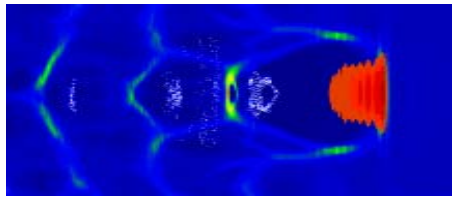












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LHC Upgrade path

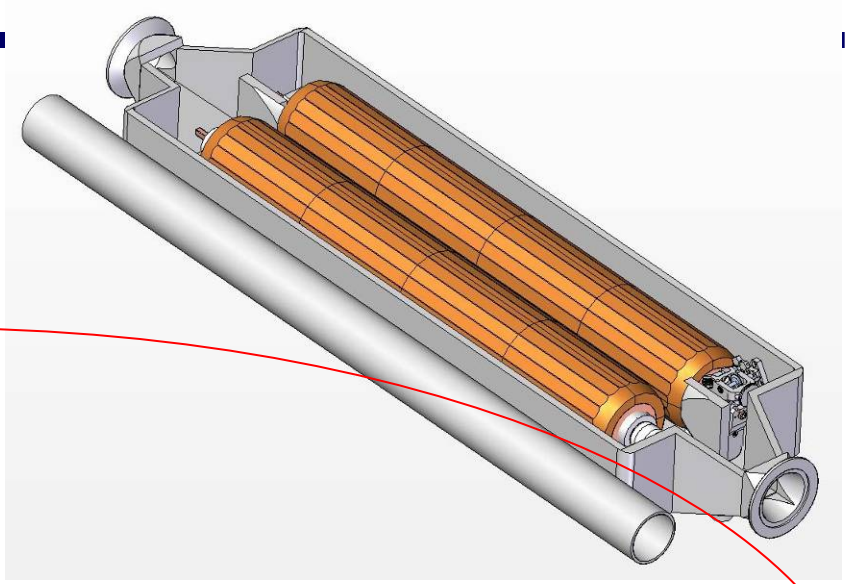
- Initial operation
  - Ramp up to 1×10^{34} $cm^{-2}s^{-1}$
- Phase I upgrade
  - After ~2 years of operation (~2012)
  - Replace 70 mm triplet quads with 120 mm quads
  - β^* goes from 50->25 cm
  - Luminosity goes to 2.5×10^{34} $cm^{-2}s^{-1}$
- Phase II upgrade
  - Second half of next decade (nominally 2016)
  - Luminosity goal: 1×10^{35}
  - Details still under study
    - New technology for larger aperture quads (Nb_3Sn)
    - crab cavities?
    - Improved injector chain (PS2?)

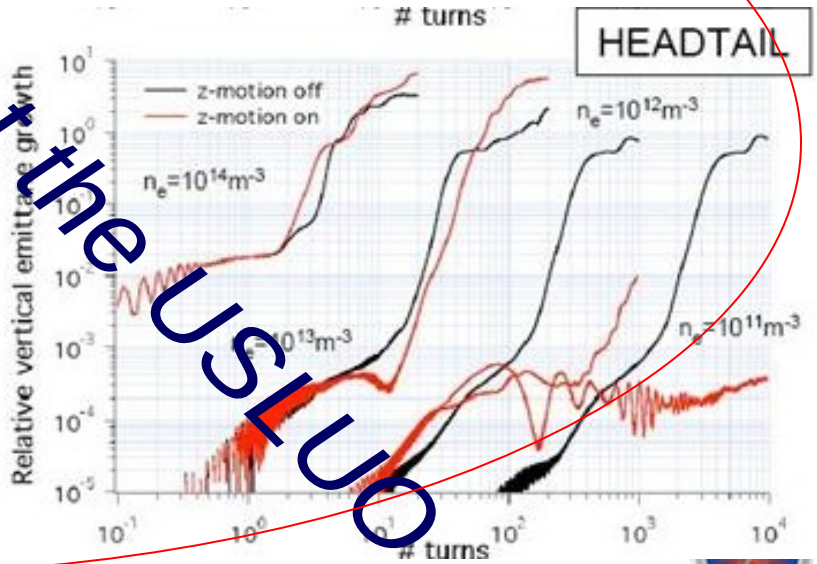
Talk by LARP Director at the USLUO

LARP Accelerator R&D for future LHC

Talk by LARP Director at the USLUO

- Rotating collimators
  - Aim for prototype in FY09
- Crystal Collimation
  - CRYSTAL Collaboration, T980
- Beam-beam studies
  - General simulation
  - Electron lens
  - Wire compensation
- Electron cloud studies
  - Study effects of electron cloud in LHC and injector chain





ComPASS major thrust areas for HPC accelerator physics

- Electromagnetics (EM): Modelling of electromagnetic fields in complex accelerating cavities and other accelerator components, to maximize acceleration while minimizing beam quality degrading effects. [Component design]
- Beam dynamics (BD): Modelling the evolution of beams through beam optics systems, including self-forces and other forces of interaction. [Machine design]
- Advanced acceleration (AA): Tools that guide the R&D for new high-gradient acceleration techniques such as plasma or laser wakefield accelerators. [New concept design]

➪ Common computer science and applied math activities to achieve performance and develop simulation environment [Enabling technologies]

Enabling Technologies: collaboration with SciDAC CET and Institutes

- Scalable parallel eigensolvers (with TOPS), to enable simulation of complete systems of rf cavities with many millions of degrees of freedom.
- Domain-specific scalable linear solvers (with TOPS), for large EM systems.
- Meshing technology for shape adaptation in EM, essential for cost effective design of rf cavities (with ITAPS and TOPS).
- Poisson solvers that perform and scale on petascale platforms (with TOPS). Essential for applications involving a mean field treatment of space charge.
- Parallel adaptive refinement for finite elements, to improve accuracy and reduce computational cost (with ITAPS and CSCAPES).
- Utilization of remote and interactive visualization tools (with ISUV).
- Deployment of performance analysis and optimization tools (with PERI) .
- Embedded boundary methods for EM structure PIC simulations (with ITAPS).
- Mesh refinement and optimized preconditioning in reduced PIC and spectral method-based dispersionless solvers (with APDEC, TOPS, and PERI).
- "Computational quality-of-service" infrastructure and interoperable components for BD applications (with TASCS, TOPS, and PERI).
- High-performance parallel data management and analysis tools for BD modelling (with VACET).
- Implementation of effective load balancing for particle-field simulations, to improve PIC performance (with ITAPS and CSCAPES).

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Electromagnetics

- Continue to develop and optimize capabilities for
  - finite difference and finite element, time and frequency domain
- Begin developing integrated environment including mechanical & thermal properties
- Application focus
  - Finalize ILC cryomodule calculations (including imperfections)
    - Transfer expertise to Project-X SRF linac applications
  - Design and optimization of LHC crab cavity; multipacting; wakefield effects in collimators; PS2 impedance calculation.
  - Wakefield effects in high-energy linac; ring impedance calculation for Project-X
  - Cavity design optimization including EM, thermal and mechanical analysis; dark current simulation; photonic crystal design for High-Gradient R&D.
  - Utilize existing application capabilities for NP, BES needs

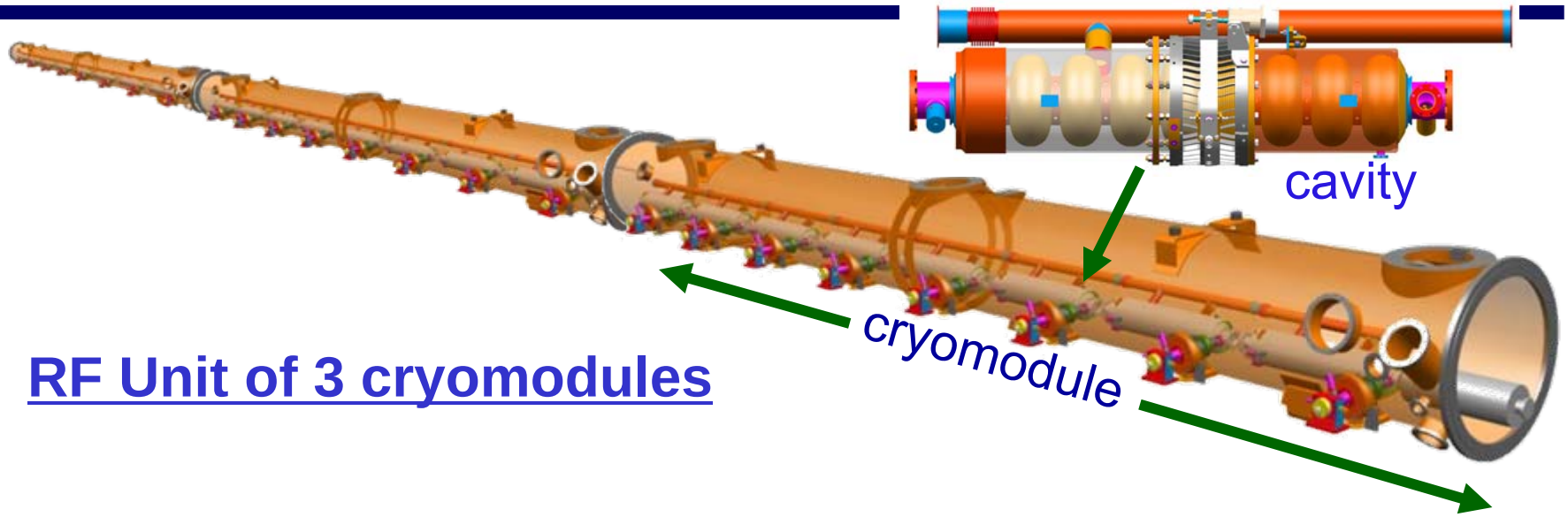
Parallel Electromagnetics & Beam Dynamics Codes

Finite-Element EM Codes:

Frequency Domain:	**Omega3P**	– eigensolver (mode damping, non-linear)
	S3P	– S-parameter
Time Domain:	**T3P**	– transients & wakefields
	Pic3P	– self-consistent particle-in-cell (PIC)
Particle Tracking:	**Track3P**	– dark current and multipacting
	Gun3P	– space-charge beam optics
Multi-Physics:	**TEM3P**	– EM-thermal-mechanical
Visualization:	**V3D**	– meshes, fields and particles

Note: Codes developed since SciDAC1 in black; Codes developed under ComPASS in green

Modeling an Entire RF Unit of ILC Linac



RF Unit of 3 cryomodules

Physics Goal: Calculate wakefield effects in the 3-cryomodule RF unit (**26** cavities) with realistic 3D dimensions and misalignments

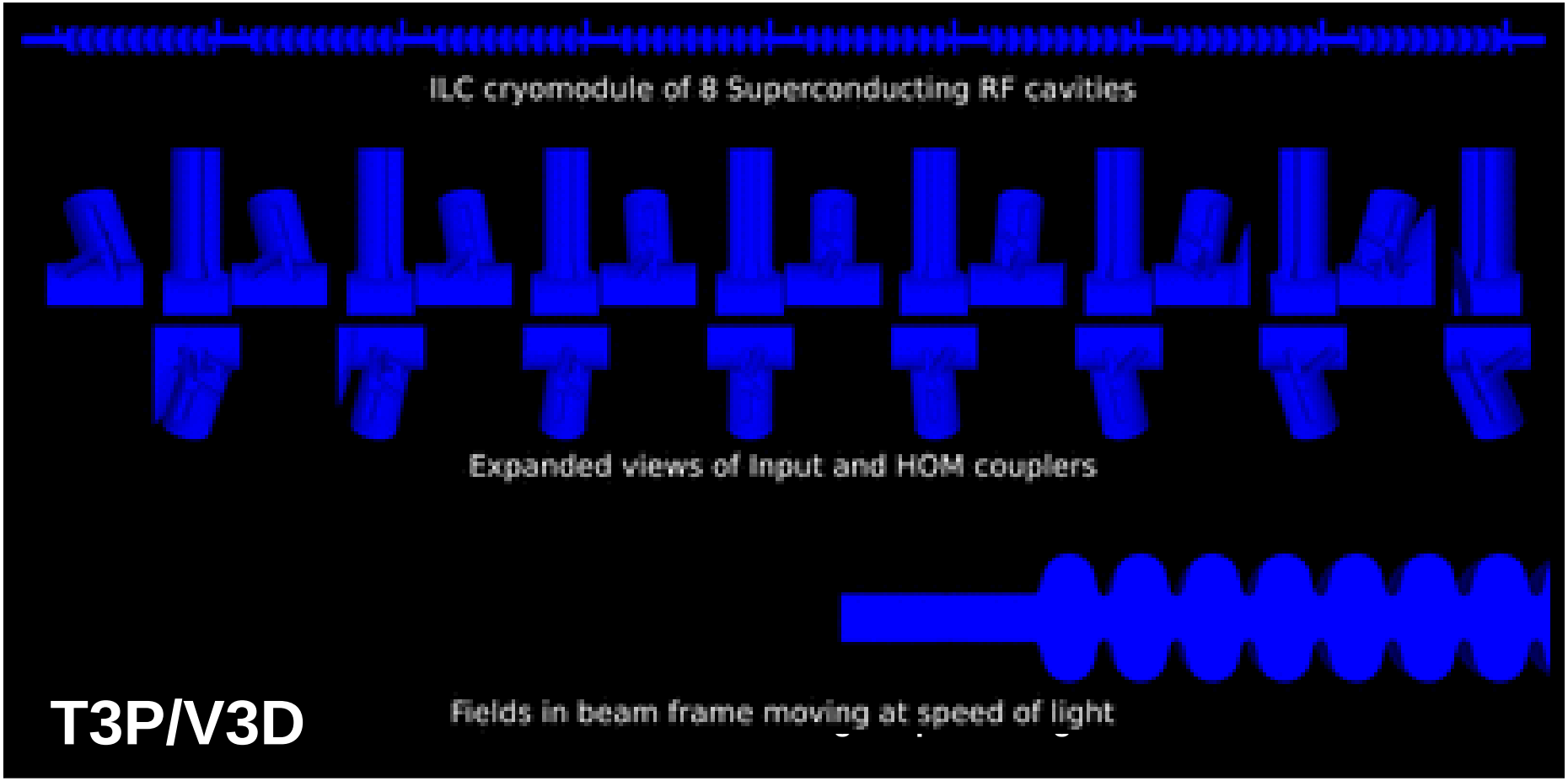
The LARGEST problem for time-domain T3P analysis

- *80 million-element mesh, ~500 million DOFs, 4096 CPUs (Jaguar), 4 seconds per time-step.*

For frequency domain Omega3P

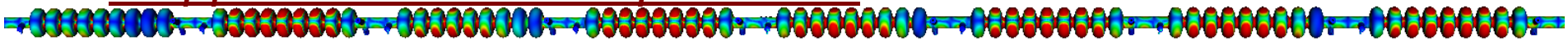
- *3 million-element mesh, ~20 million DOFs, 1024 CPUs (Seaborg), 300 GB memory, 1 hour per mode.*

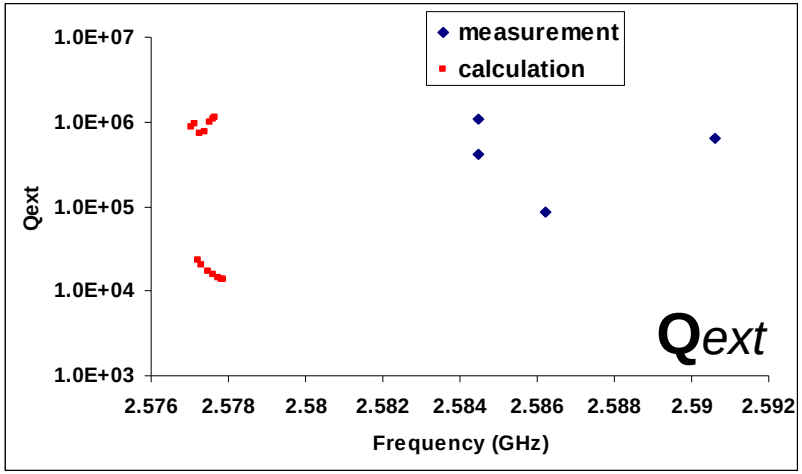
T3P - Beam Transit in Cryomodule



Omega3P - Trapped Modes in ILC Cryomodule

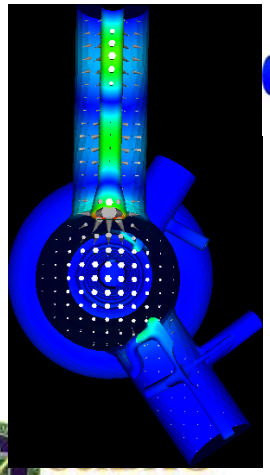
- *Trapped modes in 3rd dipole band*

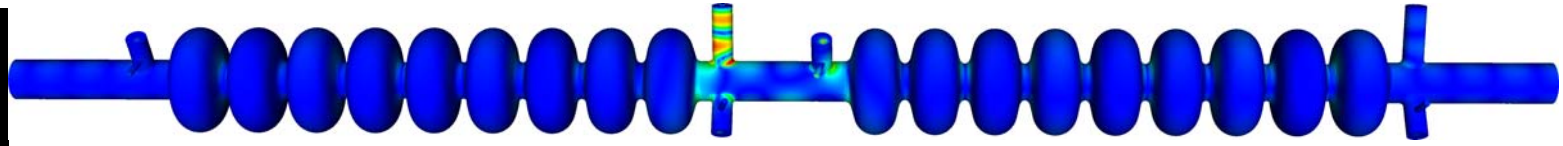




- Modes above cutoff frequency are coupled throughout 8 cavities
- Modes are generally x/y-tilted & twisted due to 3D end-group geometry
- Both tilted and twisted modes cause ***x-y coupling in the beam***

- *Trapped mode in beampipe between 2 cavities*





- TM-like mode at 2.948 GHz, higher than 2.943 GHz TM cutoff
- R/Q = 0.392 Ω, Q = 6320
- Mode power = 0.5 mW (averaged)

(not a concern for heating in this case)

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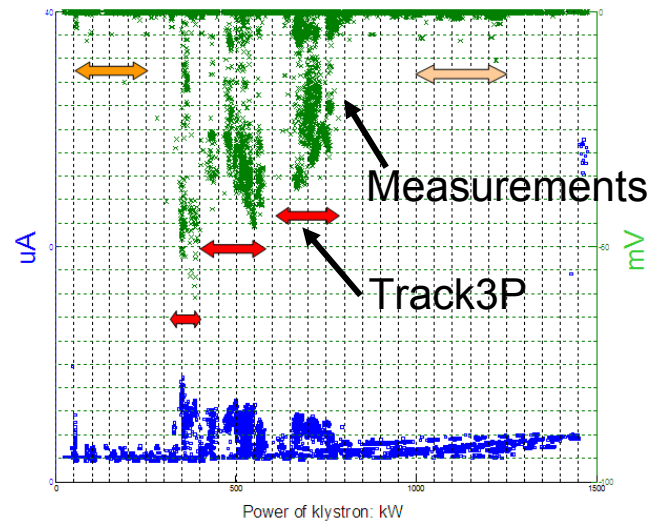
Track3P - Multipacting in SRF Cavities

ILC Linac TTF-III cavity coupler

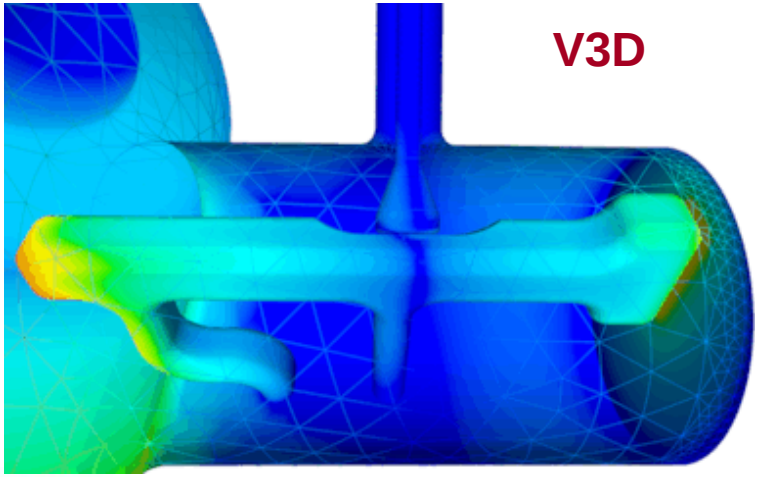
- Simulated MP bands in coaxial waveguide agreed with measurements

MP in TTF coupler

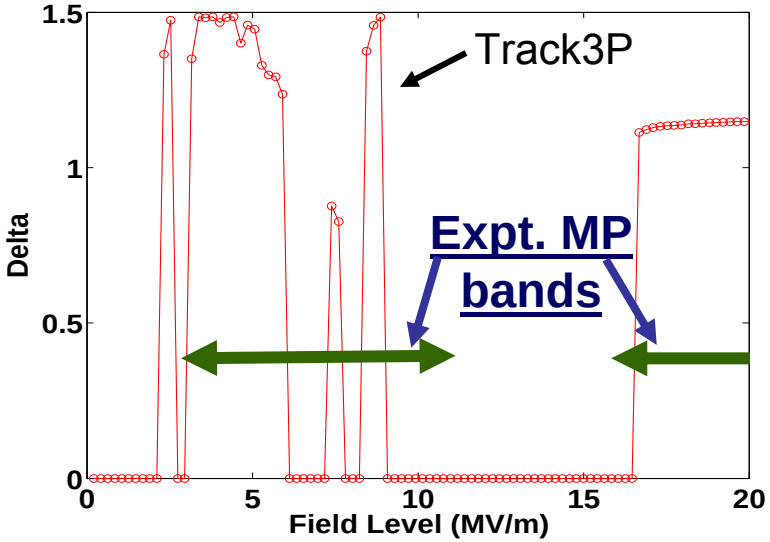


SNS SRF cavity HOM coupler

- RF heating observed at HOM coupler
- 3D simulations showed MP barriers close to measurements

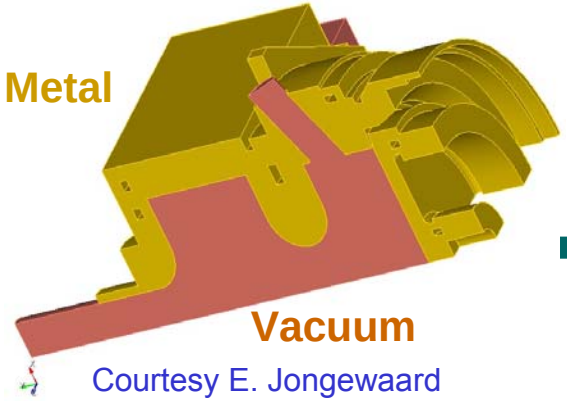


MP in SNS HOM coupler



TEM3P - EM, Thermal and Mechanical Analysis

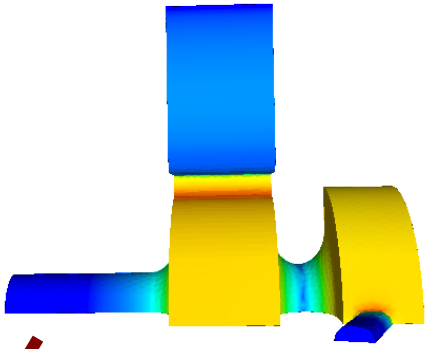
CAD model of LCLS RF gun



Courtesy E. Jongewaard

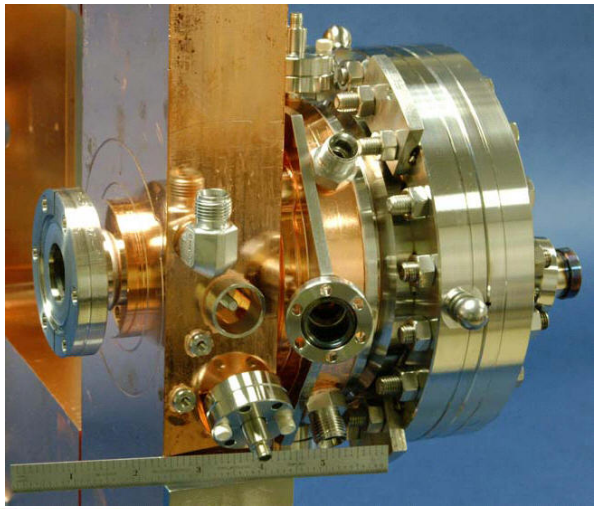
TEM3P for design and optimization

Electromagnetics



Thermal → *Mechanical*

Engineering prototype



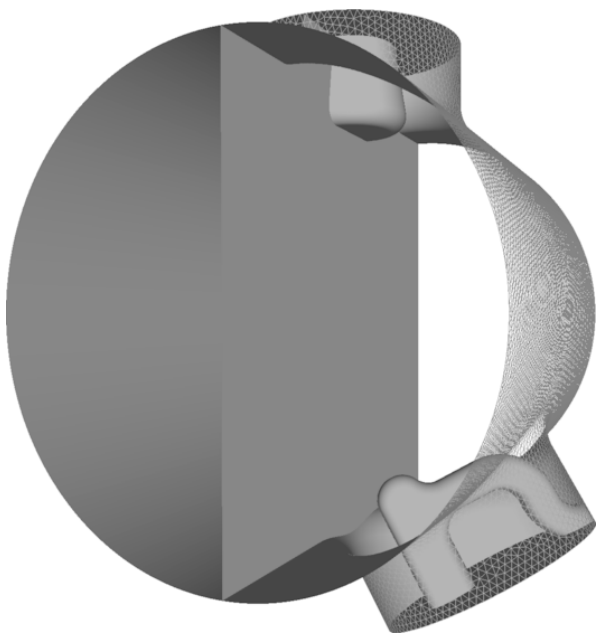
Courtesy D. Dowell

Refinement for Short-Range Wakefields - **ITAPS**

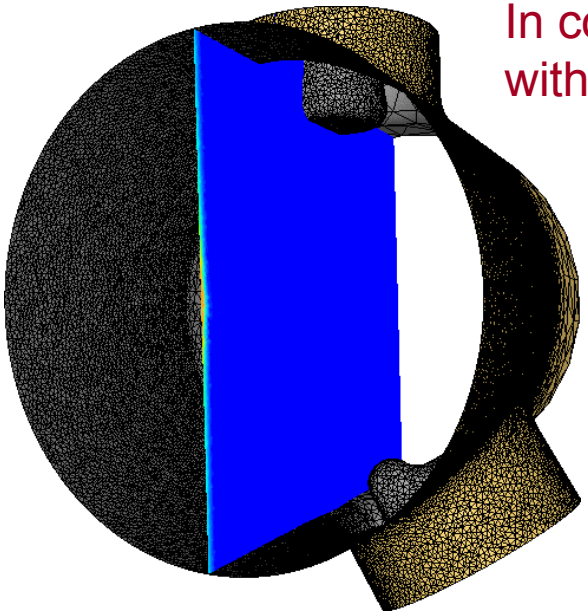
- *Provide **refined mesh only around the moving beam**, thereby reducing computational resources by orders of magnitude*
- *Applications to the ILC damping rings, LHC collimator*

In collaboration with RPI/ITAPS

T3P



p-refined moving window



h-refined moving window

Ref: X. Luo. M. Shephard, L.-Q. Lee, C. Ng, L. Ge, "Tracking Adaptive Mesh Refinement in 3D Curved Domains for Large-Scale Higher-Order Finite-Element Simulations", Best Meshing Technical Poster Award at the 17th International Meshing Roundtable, Pittsburgh, Oct. 12-15, 2008.

Linear Solvers for Large-Scale EM Simulation - **TOPS**

- Improve solvers for Karush-Kuhn-Tucker (KKT) linear systems used in shape optimization and uncertainty quantification

$$\begin{pmatrix} \mathbf{K} - \lambda \mathbf{M} & \mathbf{M}\mathbf{v} \\ (\mathbf{M}\mathbf{v})^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{t} \\ \xi \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{0} \end{pmatrix}$$

  - A sparse direct solver is applied to (0,0) block
  - Null space is removed through orthogonalization

- Enhance multi-level preconditioners in Omega3P to achieve scalable performance on computer platforms such as NERSC's Franklin with small per-node memory

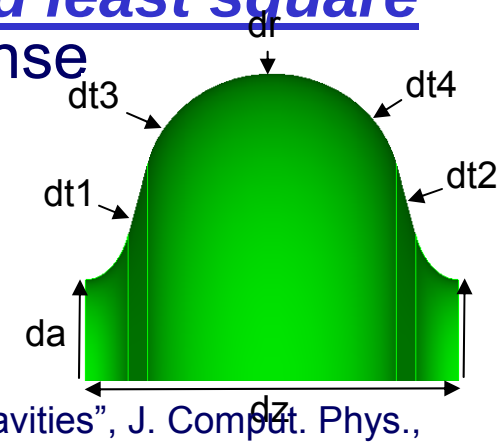
- Integrate out-of-core capabilities of direct linear solver MUMPS into Omega3P for problems with large memory usage

Shape Uncertainty Quantification - **TOPS**

*Solve an **inverse problem** to determine the **deformed cavity shape***

- Use measured rf parameters such as f, Q_{ext}, and field profile as inputs
- Parameterize shape deviations using pre-defined geometry variations
- ***Objective (function ,1) - minimize weighted least square misfit*** of the computed and measured response

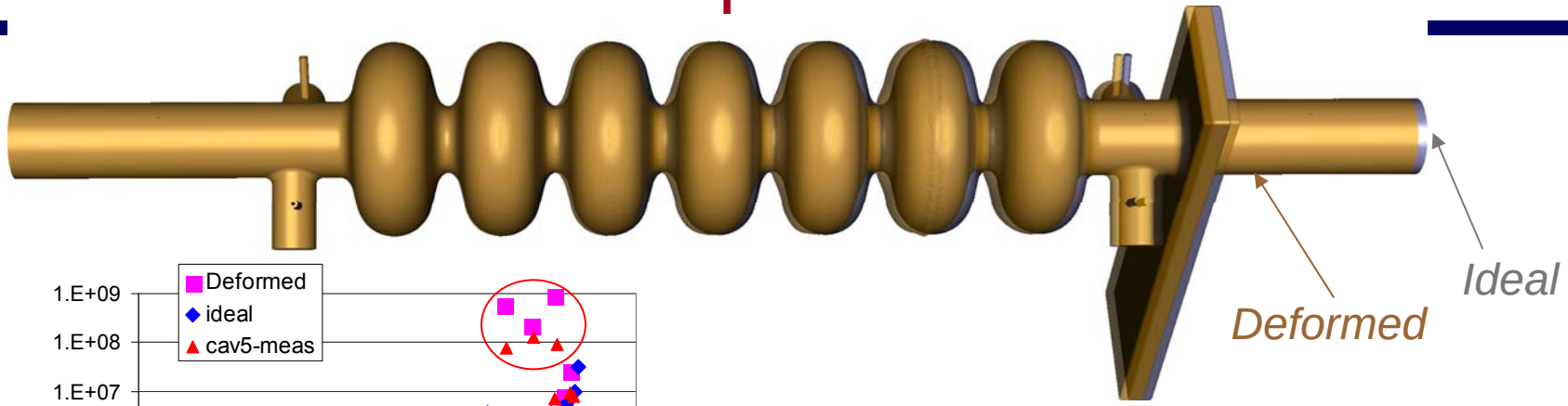
$$\begin{aligned} \underset{\mathbf{e}_j, k_j, \mathbf{d}}{\text{minimize}} \quad & \sum_i \alpha \left(f_i - \bar{f}_i\right)^2 + \sum_i \beta \left(Q_i - \bar{Q}_i\right)^2 \\ \text{subject to} \quad & \mathbf{K}\mathbf{e}_j + ik_j\mathbf{W}\mathbf{e}_j - k_j^2\mathbf{M}\mathbf{e}_j = \mathbf{0} \\ & \mathbf{e}_j^T\mathbf{M}\mathbf{e}_j = 1 \end{aligned}$$

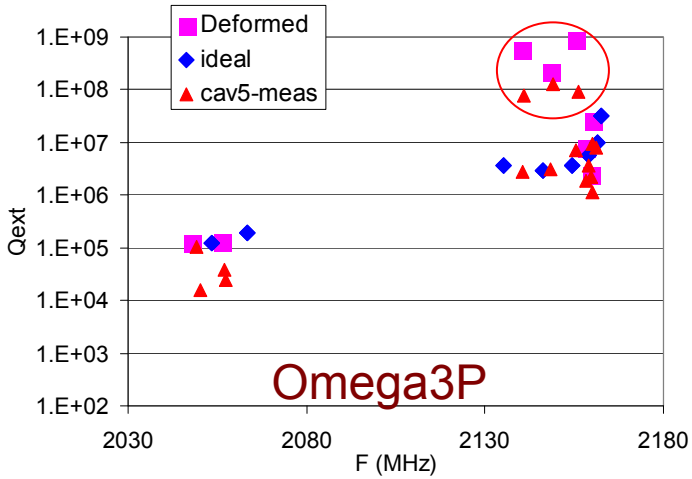


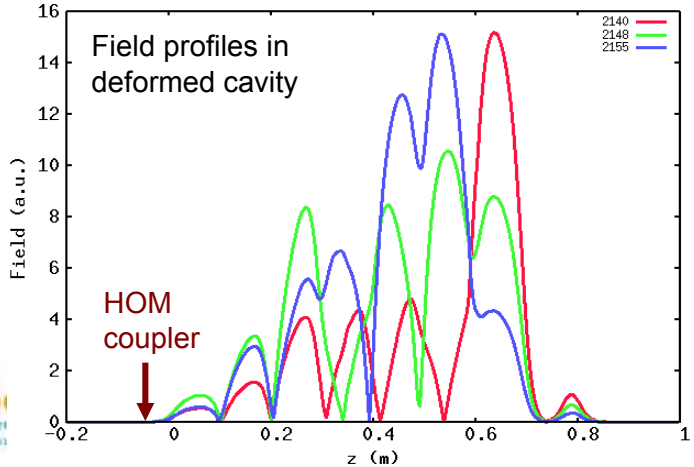
Ref: V. Akcelik et al., "Shape Determination for Deformed Electromagnetic Cavities", J. Comput. Phys., **227**, 1722 (2008).

- The optimization algorithm typically converges within a handful of nonlinear iterations

Solved CEBAF 12-GeV Upgrade Beam Breakup Problem

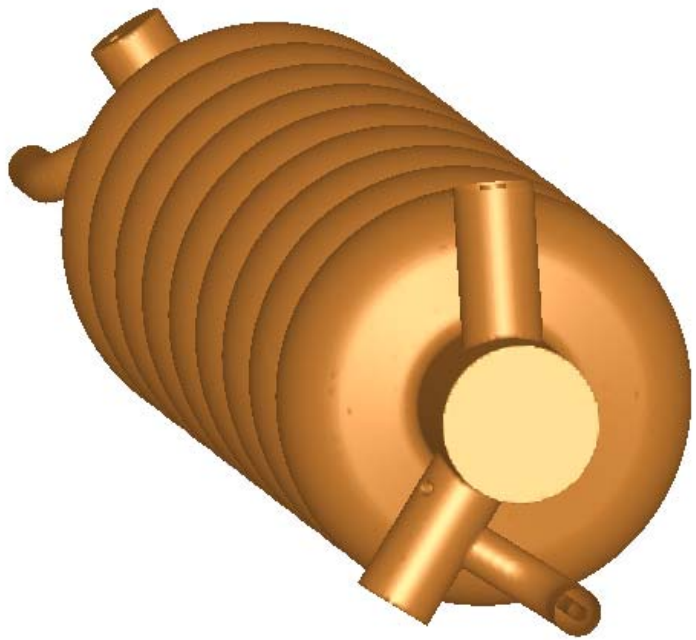


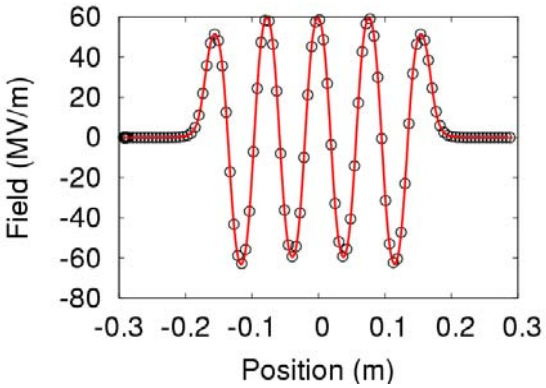




- Beam breakup (BBU) observed in CEBAF 12-GeV upgrade at beam currents well below designed threshold.
- Solutions to the inverse problem identified the main cause of the BBU instability: **Cavity is 8 mm shorter** – predicted and confirmed later from measurements
- The fields of the **3 abnormally high Q modes** are shifted away from the coupler
- This demonstrates that **Quality Control in cavity manufacturing** is essential
- Success requires **a multidisciplinary effort** in accelerator modeling, applied mathematics and RF measurements

FDTD EM Computations used to generate maps for integrated accelerator modeling





The longitudinal electric field on-axis as a function of cavity position computed using the full VORPAL results (red line) and using the interpolation technique of Ref. 1 (black circles). The values using the interpolation technique are then used to compute third-order Taylor maps of the cavity for use in Synergia.

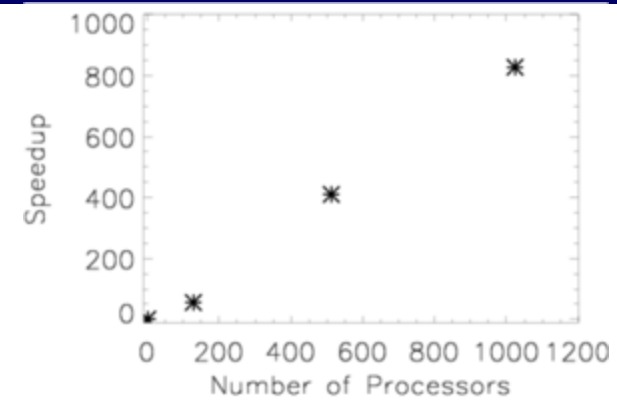
- Use EM code (VORPAL) to provide realistic rf cavity representation to Beam Dynamics codes (Synergia)

*This work funded in part by a DoE SBIR grant from the office of High Energy Physics

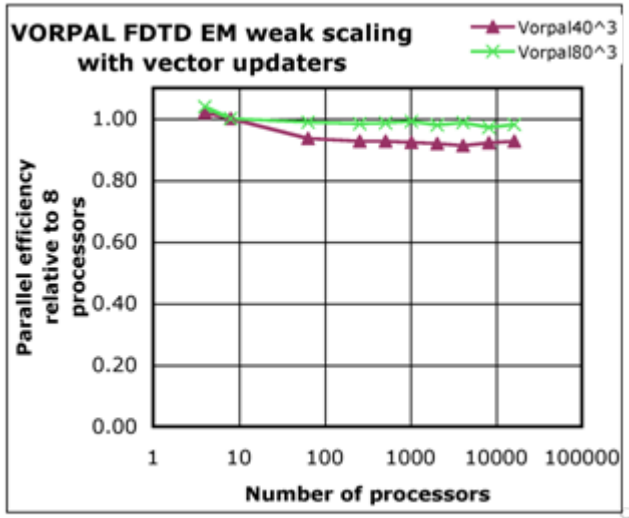
SciDAC
Scientific Discovery through Advanced Computing

FDTD EM (VORPAL) has achieved scalability supercomputer size

- FDTD computations are fast and scalable
  - No matrix inversions
  - No global solves
  - Only surface communications
- Surface area extra work explains initial loss and variation with domain size
- Scales well to 16k processors (Franklin/XT4), the max available at the time of this study



BG/L weak-scaling speedup: 192×128^2 domains

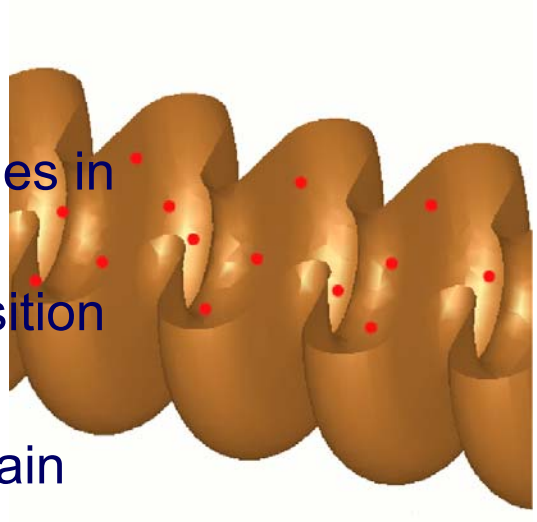


Franklin weak-scaling parallel efficiency

SciDAC
Scientific Discovery through Advanced Computing

New, scalable algorithm developed for obtaining structure modes and frequencies

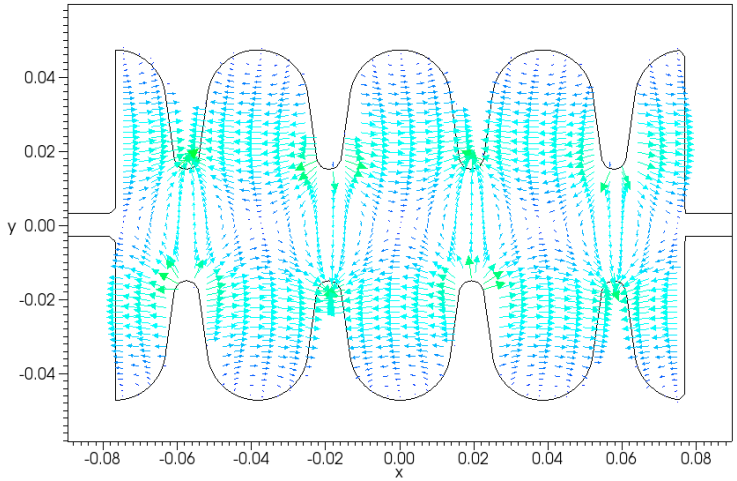
- How to take advantage of fast, scalable explicit FDTD computations?
- Developed a frequency-Filtered Diagonalization Method (FDM), origins in QM, NMR
- Beats Heisenberg! Only a few hundred oscillations to get at once multiple modes to precision of time domain computation
- Ring up finite bandwidth, compute time series of samples in subspace
- Diagonalize subspace using Singular Value Decomposition
- Multiple simulations if near degeneracies
- Turns any time-domain application into frequency domain
- Eliminates need to store a Krylov subspace in memory



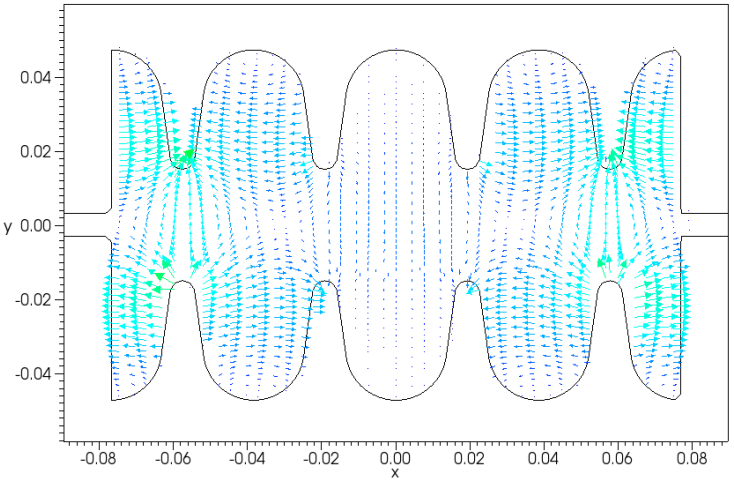
G. R. Werner and J. R. Cary, "Extracting Degenerate Modes and Frequencies from Time Domain Simulations," J. Comp. Phys. **227**, 5200-5214 (2008), http://dx.doi.org/10.1016/j.jcp.2008.01.040

Algorithm allows eigenmode (E shown) reconstruction from the dump files

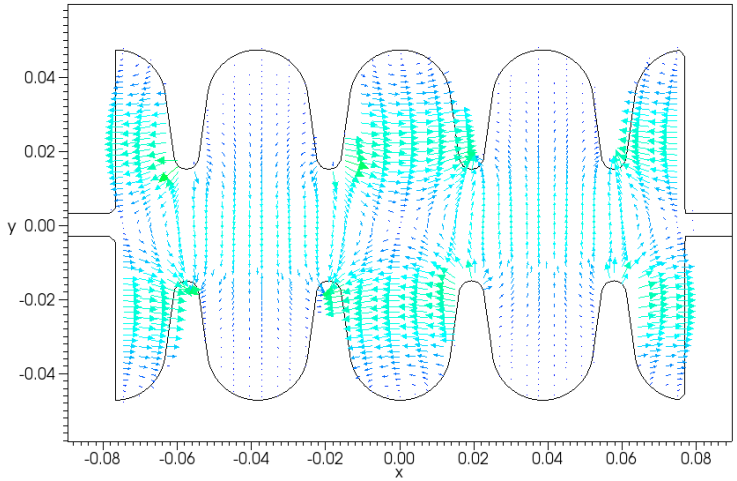
3902.810 MHz (π mode)



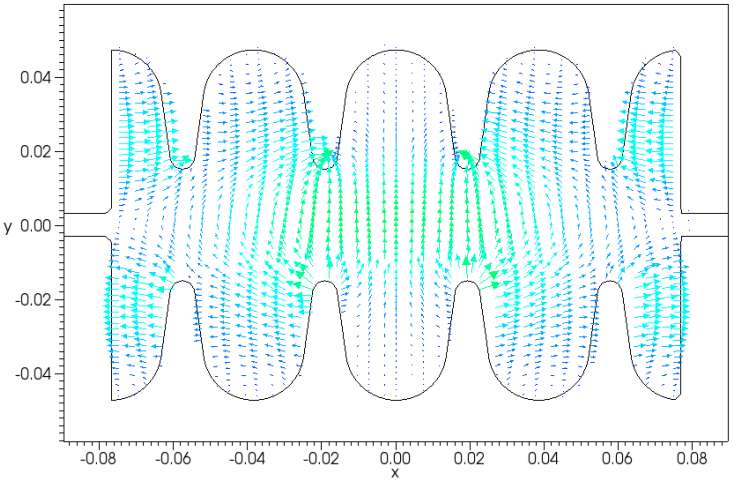
3910.404 MHz



3939.336 MHz

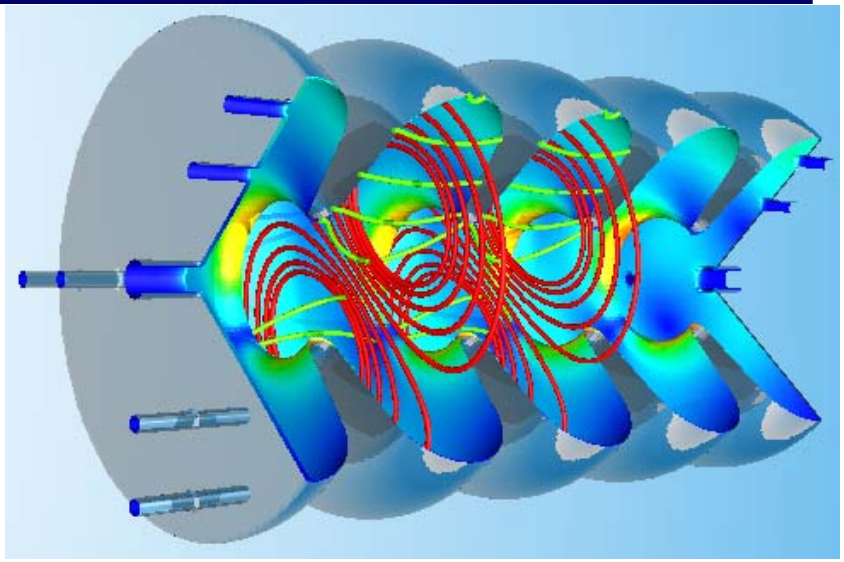


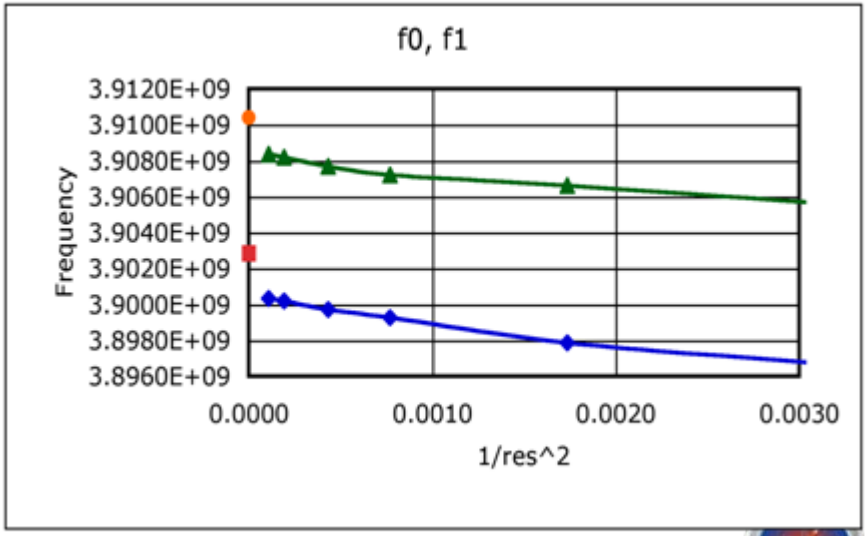
4001.342 MHz



Electromagnetic computation validation able to compute as-built cavity dimensions

- Previous computations gave frequencies low by 5 MHz out of 4 GHz.
- Ours (improved algorithm and parallelism) were low by 2 MHz, yet we had verified against exact solutions!
- Extensive tests with all diagnostic holes, dielectric corrections.
- Finally showed that reduced size cavity (0.0012 in = 30 μm) would match computations to measurements
- Cordex measurements revealed that cavities indeed had equator radius smaller by about 25 μm
- Computations sufficiently accurate to determine dimensions!

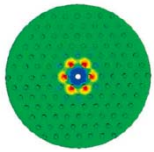




Ability to compute cavity Q allows configuration optimization

- **C. A. Bauer, G. R. Werner, and J. R. Cary, "Optimization of a photonic crystal cavity," J. Appl. Phys. 4 (105), 053107 (2008); DOI:10.1063/1.2973669.**
- Q larger by 2 orders of magnitude for optimized 18 rods compared with best truncated crystal
- Q larger for optimized 18 rods by one order of magnitude compared with 147 rods in truncated crystal
- For 24 rods, we find vacuum Q of 10^5: 100x improvement in Q, 1/6 the number of rods, ¼ the volume!

STUDY OF HYBRID PHOTONIC BAND GAP RESONATORS FOR PARTICLE ACCELERATORS



M. R. Masullo,[1] A. Andreone,[2] E. Di Gennaro,[2] S. Albanese,[3] F. Francomacaro,[3] M. Panniello,[3] V. G. Vaccaro,[3] and G. Lamura[4]

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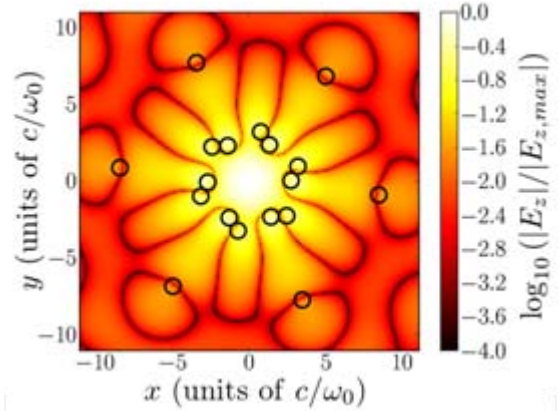
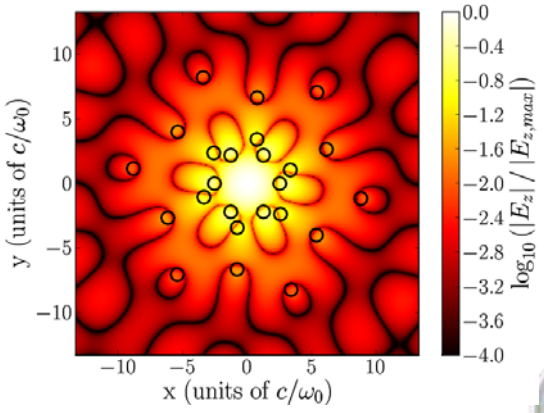
room temperature confirm the monomodal behavior, but the Q value is lower than expected (roughly 10^3). This is mainly due to





SciDAC
Scientific Discovery through Advanced Computing

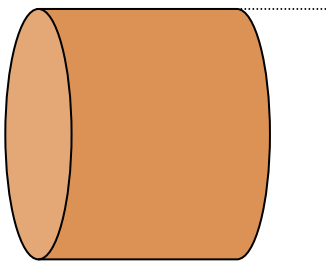
Combined framework allowed immediate evaluation of wake fields

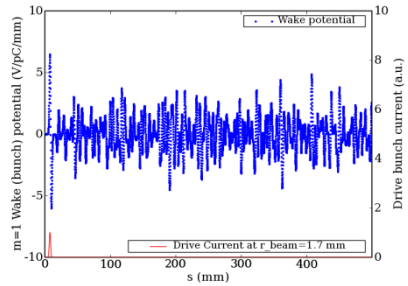
Dipole in time

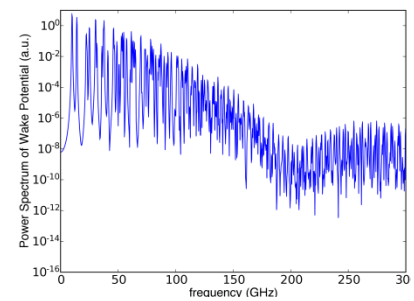
Dipole 20x mag

Accel mode Fourier

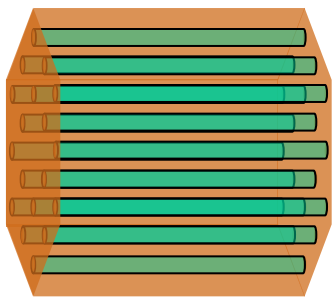
metal pillbox

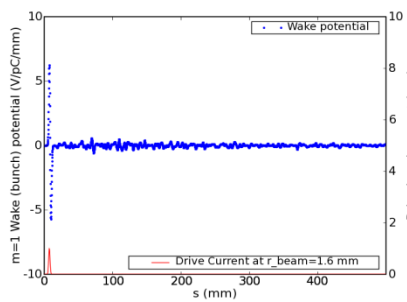


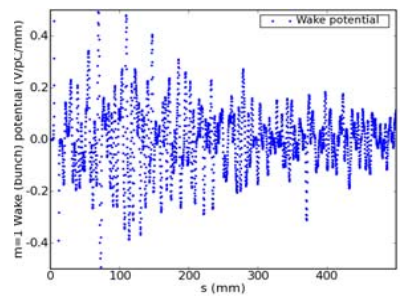


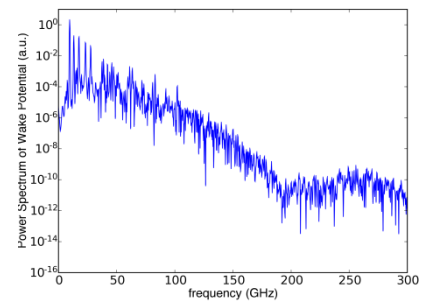


PhC trunc. crystal

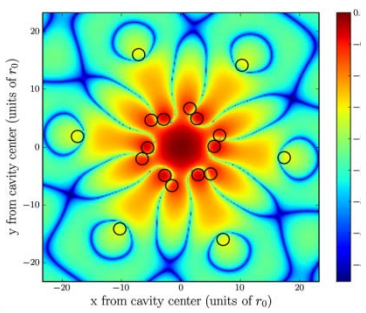


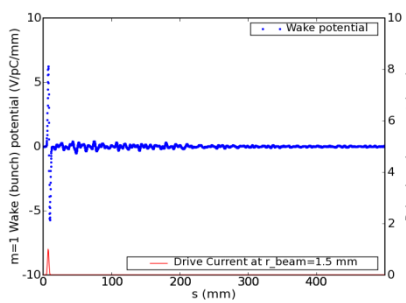


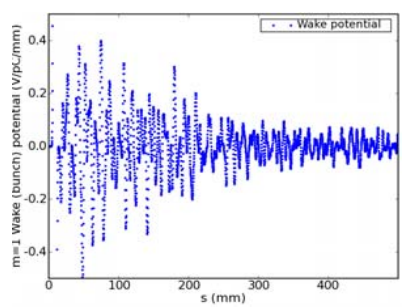


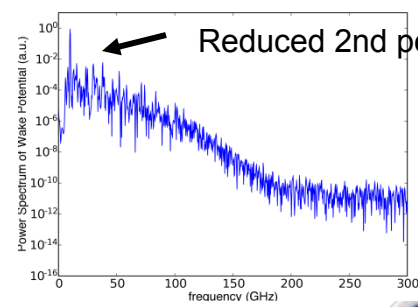


opt. loc.



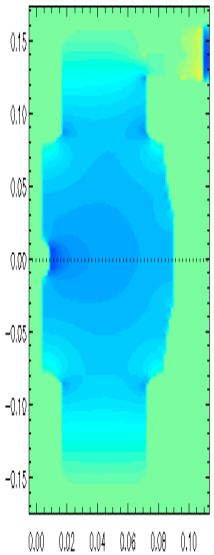


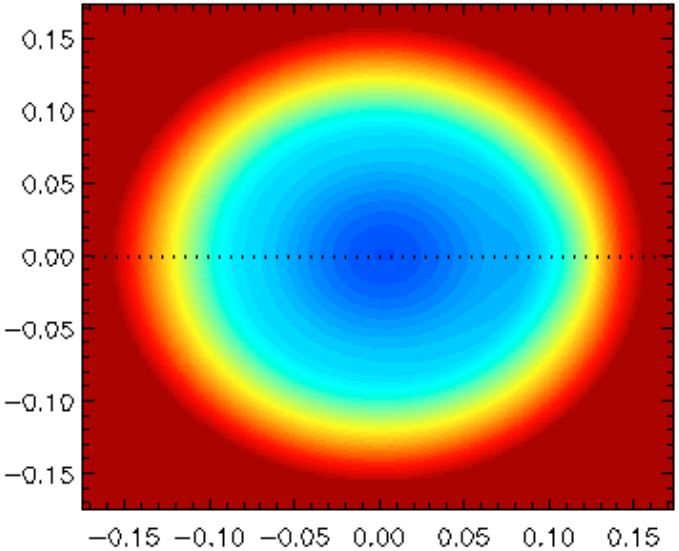


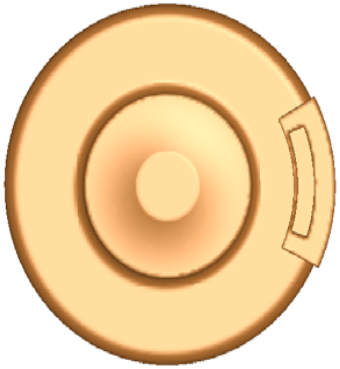


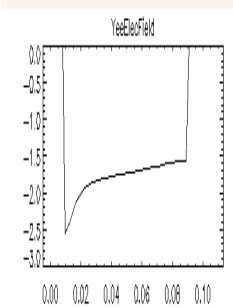
SciDAC
Scientific Discovery through Advanced Computing

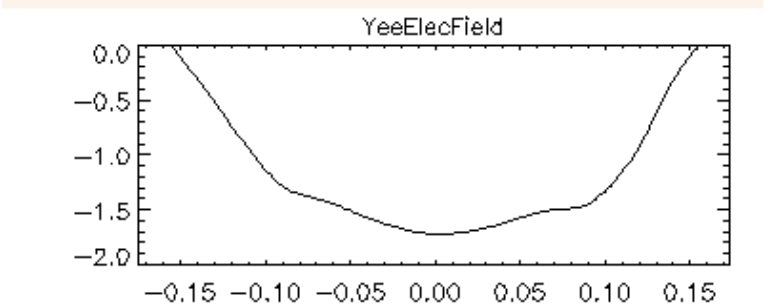
Muon collider cavity analysis started with field analysis (and verification)







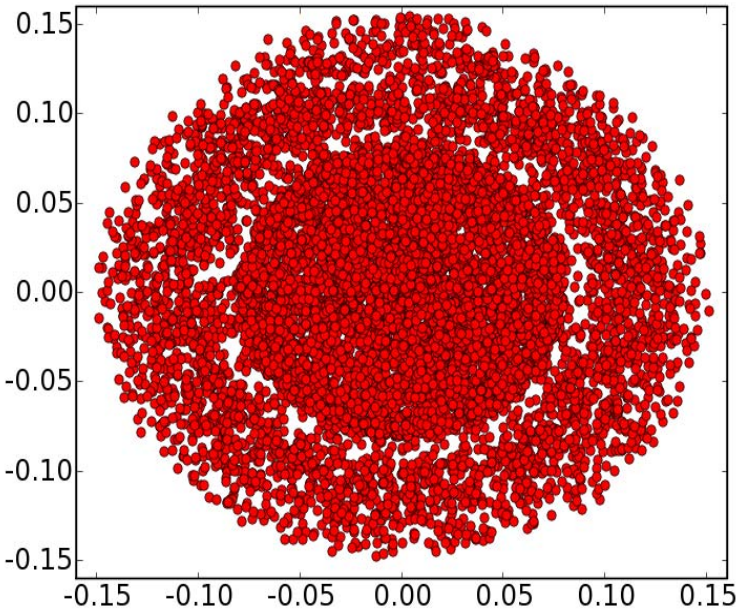




VORPAL results (in agreement with MAFIA) show degree of field asymmetry due to couplers

VORPAL used to understand multipacting and breakdown in muon collider cavities

800 MHz rf structure used for testing cavity designs for **muon collider** applications

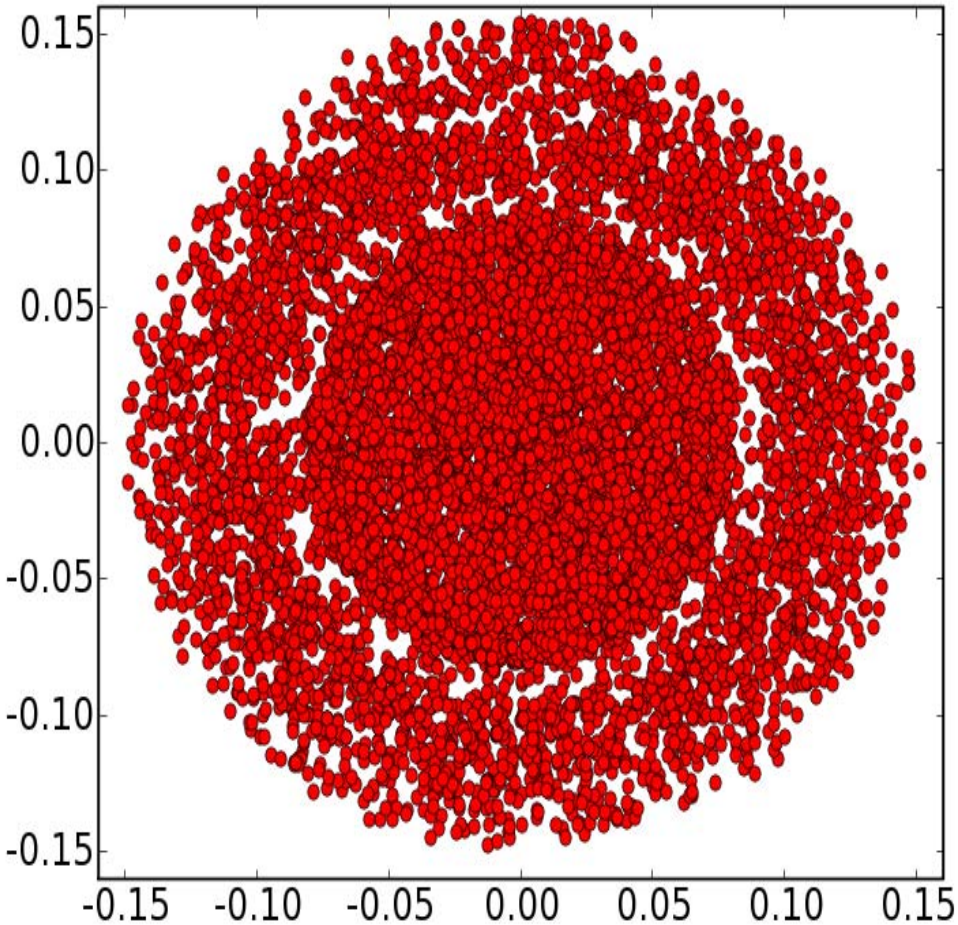


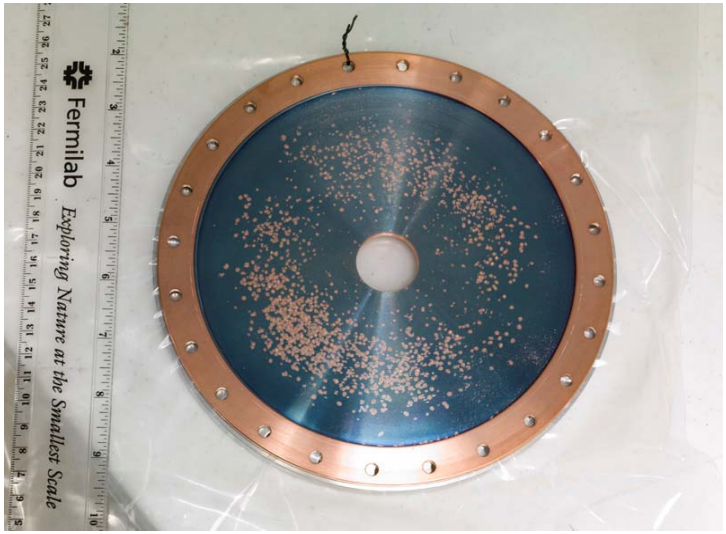
Electrons due to secondary emission after many rf periods

*This work funded in part by DoE SBIR grants from the offices of High Energy and Nuclear Physics

Secondary electrons match observed damage pattern

t =35 ns





Damage pattern in 800 MHz structure

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Scientific Discovery through Advanced Computing

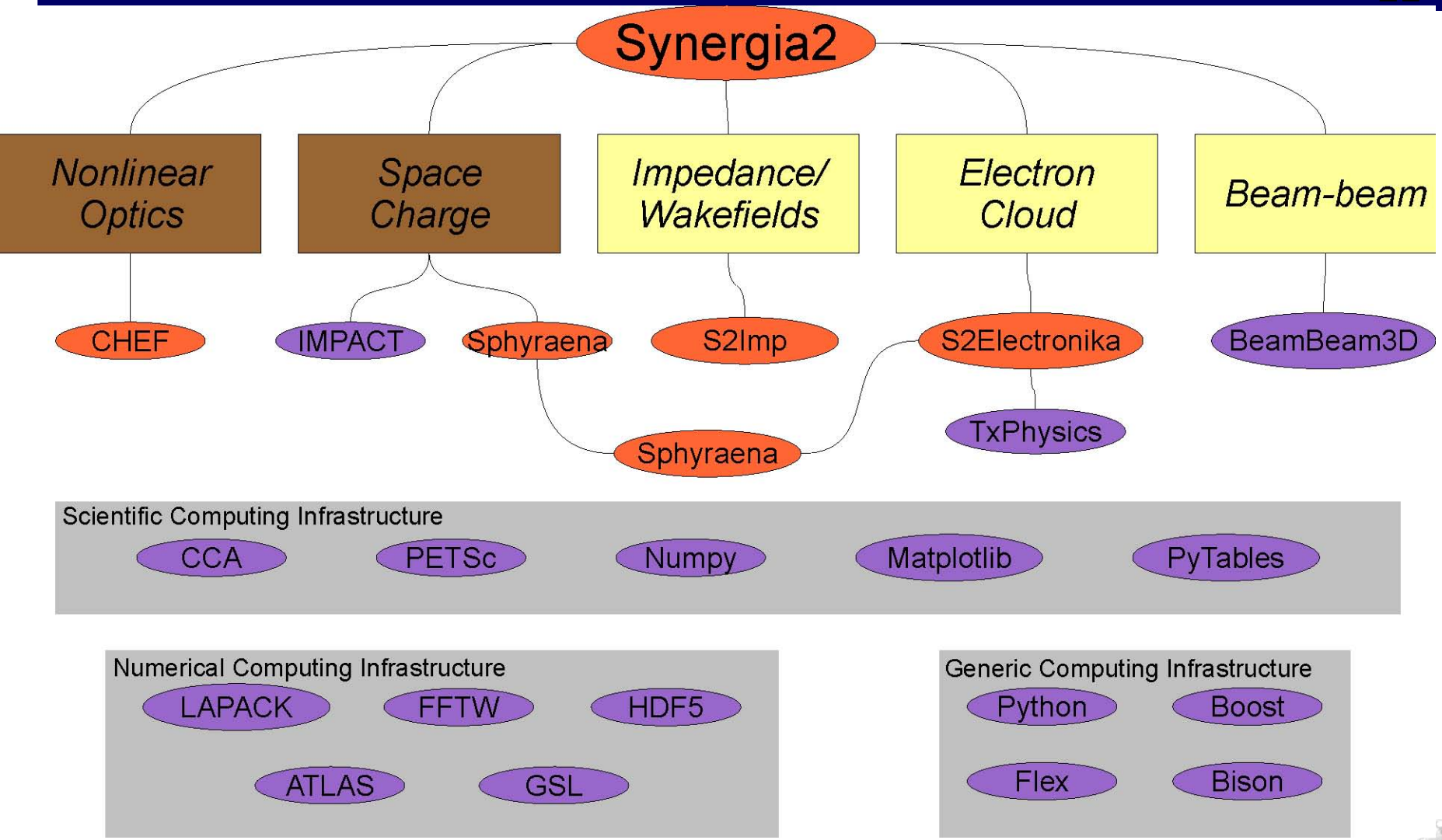
Computational Science Needs

- **Scalable linear systems and eigensystems (TOPS)**
  - Investigate memory-usage scalable solvers for large problems on small per-node memory computers such as Jaguar and Franklin
  - Develop novel algorithms for non-linear eigenvalue problems
- **Shape uncertainty quantification and optimization (ITAPS/TOPS)**
  - Improve algorithms for cavity optimization with different design objectives
  - Incorporate CAD model and advanced meshing services
- **Adaptive refinement (ITAPS)**
  - Develop online mesh generation for h-refined moving window
  - Combine h- and p- refinements for moving window
- **Dynamic load balancing (CSCAPES)**
  - Implement mixed partitioning schemes in Pic3P to dynamically balance particle and field computation in time domain
- **Visualization (IUSV)**
  - Visualize fields and particles on unstructured grids within Paraview *parallel* framework

Beam Dynamics

- Mainly electrostatic PIC codes. Continue to
  - work on PIC infrastructure performance optimization
  - work on solver performance enhancement and new solver development
  - work on pipeline algorithm optimization
  - enhance infrastructure to allow multi-physics capabilities
  - benchmark, share physics modules between different frameworks
- Applications
  - Finalized ILC applications (RTML, ML, DR)
  - Begun involvement with Project-X (space-charge, e-cloud, impedance, …)
  - Increased Tevatron and LARP involvement (utilizing existing capabilities)
    - Beam-beam effects and mitigation
    - PS2 design (space-charge, impedance, e-cloud)
  - Continued/increased emphasis on NP applications
    - Beam-beam
    - Electron Cooling
  - Continued light source applications for BES
    - Microbunch instability
    - Emittance preservation

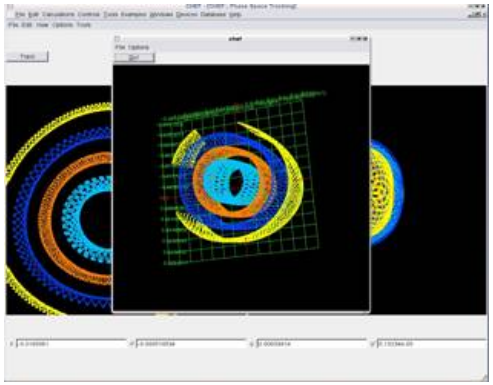
Framework Development

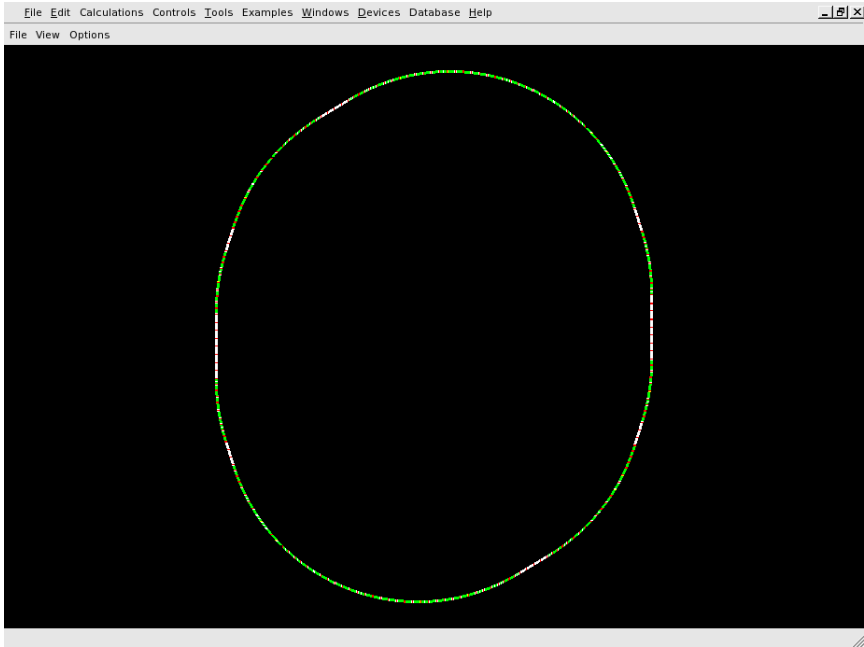


SciDAC
Scientific Discovery through Advanced Computing

Single-particle tracking: CHEF

- 6D Particle tracking code
  - Arbitrary-order maps
  - Individual particle (non-map) tracking available
    - particularly useful for longitudinal dynamics in beam capture when accurate description of entire bucket is necessary
  - Accepts MAD(8) and XSIF
    - MADX in development
  - Provides a GUI





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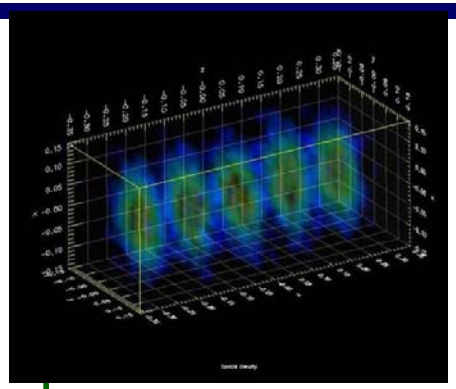
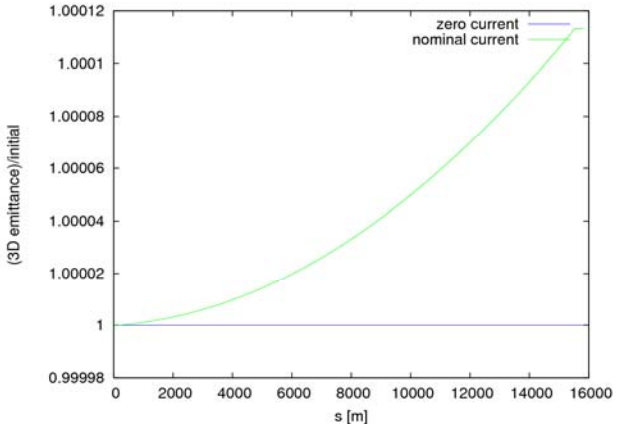
Space charge physics



- Extensively validated, utilized for
  - Fermilab Booster & ILC RTML studies
- New 3D solver suite, Sphyraena
  - Arbitrary number of loosely-coupled bunches
    - previous strongly-coupled Synergia implementation does not scale past a few bunches
  - FFT based solvers
    - Open boundary conditions
    - Conducting circular pipe
  - Finite Difference solver
    - Arbitrary BCs possible
    - First multigrid version too slow for production
    - Non-MG version under development



SciDAC
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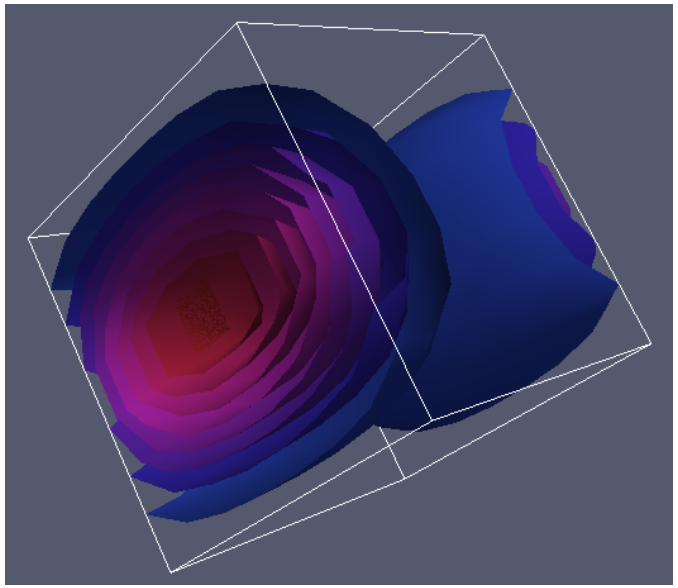
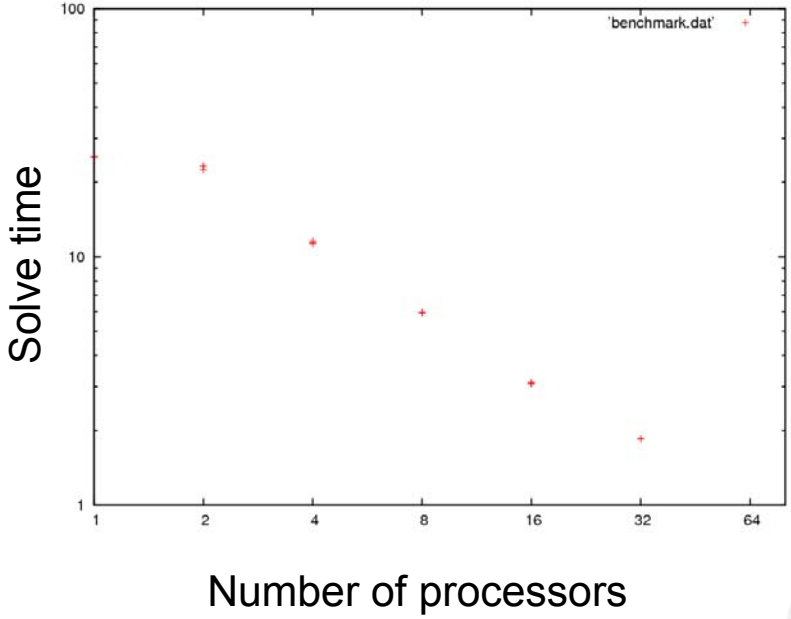
Sphyraena solver development for Synergia2

- FFT based Poisson solver implementations use open, closed rectangular, or closed circular boundary conditions
  - Fermilab Main Injector has an elliptical beam pipe
- We developed a PETSc-based finite-difference Poisson solver
  - can accommodate elliptical pipes

Field solution for benchmark problem



excellent parallel scaling performance provided by PETSc libraries



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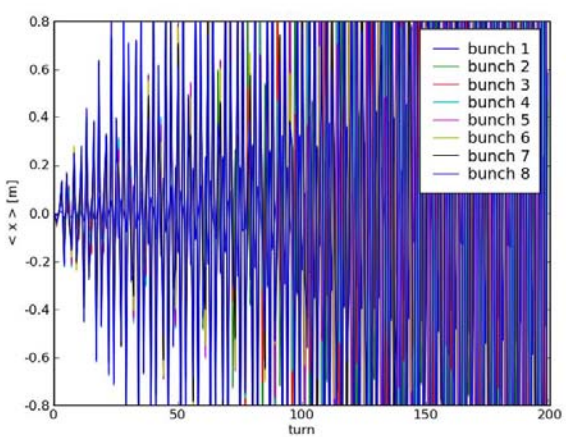
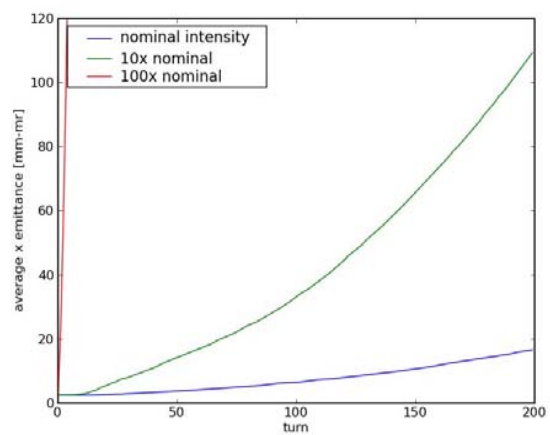
Resistive Wall Impedance Module

- Developed for BeamBeam3D simulations of Tevatron
- Longitudinal charge density is calculated using 3D PIC and cloud-in-cell slices
- Utilized for Fermilab MI studies





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Accelerator Simulation using CCA Components (CCA/Synergia)

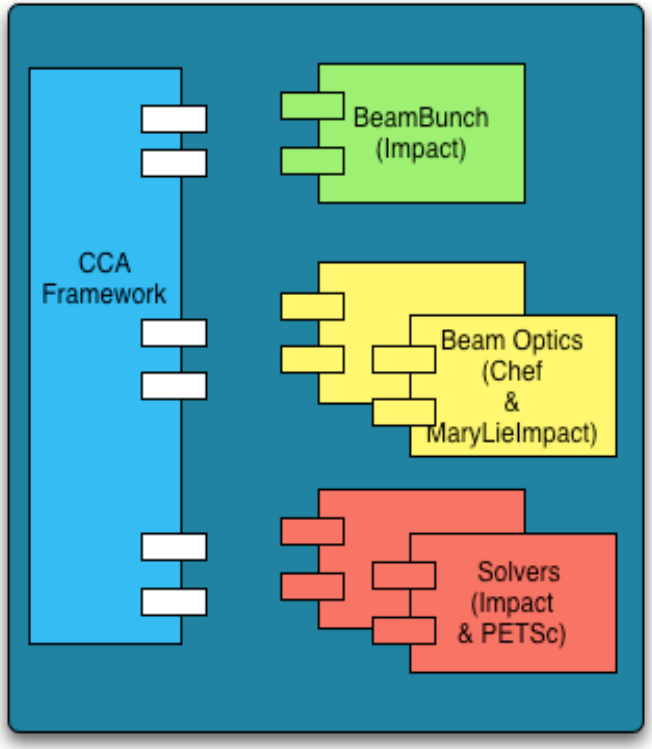
- **Motivation:**
  - **Computational accelerator community:** Tremendous investment in software applications, codes written in a variety of languages, targeting a range of computational platforms
  - **Common Component Architecture (CCA) component vision:** Enable the HPC community to leverage existing applications, creating modular, reusable software components that facilitate the combined use of historically independent codes to add new capabilities (see www.cca-forum.org)
- **Approach:**
  - Using CCA tools and specifications, prototype an accelerator simulation from existing codes that were not originally designed to work together
  - Develop components based on codes for beam dynamics; also incorporate external numerical libraries:
    - Synergia2 beam physics framework (FNAL)
    - MaryLie/Impact beam physics application (LBNL/U. Maryland)
    - High-performance numerical tools via TOPS CET (including PETSc (ANL), LBNL numerics)
- **SciDAC Math/CS Collaborators:** TASCS, TOPS, and PERI
- **Long-term Goal:** Foster a component community in computational accelerator physics

Benefits

- Improved Productivity
  - Reuse physics components across COMPASS project and the accelerator community
  - Leverage tools and libraries developed by experts in other specialties (math/cs)
- Enhanced Performance
  - Exploit highly optimized numerical software (e.g., TOPS)
  - Enable adaptive method configuration and selection to better match dynamically changing computational requirements

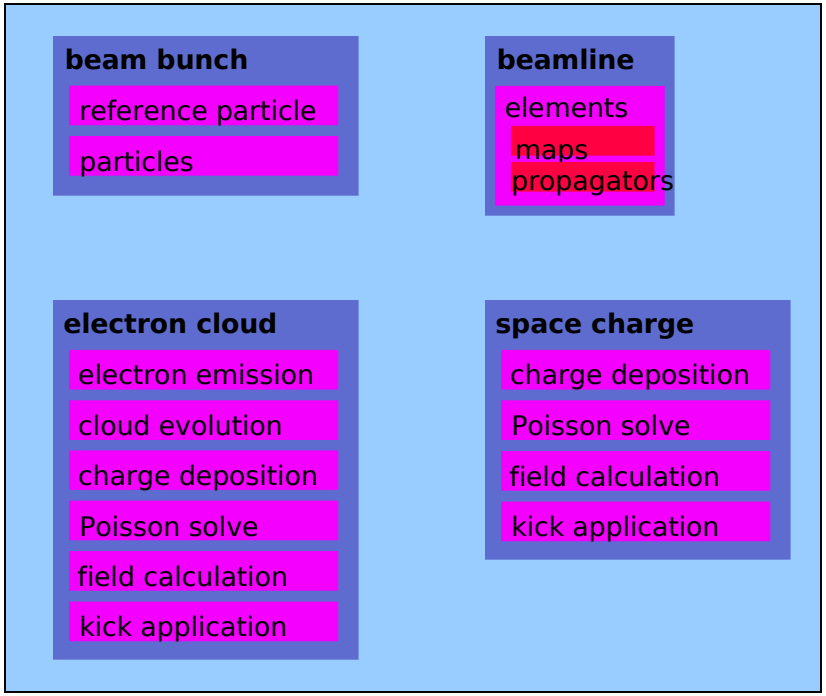
Initial Work: Beam Dynamics Components

- Accelerator modelling components (collaboration with TASCS):
  - F90-based beam optics components (quadrupoles and drifts) from the MaryLie/Impact application (LBNL)
  - C++ and F90 particle store components from the Synergia2 framework (FNAL)
  - A newly implemented C++-based space charge solver, Sphyraena, that makes use of Synergia2, PETSc (ANL), and FFTW.
- Component interfaces allowed us to capture and make available only the functionality that was desired from the existing codes.
- Reference: D. Dechow, B. Norris, and J. Amundson, *The Common Component Architecture for Particle Accelerator Simulations*, Proceedings of HPC-GECO/CompFrame'07, October 21-22, 2007, Montreal, Quebec, Canada, ACM, 2007.



Beam Dynamics Interface Issues

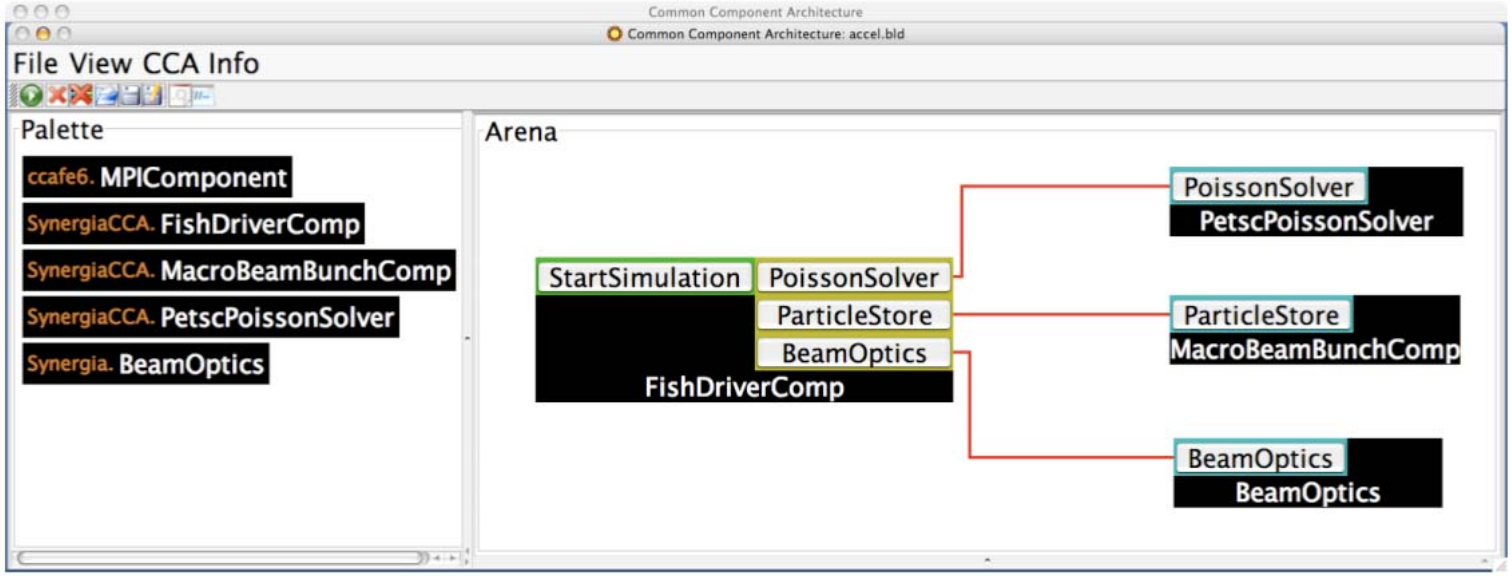
- Refactoring Synergia2 and exploring interface issues for common functionalities
  - Beam bunch
  - Beamline
    - Demonstrated interchanging CHEF and MaryLie beamline components at the map level, even though beamline models themselves are very different
  - Space charge
    - Synergia2 can use space charge modules from either IMPACT or Sphraena
  - Electron cloud
- Challenges
  - **Granularity:** Overheads that apply *per particle* get an extra factor of ~10^7
    - unacceptable … use aggregation
  - **Parallel decomposition** of fields, etc., must be compatible: may force coarser granularity



Reference: *Multiscale, Multiphysics Beam Dynamics Framework Design and Applications,* J. Amundson, D. Dechow, L. McInnes, B. Norris, P. Spentzouris and P. Stoltz, J. Phys.: Conf. Ser. 125 (2008) 012001, available via: http://www.iop.org/EJ/abstract /1742-/125/1/012001

Recent Accomplishments

- Developed prototype Contractor-enabled CCA beam dynamics toolkit
  - Demonstrated new beam optics with Fortran90 and Python, ChannelDriver basis component, new Synergia BeamBunch component
- Performed initial simulations using Synergia2 components
  - FODO cell demo, Apply space charge kick
    - Poisson solvers and beam dynamics, Sphyraena-based implementation

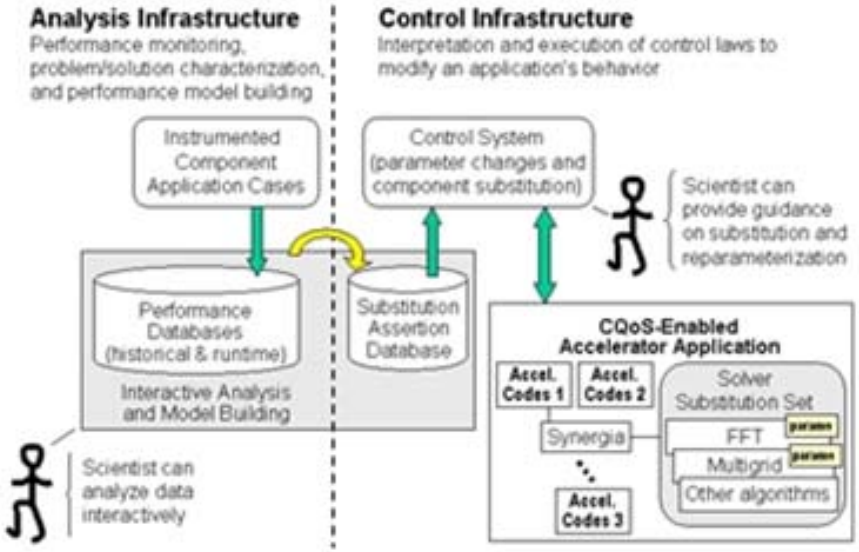


Ongoing and Future Work

- **Immediate priorities:** Critical for COMPASS component integration
  - Collaborate with TASCS to address
    - Babel/SIDL interlanguage capabilities with struct support, broad support of Fortran compilers
    - Ability to run on leadership class facilities (including Cray XT4, BG/P)
  - Complete initial componentization of Synergia2
  - Evaluate performance of original Synergia application and component variant on Project-X and LARP simulations, with emphasis on beam dynamics applications for space charge and wakefields
- **Longer-term challenge:** Collaborate with TASCS, PERI, and TOPS to address issues in Computational Quality of Service (CQoS) for accelerator simulations,
  - How, during runtime, can we make make sound choices for reliability, accuracy, and performance, taking into account the problem instance and computational environment?
    - **Composition:** select initial component implementations and configuration parameters
    - **Reconfiguration:** change parameters
    - **Substitution:** change implementations
  - Recent work: Developed an initial catalog of Syn2CQoS Components

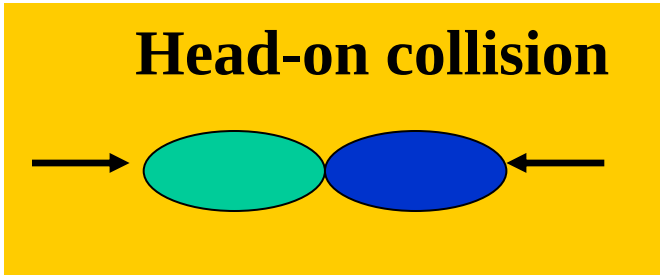
Simulation Environment

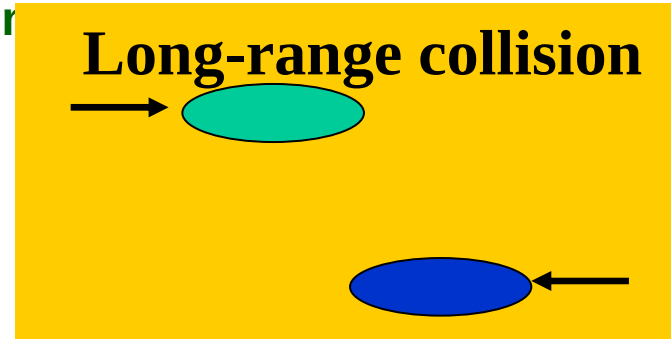
- Many different applications → no single solver or solution strategy spans entire spectrum. Develop framework environment to help automate application configuration
  - Analysis Infrastructure
    - Performance information from historical and runtime databases
  - Control Infrastructure
    - Decision making tools, tools to enable runtime configuration
- increased requirements on target computing platforms
  - Run time environment, libraries

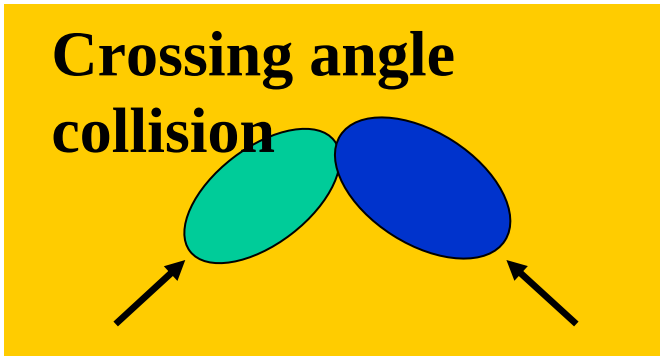


BeamBeam3D

- **Code Features**
  - **Both strong-strong and weak-strong models**
  - **Multiple-slice model for finite bunch length effects**
  - **New algorithm -- shifted Green function -- efficiently models long-range parasitic collision**
  - **Parallel particle-field based decomposition to achieve perfect load balance**
  - **Crossing angle collisions**
  - **Multiple bunches, multiple collision points**
  - **Crab cavity and conducting wire compensator**
- **Applied to**
  - **Tevatron, RHIC, LHC**
  - **e-RHIC and ELIC design**
- **Used by researchers at FNAL and JLab**
- **Close collaboration with FNAL, BNL, JLab**
  - **Code feedback, code enhancement (FNAL)**

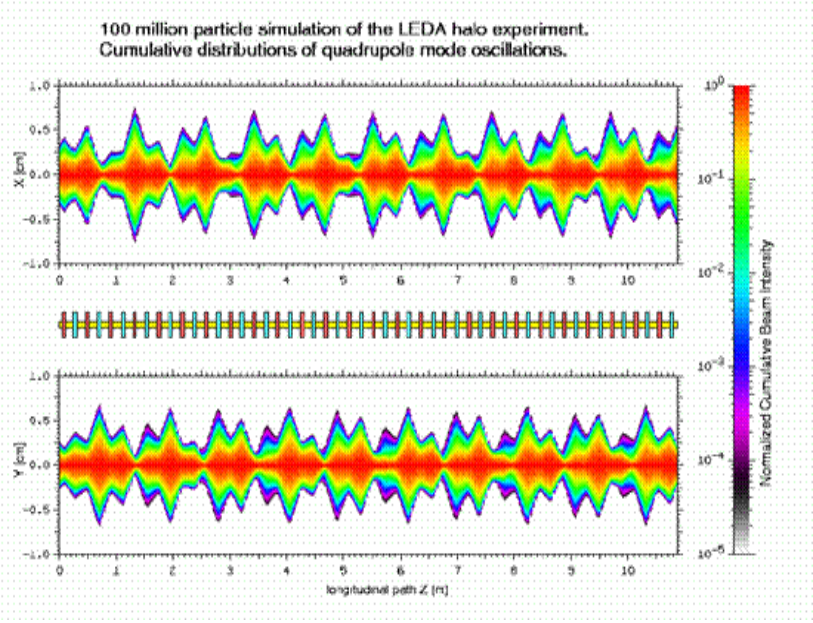






IMPACT-Z

- Parallel PIC simulation using coord “z” as the independent variable
- **Key Features**
  - **Multiple Poisson solvers**
    - **Variety of boundary conditions**
    - **3D Integrated Green Function**
    - **point-to-point**
  - **Multi-charge state**
  - **Machine error studies and steering**
  - **Wakes**
  - **CSR (1D)**



- **In use at SNS for linac commissioning**
- **Also applicable to Project-X design**

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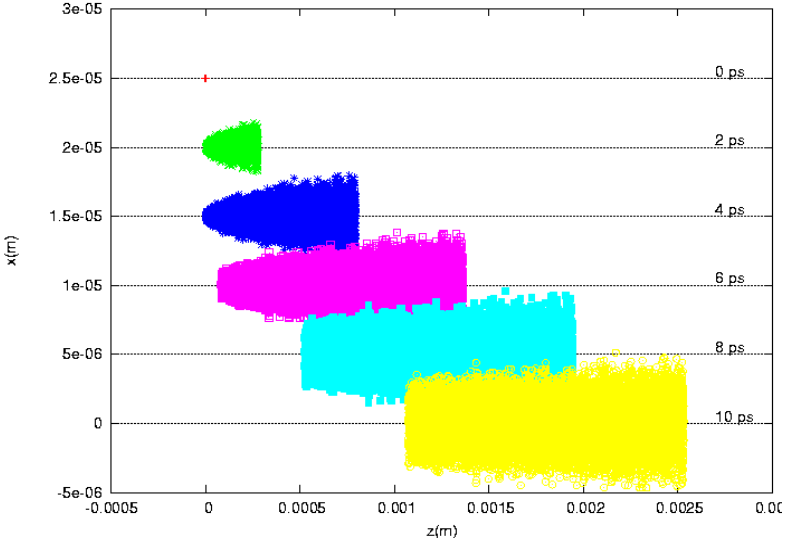
IMPACT-T

- Parallel PIC simulation using time as the independent variable

- **Key Features**
  - **Multiple Poisson solvers**
    - **3D Integrated Green Function**
    - **point-to-point**
  - **Energy Binning**
  - **Cathode image effects**
  - **Wakes**
  - **CSR (1D)**

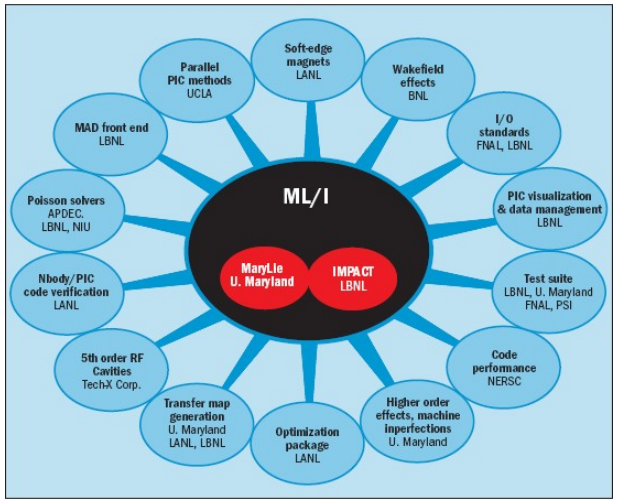


Emission from nano-needle tip including Borsch effect

- **Has been used to study photoinjectors for BNL e-cooling project, Cornell ERL, FNAL/A0, LBNL/APEX, ANL, JLAB, SLAC/LCLS**

MaryLie/IMPACT (ML/I)

- Combines capabilities of MaryLie code (from U. Md.) with IMPACT code (from LBNL) + new features
- Multiple capabilities in a single unified environment:
  - Map generation
  - Map analysis
  - Particle tracking w/ 3D space charge
  - Envelope tracking
  - Fitting and optimization
- Applied to RHIC, ILC



- **Parallel**
- **5th order optics**
- **3D space charge**
- **Fitting/Optimization**
- **5th order rf cavity model (Tech-X)**
- **Crab cavity model (Tech-X)**
- **Multiple ref traj for rf cavities**
- **3D integrated Green function**
- **Envelope tracking**
- **Soft-edged magnets (LANL)**
- **Coil stacks (LANL)**
- **MAD-style input compatibility**
- **Test suite, regression tests**
- **“Automatic” commands**

Improvement of the Poisson Solver in IMPACT

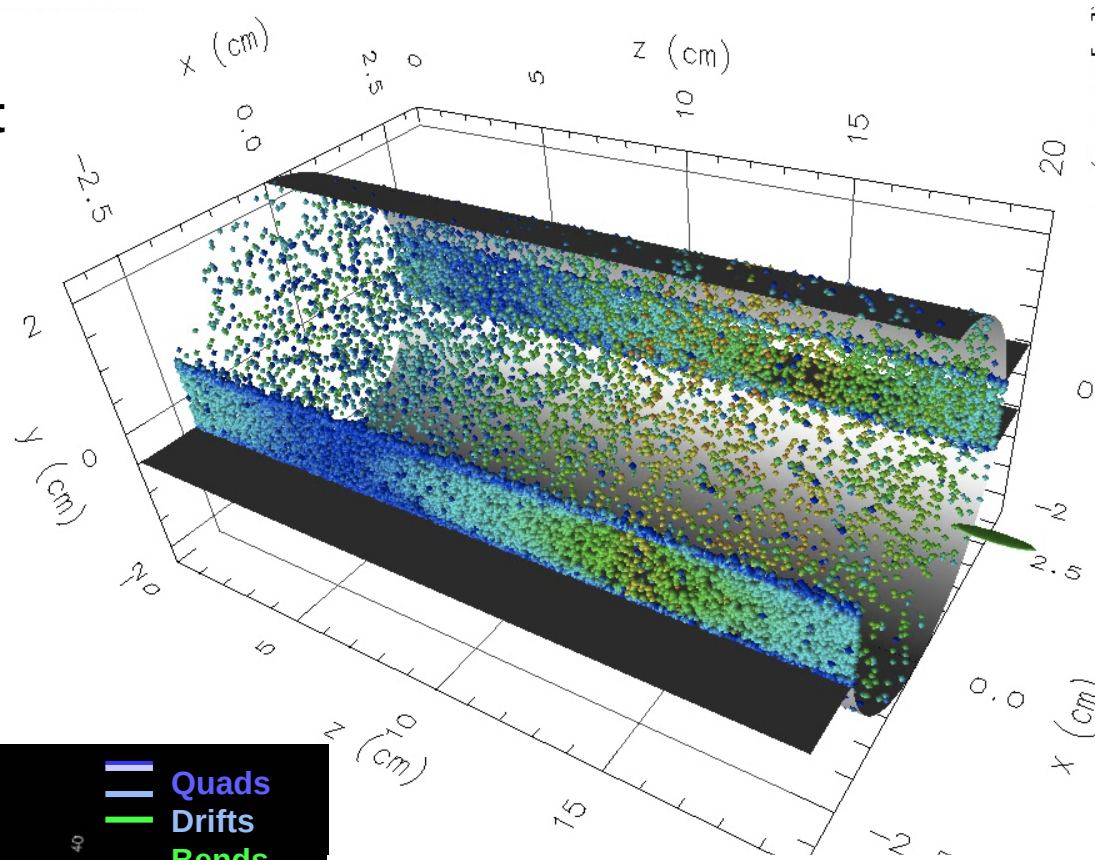
- IMPACT
  - Model high intensity, high brightness beams in linear accelerators (Poisson-Vlasov integral equation)
  - 3D Particle-In-Cell code, domain decomposition
  - Simulation cycle : deposit charge density on grid points, solve Poisson equation (FFT-based) for field vector, interpolate the field vector, advance particles
- Optimizations of Poisson solver – better use of FFTW
  - Exploit multiple 1D FFT calls of same length
  - Exploit real-complex mixed-data transformations
- Improved results
  - Benchmarked on bassi (Power5), franklin (XT4), jacquard (AMD cluster); up to 40 M particles, 1024 processors
  - Up to 10x faster for Poisson, and 2.5x faster for entire code
- Future
  - Closed boundary conditions
  - Multigrid-based Poisson solver

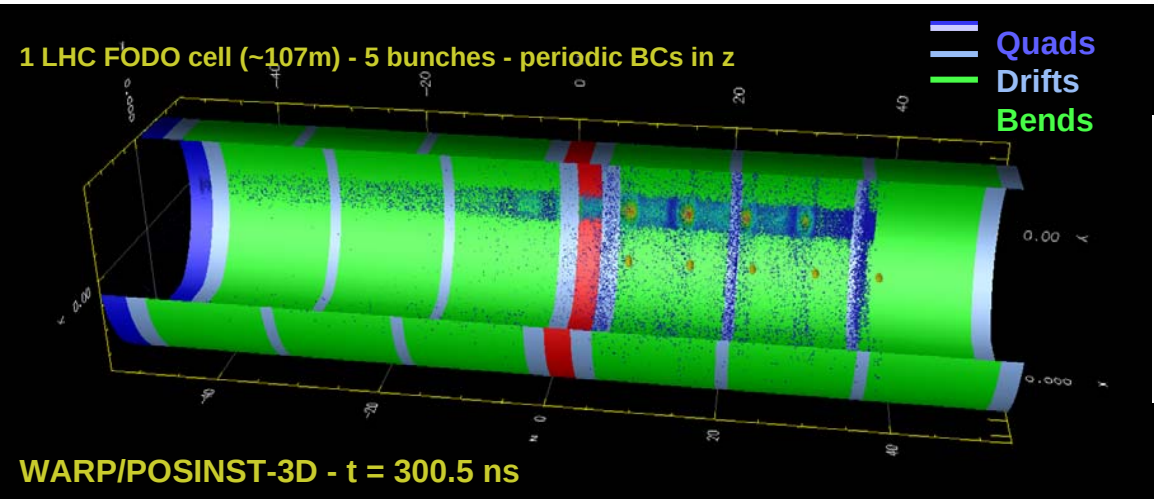
E-cloud modeling using WARP-POSINST

- 3D field dynamics and dynamics
- Fully self-consistent
- Realistic boundary conditions
- Detailed electron generation models (POSINST, including energy spectrum)
- Drift Lorentz electron “mover” (correct space charge w/out resolving cyclic orbit)
- Mesh refinement
- Velocity sub-cycling (small Δt only for particles that need it)
- Parallelized

Electron-Cloud Examples

- **Hybrid WARP/POSINST code yields first 3D self-consistent e-cloud simulations**
- **Applied to**
  - **LHC and and LHC upgrade design**
  - **ILC design**





Above: WARP/POSINST simulation of electron-cloud formation in an ILC wiggler magnet.

Left: WARP/POSINST simulation of electron-cloud formation in LHC

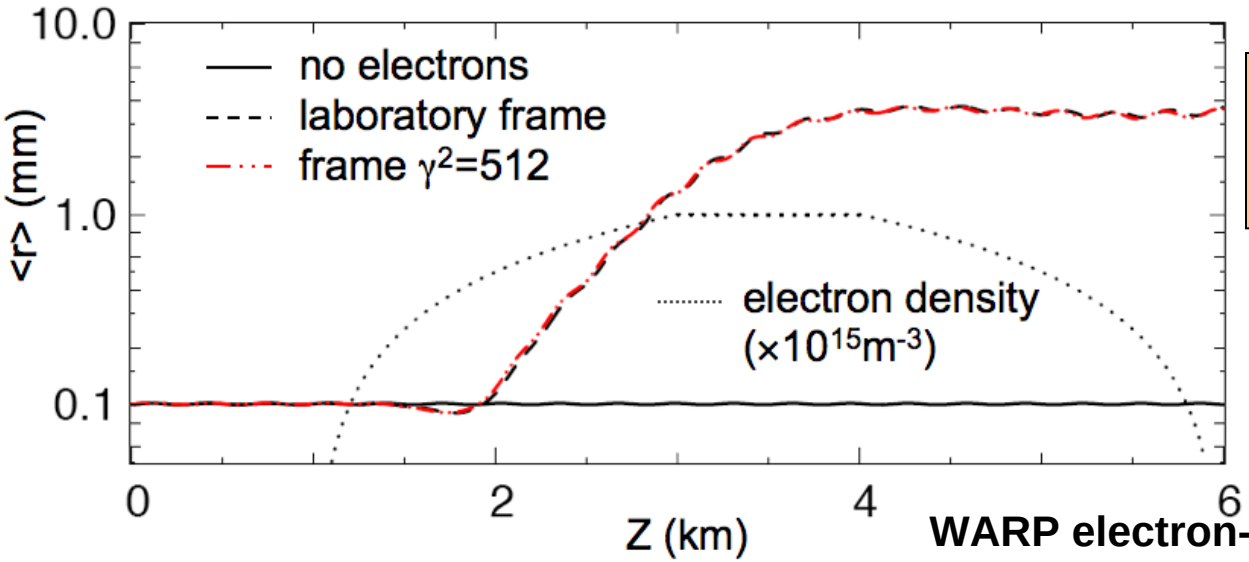
Noninvariance of space- and time-scale ranges under a Lorentz transformation (J.-L. Vay)

Key observation: ***range*** of space and time scales is ***not*** a Lorentz invariant; the ***optimum*** frame to minimize the range is ***not necessarily*** the lab frame

Choosing optimum frame of reference to minimize range can lead to dramatic speed-up for relativistic matter-matter or light-matter interactions.

speedup (PIC in boosted frame vs PIC in lab frame) reported so far:

- x1000 **3-D e-cloud driven beam instability (LBNL),**
- x45,000 **2-D free electron laser toy problem (LBNL),**
- x1,500 **1-D laser-plasma acceleration (Tech-X),**
- x150 **2-D,** x75 **3-D laser-plasma acceleration (UCLA, IST Portugal).**



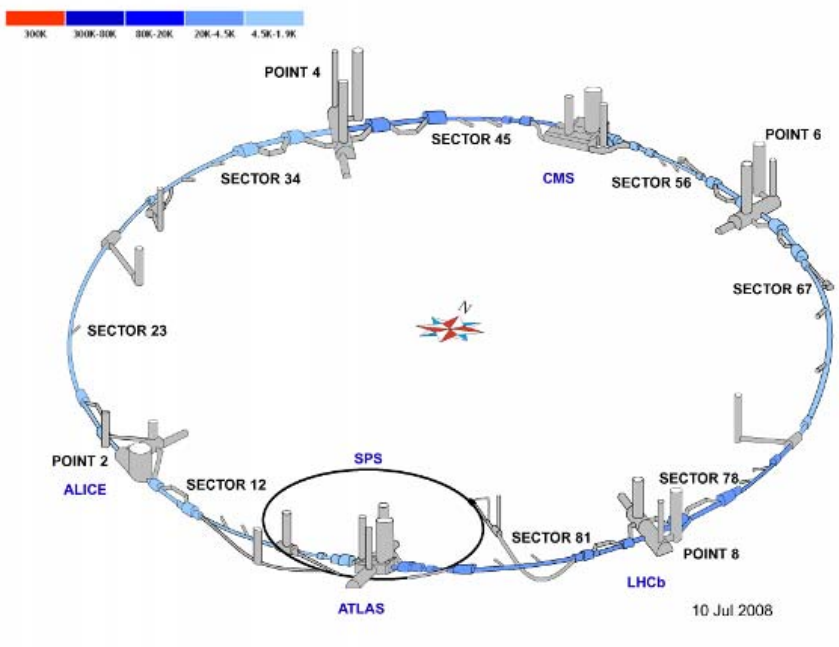
CPU time (8 procs):
- lab frame: >2 weeks
- frame γ^2=512: <30 min

Speedup x1000

WARP electron-cloud instability simulation

LHC application examples

- LHC optimal operation parameters and beam lifetime affected by
  - Beam-beam
  - Electron cloud
- ComPASS applications include simulation of the effects and methods to minimize their impact



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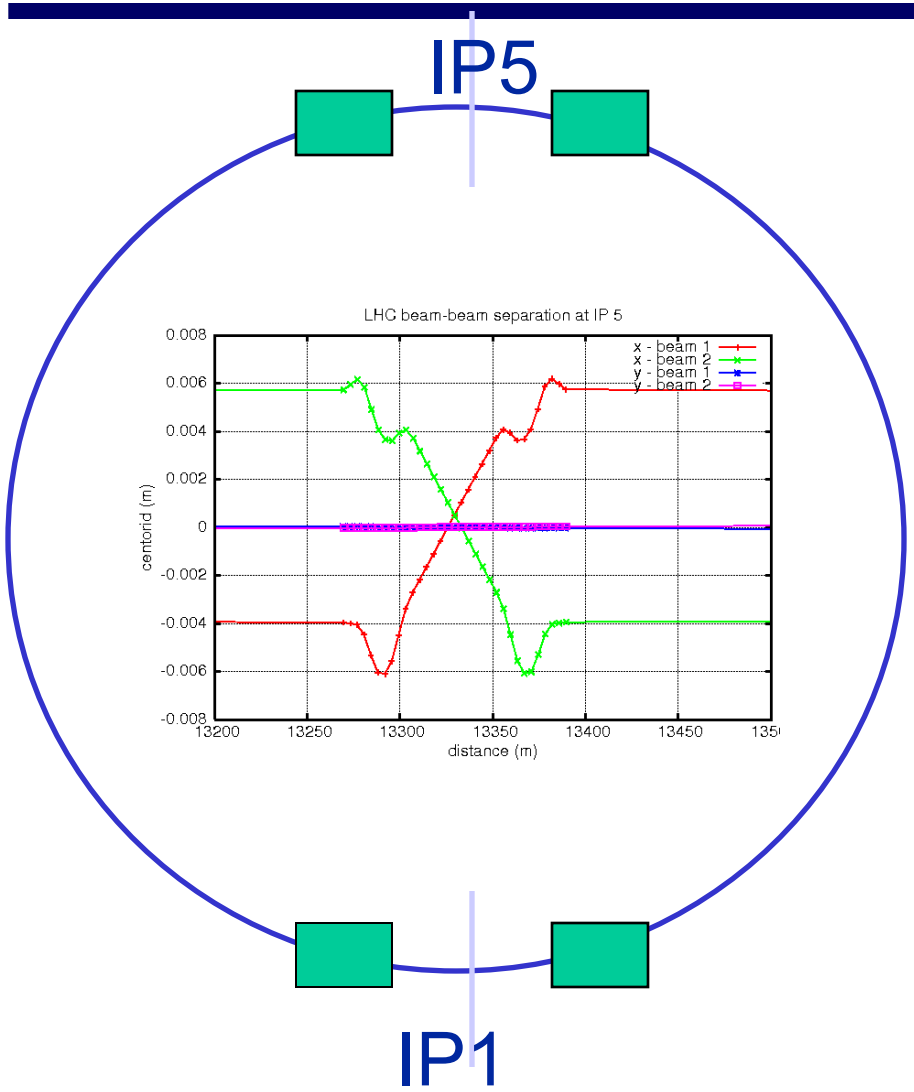
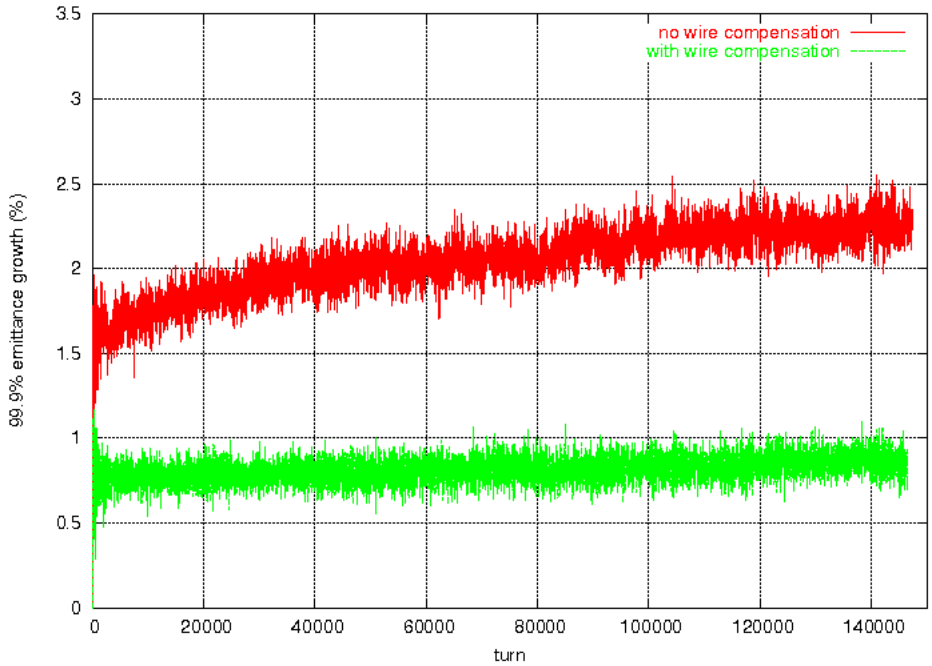
Strong-Strong Beam-Beam Simulation LHC Wire Compensation (2 Head-On + 64 Long Range)





J. Qiang, LBNL

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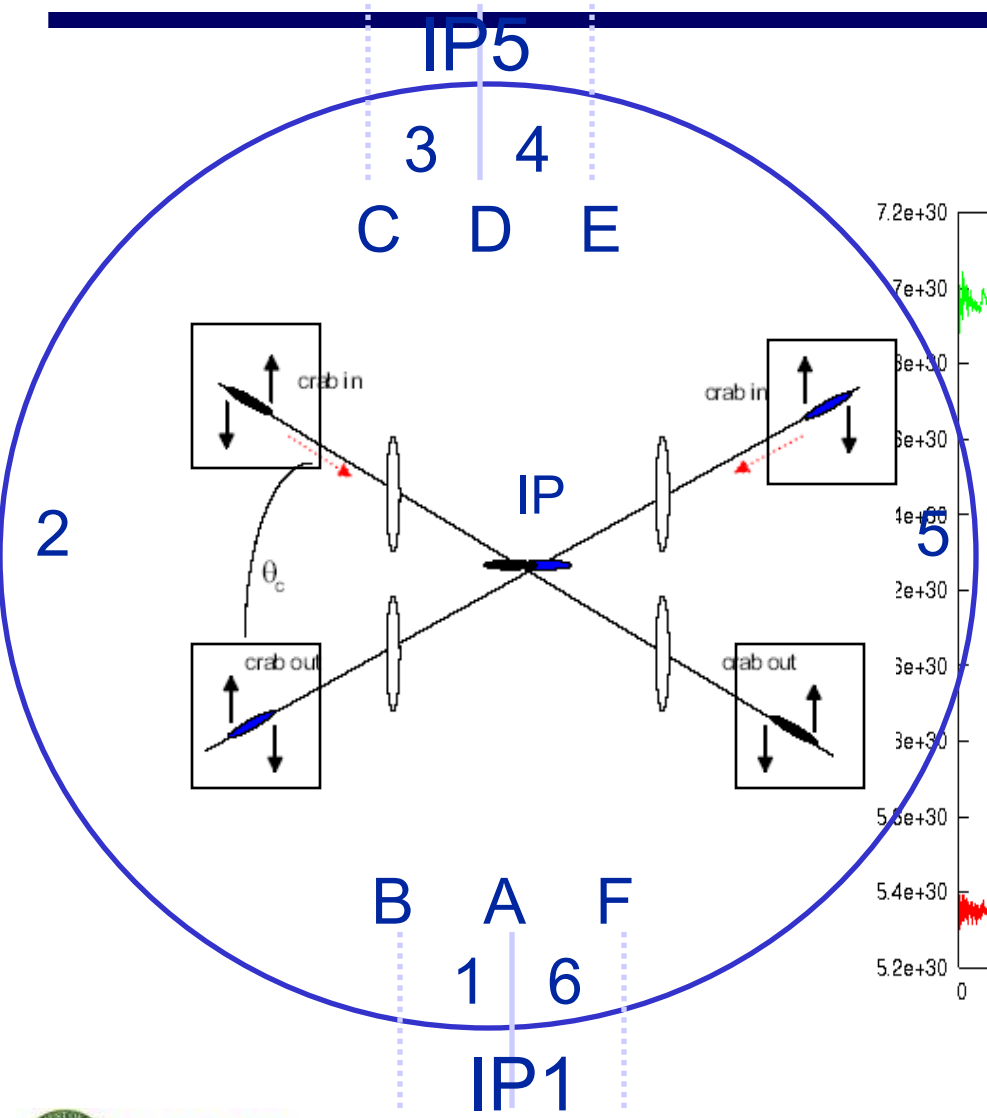
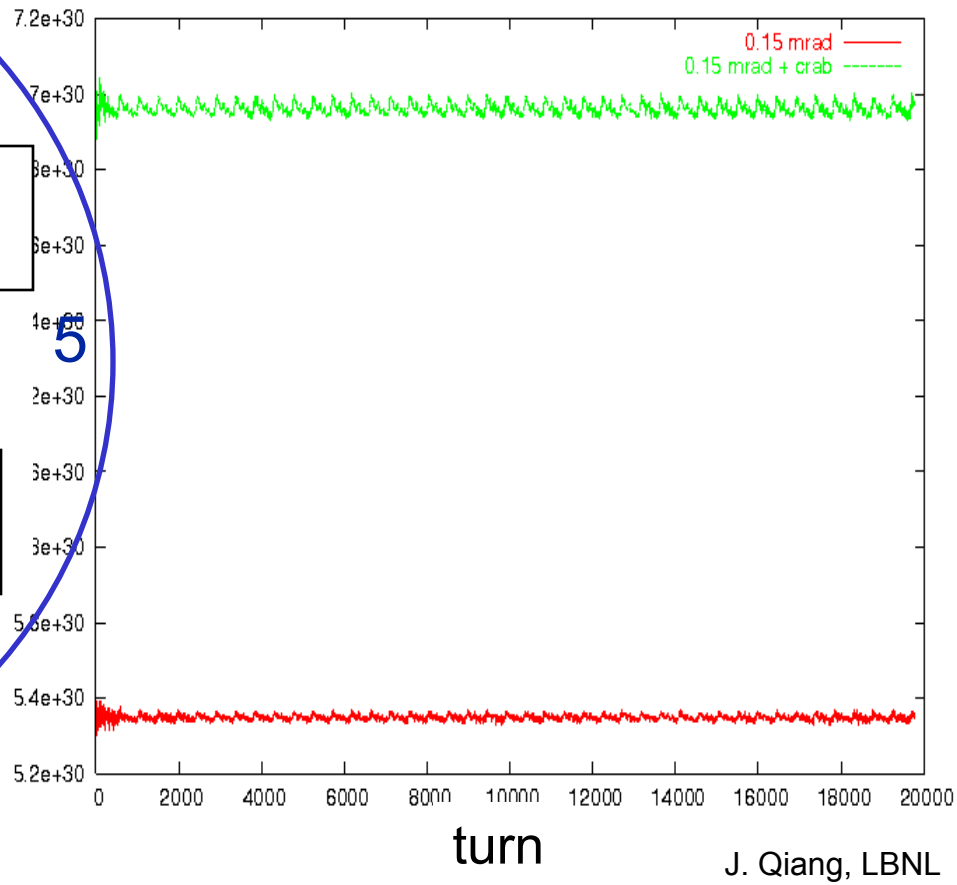
Luminosity Evolution with 0.15 mrad Half Crossing Angle with/without Crab Cavity for LHC Upgrade





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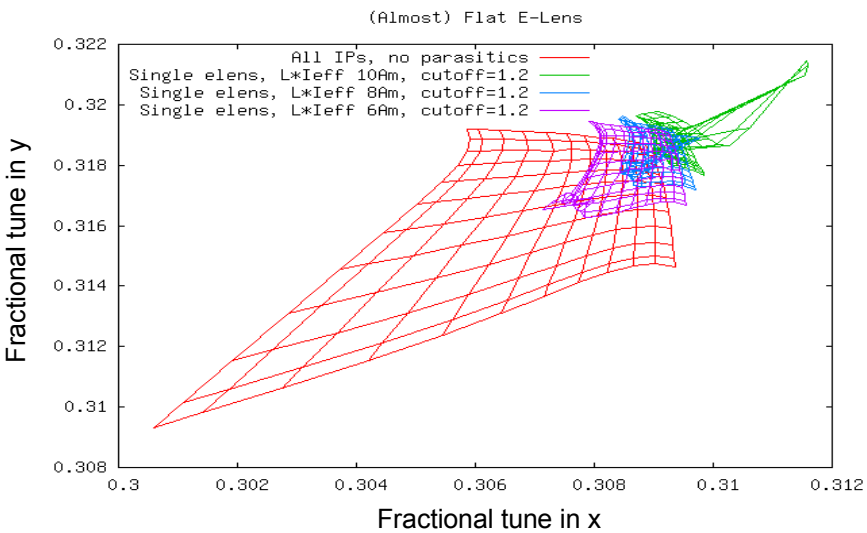
PliBB - Parallel Tracking Framework

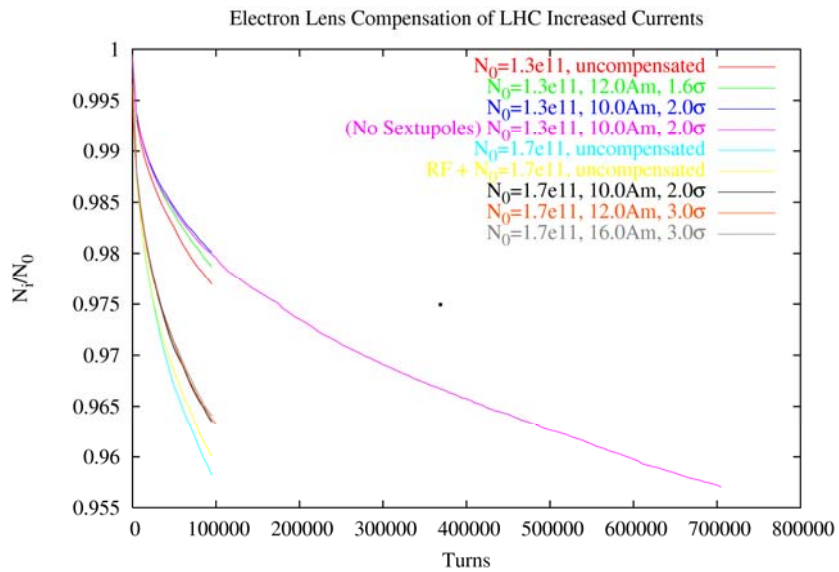
A parallel framework for long-time tracking studies of storage rings:

- **'PliBB'** library for symplectic algebra, magnetic elements, beam-beam
- **LHC studies *(LARP)*:** LHC upgrade scenarios: loss-rate studies show efficacy of electron lens for beam-beam compensation
- **Parallel computation:** LHC: 4 interaction points + all parasitics + non-linear lattice: 10^{10}-10^{11} particles · turns are achievable on NERSC computers

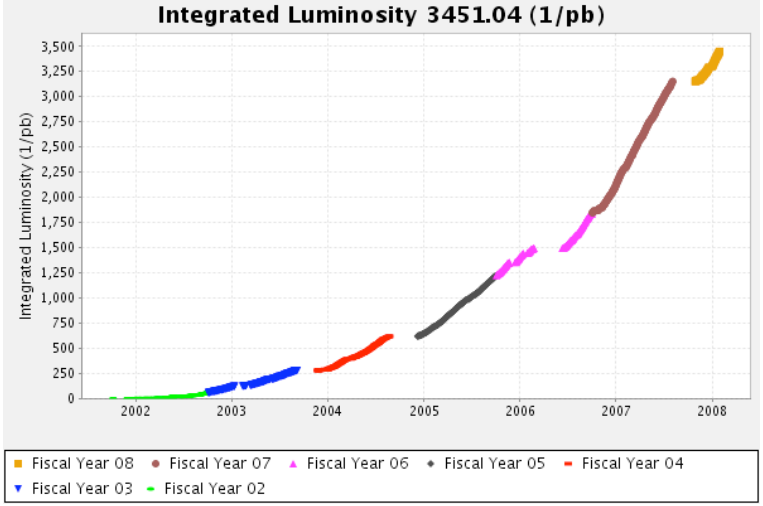
Tune footprint in LHC with electron lens

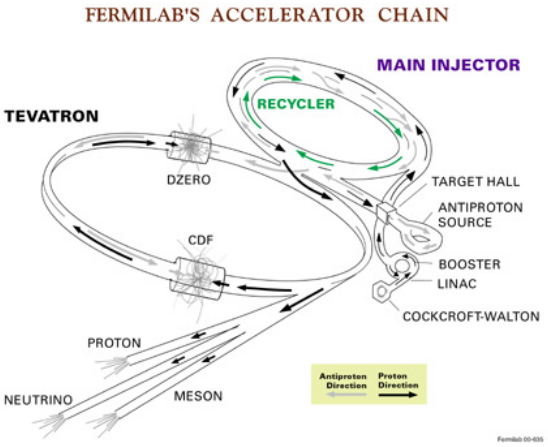


Particle loss rate

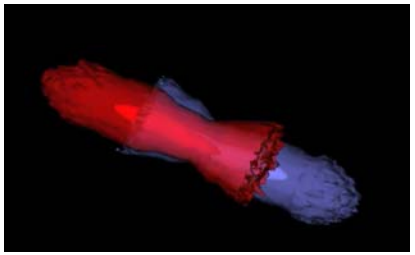


Tevatron Run II application example





- Performance increase due to 5 areas of improvement
  - Antiproton production
  - Proton slip-stacking in MI
  - Recycler electron cooling
  - Improved diagnostics
  - Control of parasitic (long range) collisions



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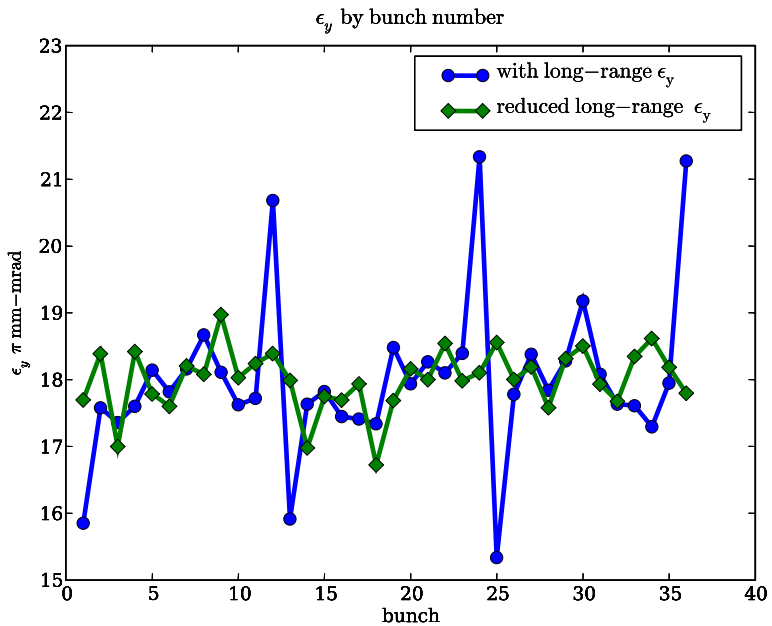
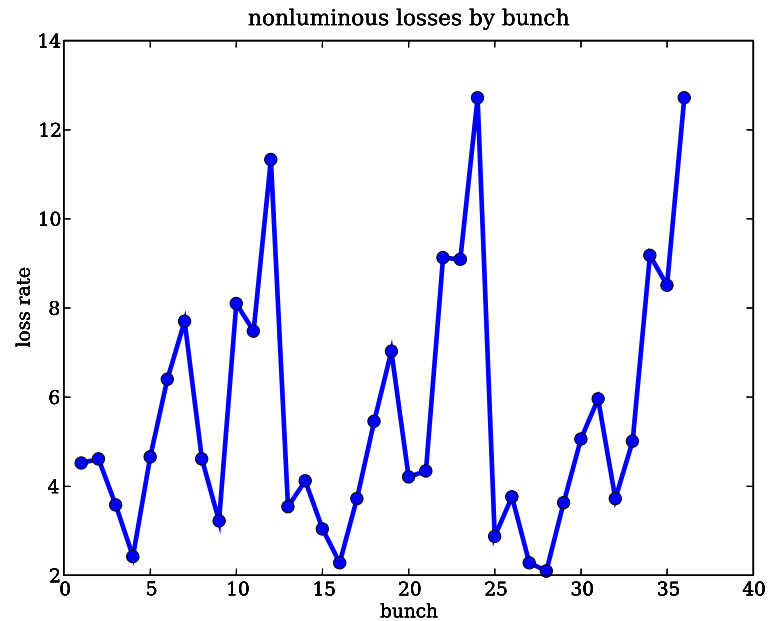
BeamBeam3D Tevatron simulation: 36-on-36 bunch run for 50,000 turns





- Realistic "geometry" (machine lattice) from measurements
- Full simulation (beam-beam & impedance) shows the same bunch to bunch variation of beam "size" (emittance) as the measured loss pattern
  - Simulations utilized Franklin @ NERSC and BG/L @ ANL

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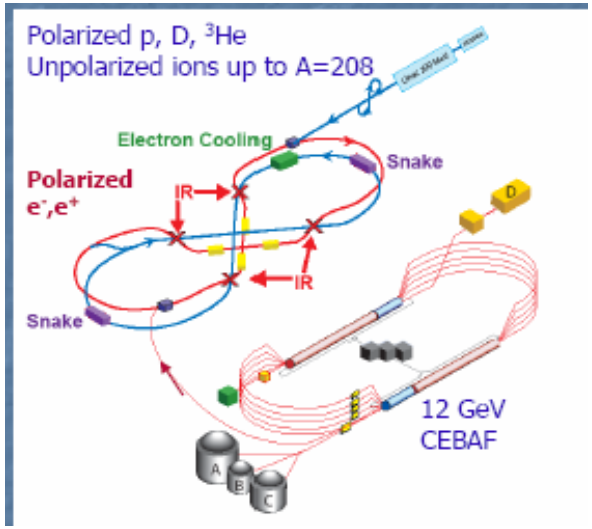
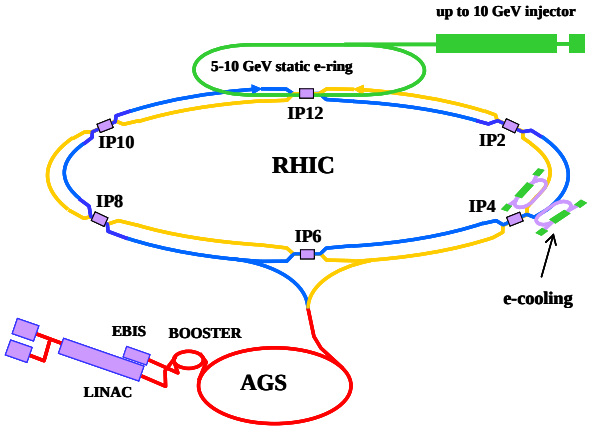
Eric Stern et al., FNAL

ComPASS NP application examples

- Understanding beam-beam effects, and understanding and optimizing electron cooling solutions is important both for operating and future NP accelerators





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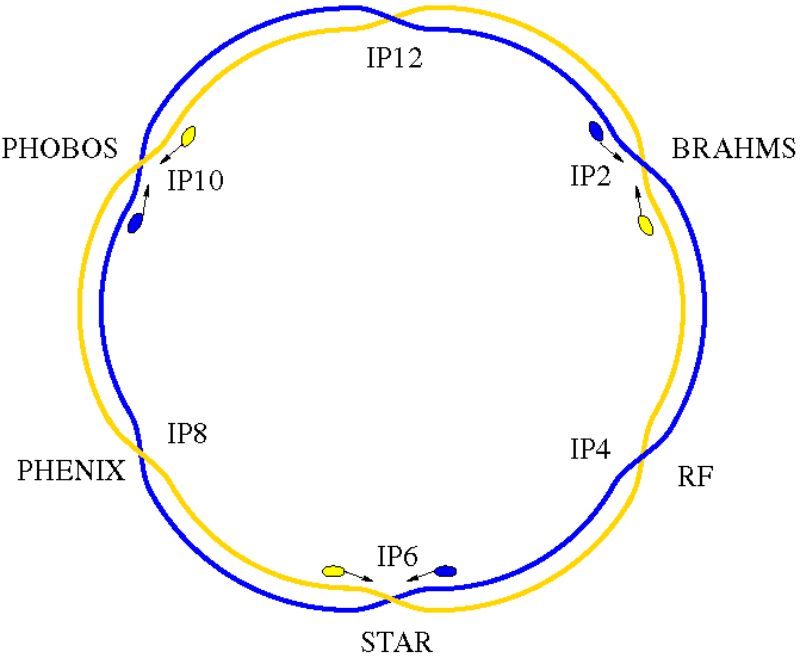
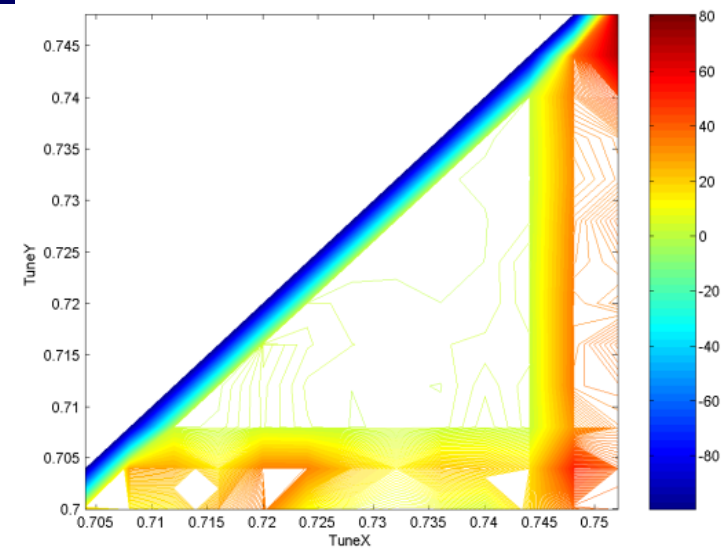
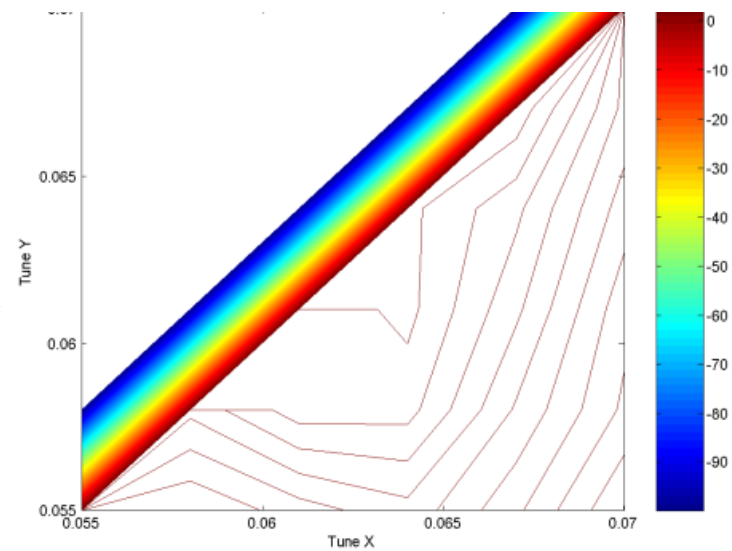
BeamBeam3D applied to RHIC







Emittance growth scan in tune space for a nominal working point (top right) and for a new working point (bottom right) at RHIC from BeamBeam3D simulation

J. Qiang, LBNL, W. Fischer, BNL

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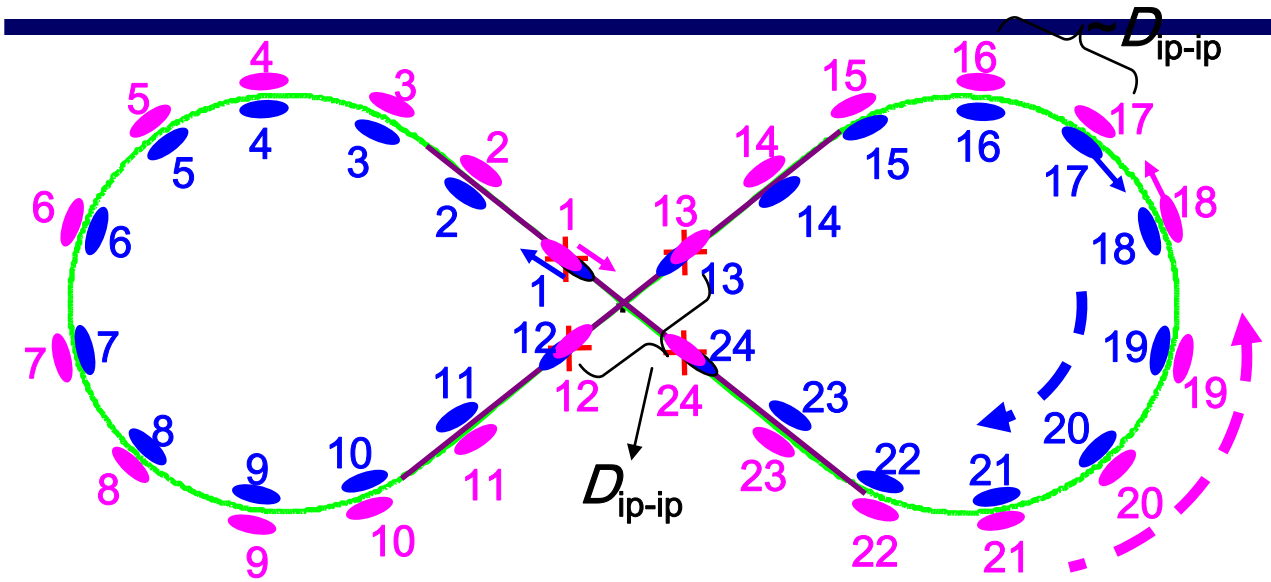
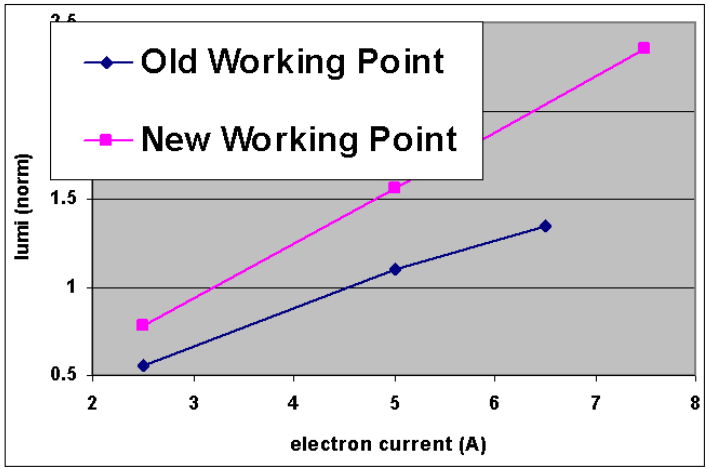
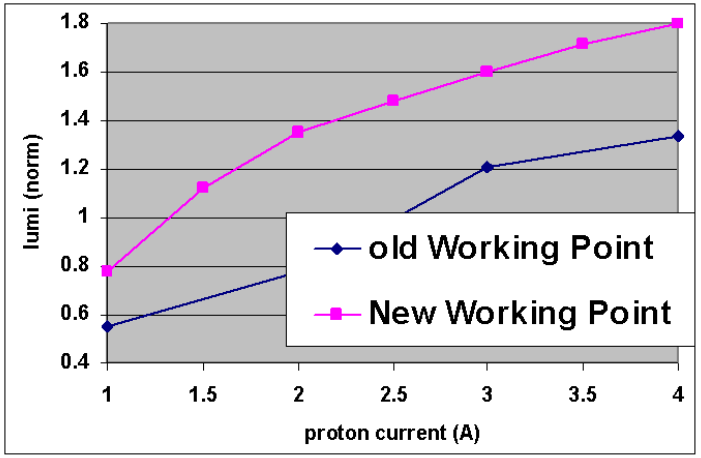
Strong-Strong Multi-Bunch (24) Multi-IP (4) Simulation of ELIC Design using BeamBeam3D



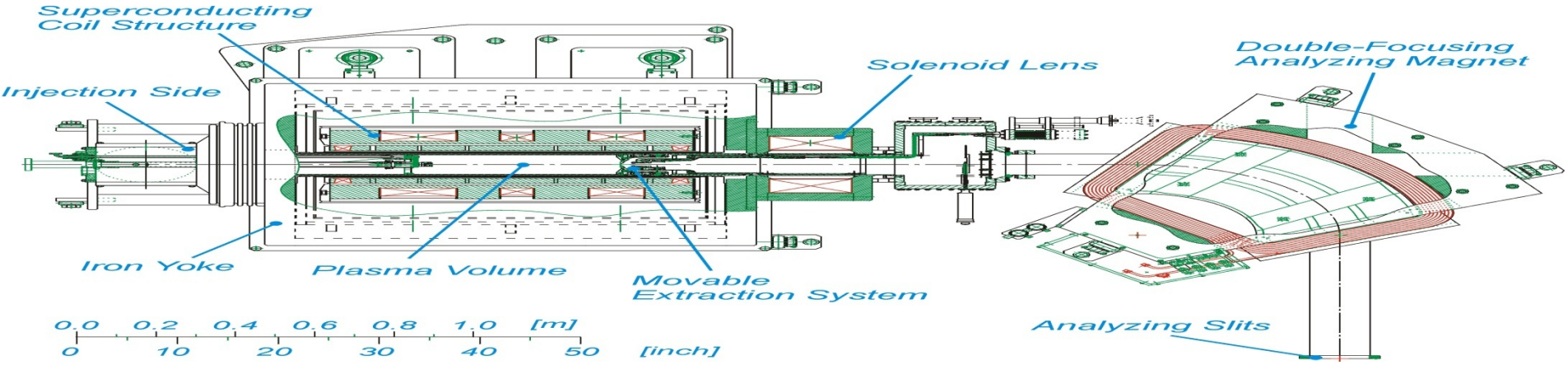
Luminosity as a function of electron (left) and proton (right) current at the JLab proposed ELIC collider from BeamBeam3D simulation.

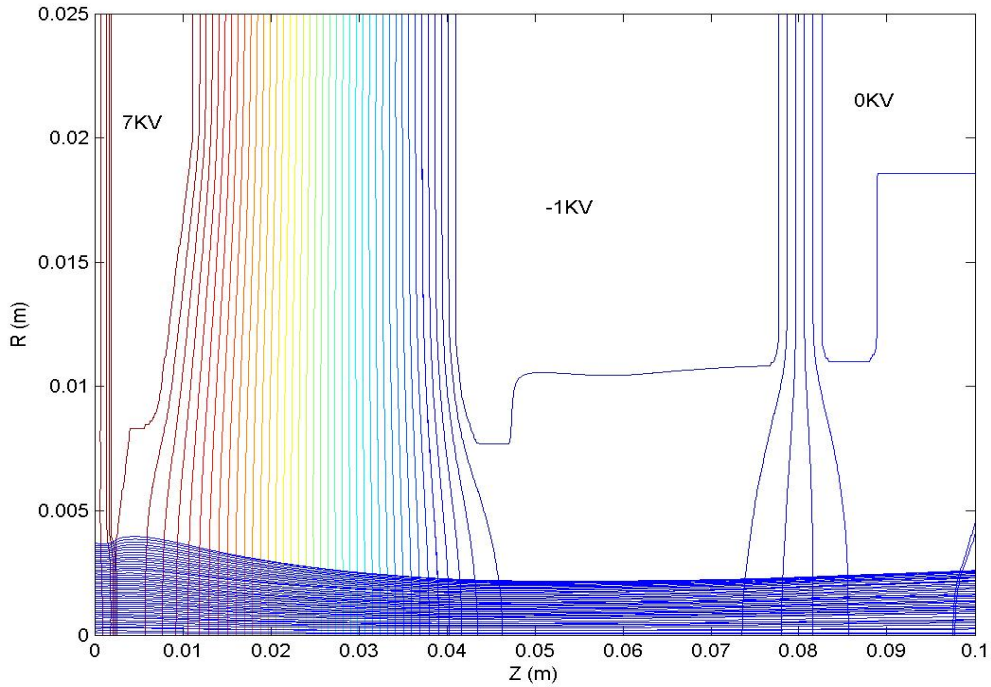




Y. Zhang, JLab, J. Qiang, LBNL

IMPACT Self-Consistent Modeling of H+ Extraction from an ECR Ion Source





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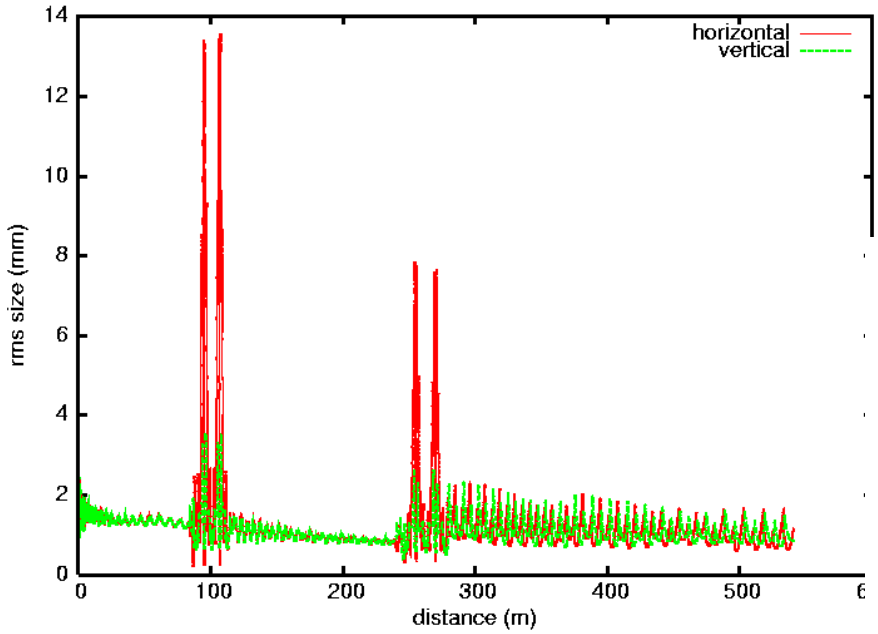
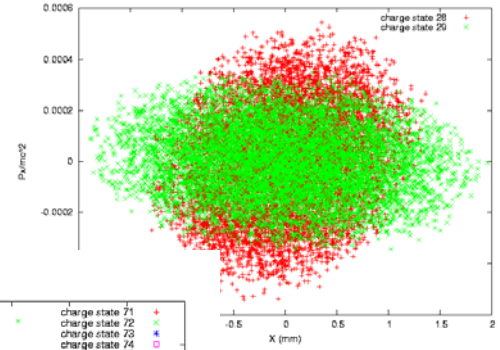
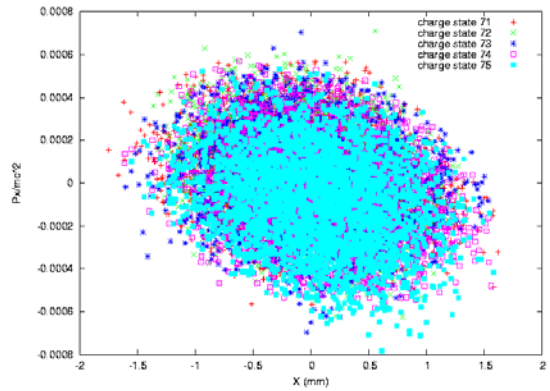
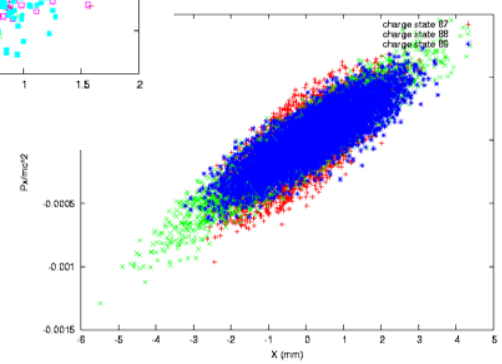
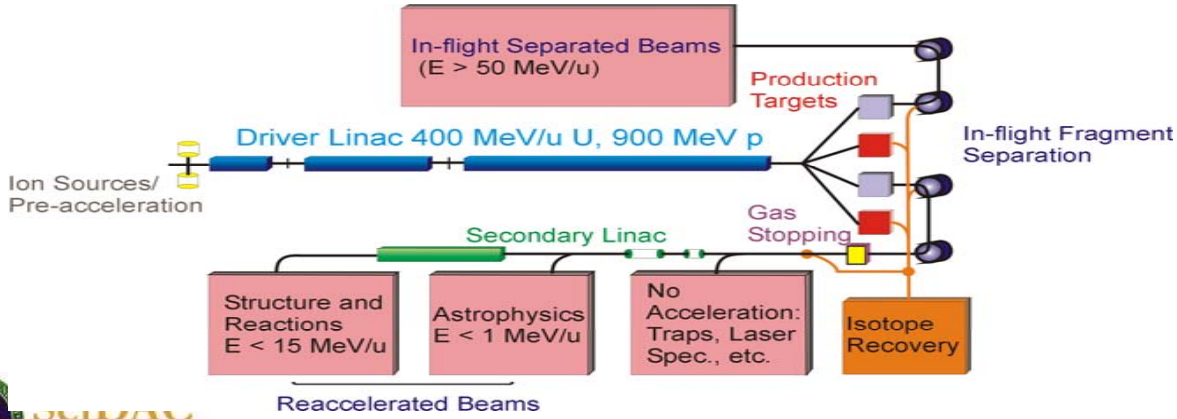
IMPACT-Z multi-charge-state simulation of beam dynamics in proposed MSU RIA linac











J. Qiang, LBNL

SciDAC
Scientific Discovery through Advanced Computing

Physics Motivation for Electron Cooling of Ion Beams

- A future polarized e-/ion collider (EIC) is required to better probe the hadronic structure of matter
  - priority for the international nuclear physics community
  - ion luminosity of order 10^{30}-10^{35} cm^{-2} s^{-1} is required
    - depending on ion, e- vs. e+, degree of polarization, other factors
    - orders of magnitude larger than present state-of-the-art
  - Office of Nuclear Physics has two long-term concepts:
    - eRHIC (add ERL e- accelerator to the RHIC complex)
    - ELIC (add e- and ion rings to Jefferson Lab complex)
- Higher luminosity requires cooling of ion beams
  - electron cooling is included in all present designs
- Some RHIC upgrade scenarios require e- cooling
  - near-term needs are being met by stochastic cooling

SciDAC Scientific Discovery through Advanced Computing

Office of Nuclear Physics Exploring Nuclear Matter - Quarks to Stars

VORPAL

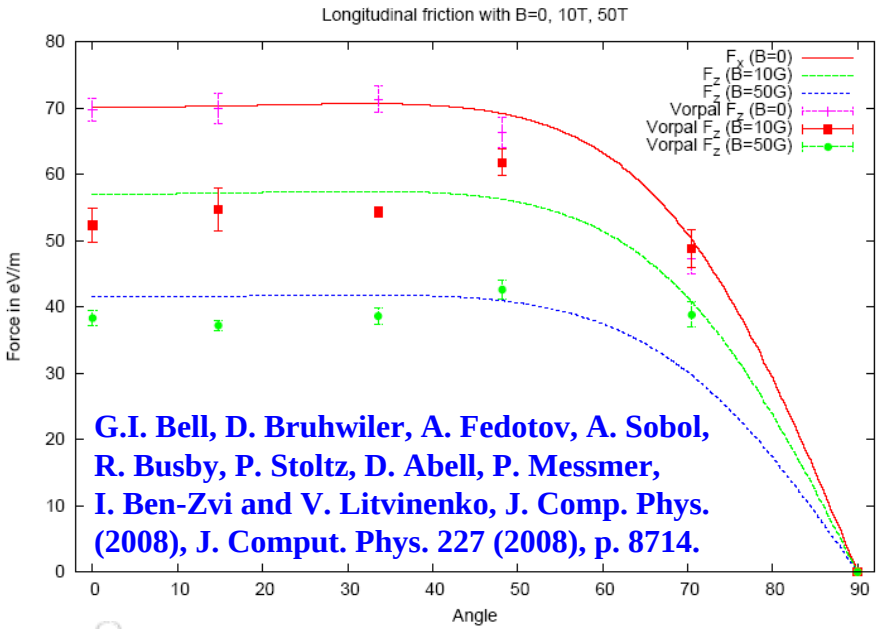
Parallel VORPAL simulations accurately calculate friction force on relativistic Au^{+79} ions in support of electron cooling designs

- Electron cooling of relativistic ion beams is required for high luminosities of electron-ion collider (EIC) concepts
  - in the mid-term, RHIC luminosity could be increased ~10x
    - conventional wiggler could replace expensive solenoid
    - e- "wiggle" motion suppresses recombination with ~10 Gauss
    - provides focusing; reduces risk
    - friction force should be reduced only by $\rho_{min} \rightarrow \rho_w$ in Coulomb log

$$\rho_w = \frac{\Omega_{gyro}}{k_w^2 v_{beam}} \sim 1.4 x 10^{-3} \lambda_w^2 [m] B_w [G] / \gamma$$

      - suggested independently by V. Litvinenko and Ya. Derbenev
      - confirmed via VORPAL simulations

I. Ben-Zvi *et al.*, "Status of the R&D towards electron cooling of RHIC," Part. Accel. Conf. (2007).

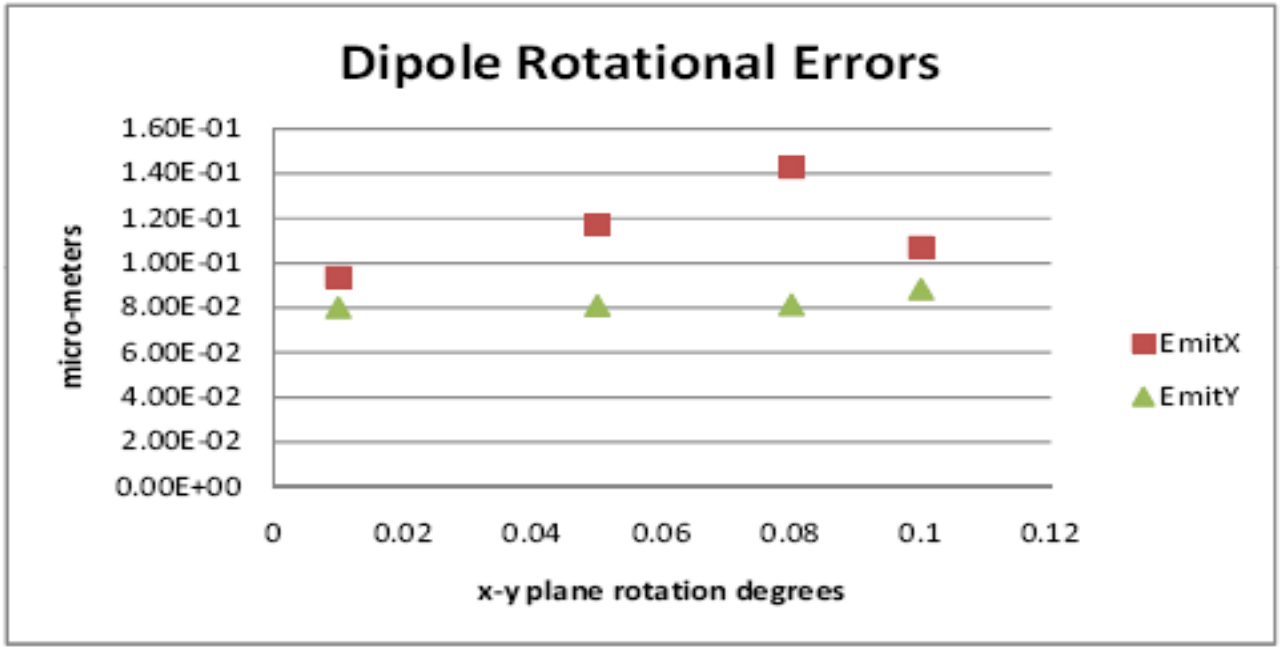


G.I. Bell, D. Bruhwiler, A. Fedotov, A. Sobol, R. Busby, P. Stoltz, D. Abell, P. Messmer, I. Ben-Zvi and V. Litvinenko, J. Comp. Phys. (2008), J. Comput. Phys. 227 (2008), p. 8714.

ML/I application to RHIC e-cooling

- **ML/I has been used to study beam transport through the e-cooling linac including the impact of misalignments on emittance.**

- **Results indicate sensitivity primarily to bend magnet misalignments. In all these cases emittance growth was kept well within tolerances at the level of 0.6 mm displacements or 0.1 degree planar rotations.**



Emittance response to x-y plane rotational misalignments of dipole magnets (D. Abell,V. Ranjbar, Tech-X; J. Jensen, BNL)

SciDAC
Scientific Discovery through Advanced Computing

Parallel VORPAL simulations of a coherent electron cooling (CEC) modulator are underway

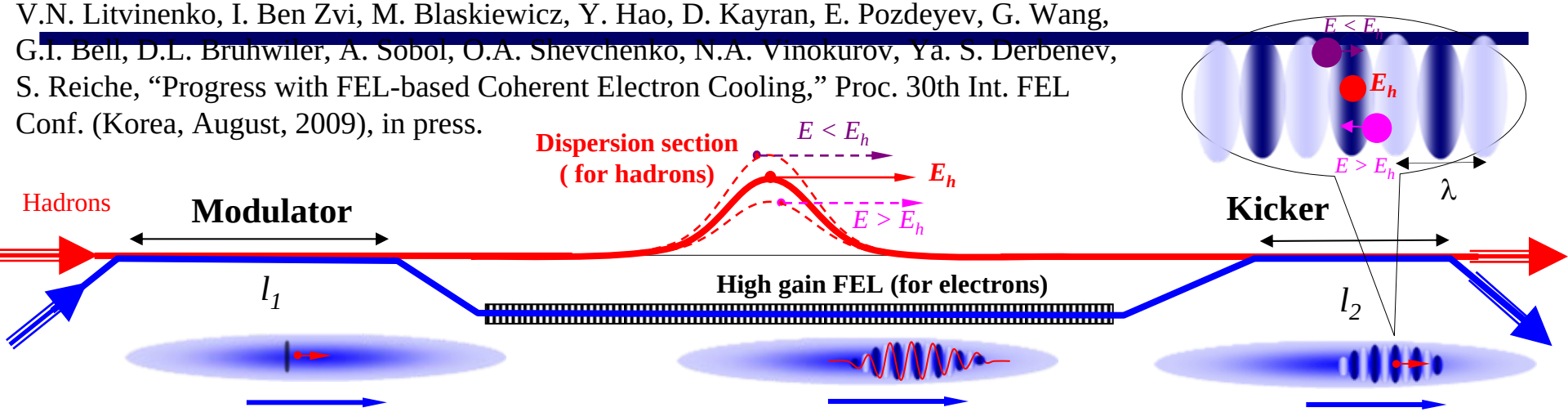
- Coherent Electron Cooling concept
  - uses FEL to combine electron & stochastic cooling concepts

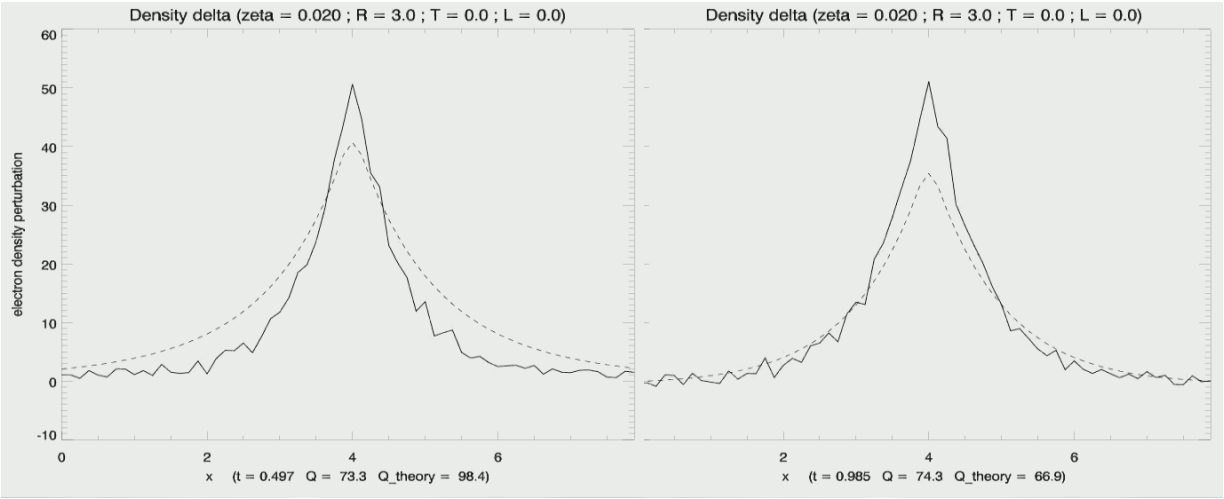
    Litvinenko & Derbenev, "Free Electron Lasers and High-Energy Electron Cooling," FEL'07 Proc.

    Litvinenko *et al*., "Progress with FEL-based Coherent Electron Cooling," FEL'08 Proc., in press.
  - a CEC system has three major subsystems
    - **modulator**: the ions imprint a "density bump" on e- distribution
    - **amplifier**: FEL interaction amplifes density bump by orders of magnitude
    - **kicker**: the amplified & phase-shifted e- charge distribution is used to correct the velocity offset of the ions
  - standard electron cooling should work well for RHIC II,
  - but CEC could be orders of magnitude better:
    - stronger interaction implies shorter cooling times
    - effectiveness does not scale strongly with ion beam energy
      - could even be relevant to the LHC
  - modulator is being simulated with VORPAL

Schematic of the CEC concept

V.N. Litvinenko, I. Ben Zvi, M. Blaskiewicz, Y. Hao, D. Kayran, E. Pozdeyev, G. Wang, G.I. Bell, D.L. Bruhwiler, A. Sobol, O.A. Shevchenko, N.A. Vinokurov, Ya. S. Derbenev, S. Reiche, "Progress with FEL-based Coherent Electron Cooling," Proc. 30th Int. FEL Conf. (Korea, August, 2009), in press.

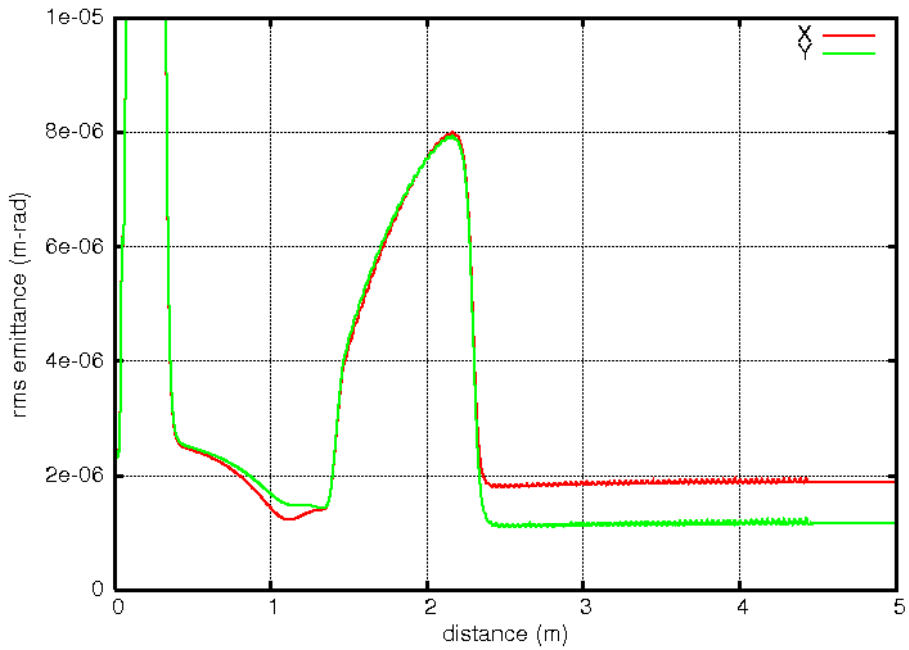




VORPAL simulations (electrostatic PIC) of the modulator, for a single ion in a semi-infinite e- beam, show e- density enhancement consistent with theory of Wang & Blaskiewicz, Phys. Rev. E. (2008); shot noise is suppressed; boundary conditions require careful treatment.

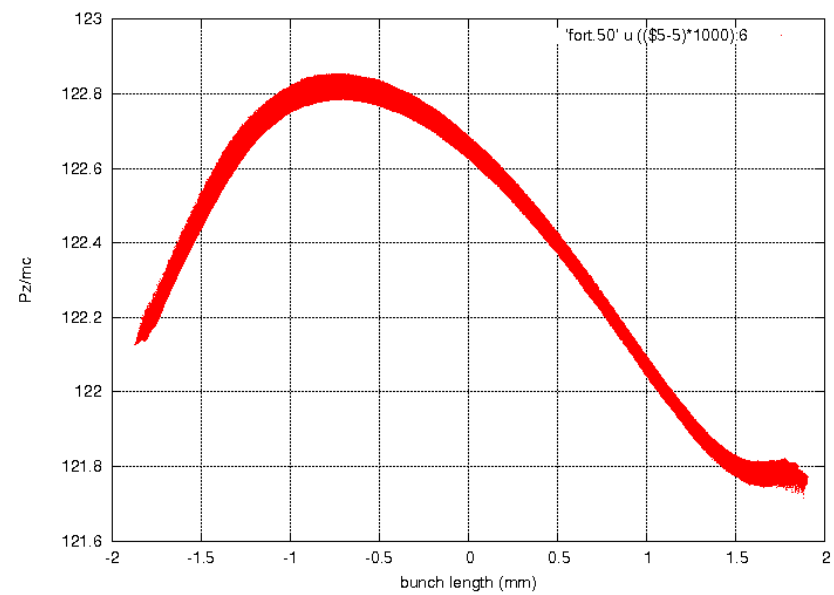
BROOKHAVEN NATIONAL LABORATORY · TECH-X · Jefferson Lab · Particle Beam Physics Laboratory

IMPACT-T Simulation of LCLS Photoinjector



Transverse emittance evolution at LCLS photoinjector with initial 0.5 mm offset

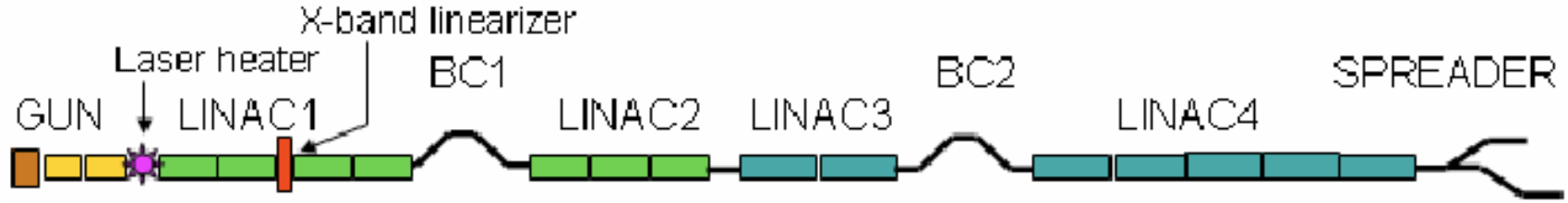
Longitudinal phase space at the end of photoinjector



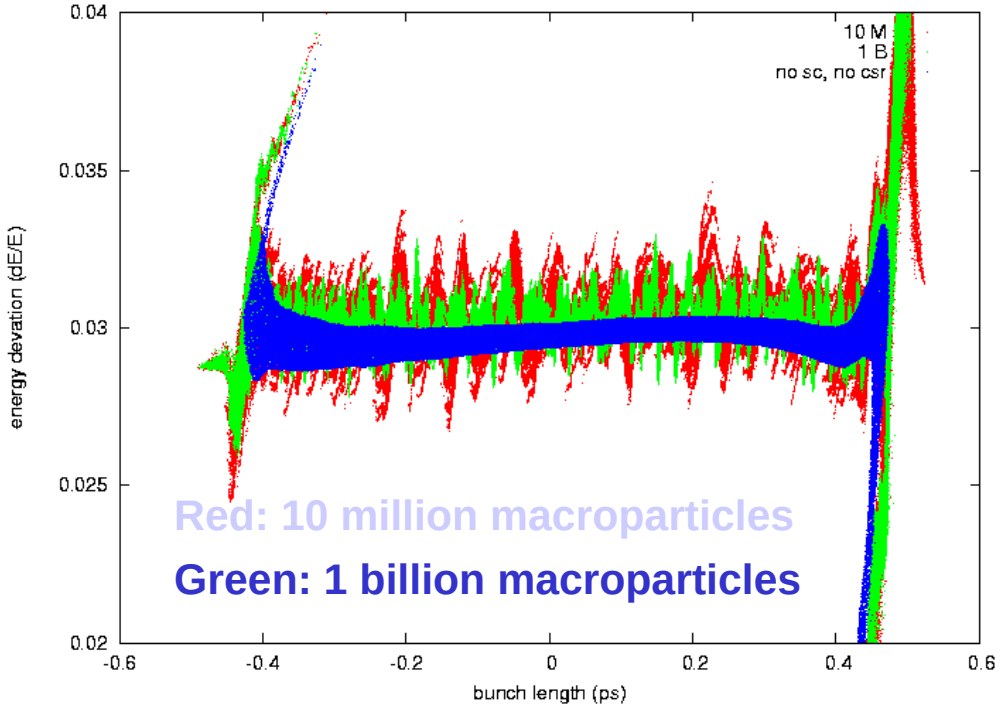
J. Qiang, LBNL, C. Limbourg, SLAC

SciDAC
Scientific Discovery through Advanced Computing

Application example: large scale modeling of the microbunching instability for light source design

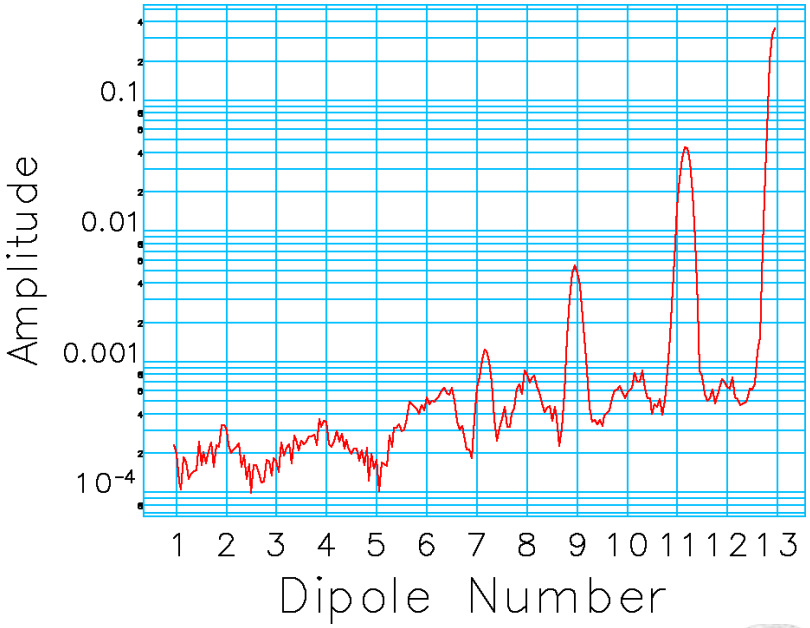


IMPACT-Z simulation showing final longitudinal phase space using 10M and 1B macroparticles



J. Qiang, LBNL

Simulation of microbunching instability with ELEGANT code



M. Borland, ANL

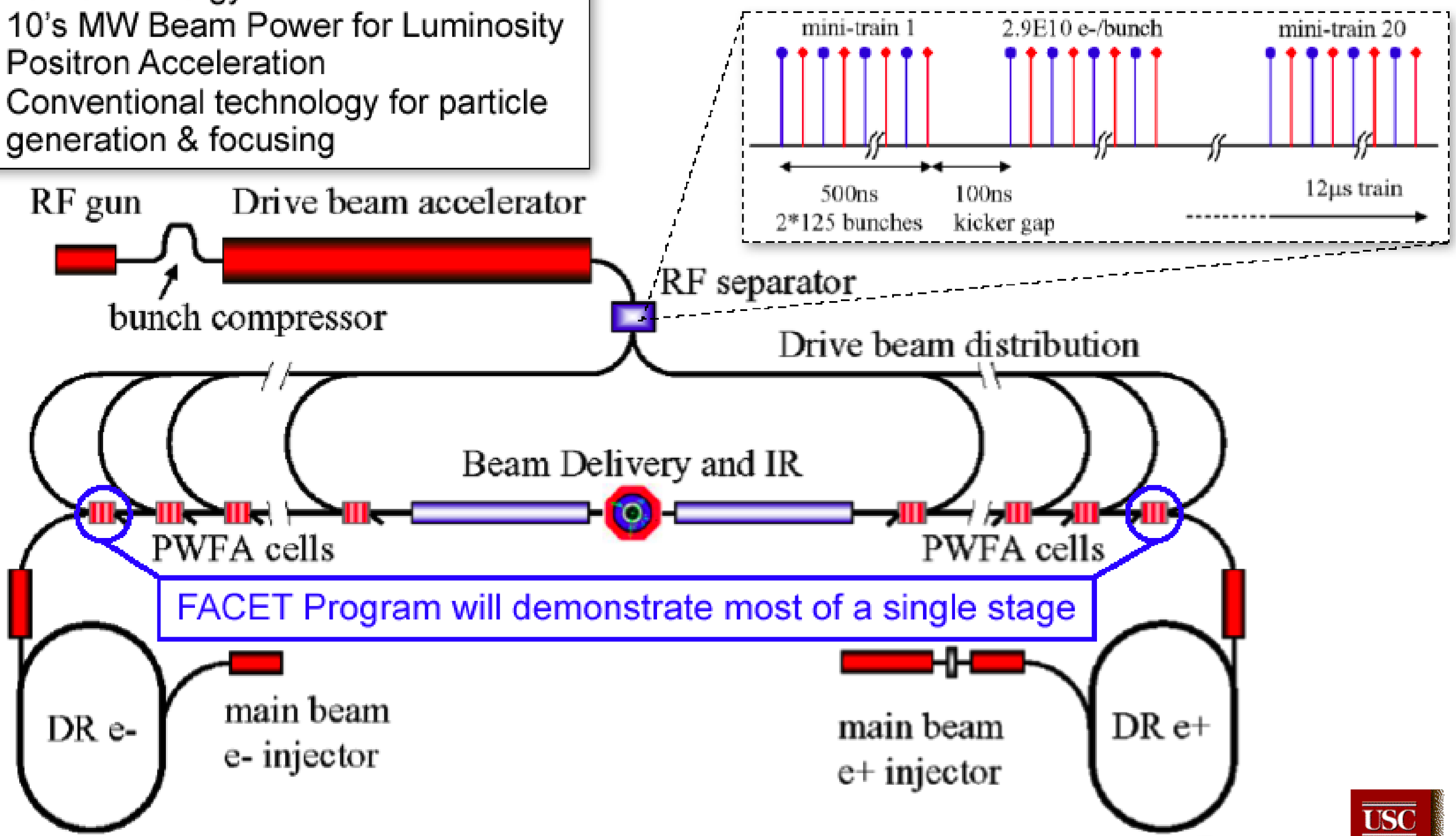
SciDAC
Scientific Discovery through Advanced Computing

Goals and vision for enabling advanced accelerator modeling under SciDAC

- Help in designing linear colliders based on staging PWFA or LWFA stages
  - Develop integrated codes for modeling a staged wakefield "system".
  - Develop high fidelity modeling for optimizing a single LWFA or PWFA stage.
  - Enable routine modeling of experiments:
    - Bella
    - FACET
    - Real time steering of experiments?
    - Code validation against numerous worldwide experiments
  - Code Verification

A Concept for a Plasma Wakefield Accelerator Based Linear Collider

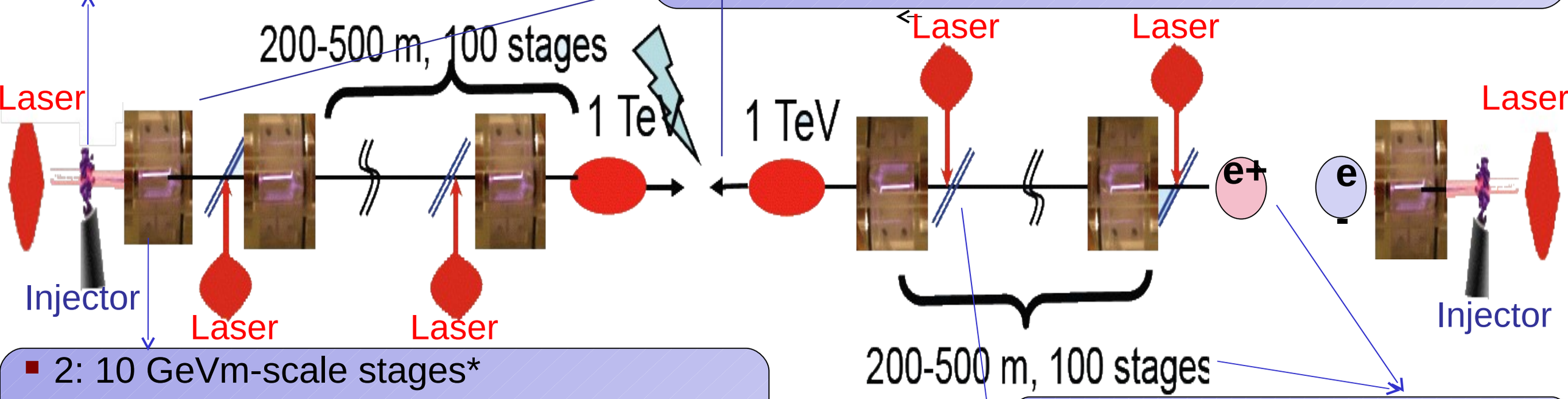
- TeV CM Energy
- 10's MW Beam Power for Luminosity
- Positron Acceleration
- Conventional technology for particle generation & focusing



Simulating a laser - plasma collider

- 1: Low emittance injector*
  - Envelope – Downramp
  - Explicit – Ramp or Colliding

- 5: Bunch emittance
  - Accurate momentum advance (weighting, mesh refinement, high order models)
  - Noise control(fluids, EM dispersion,Cerenkov)



- 2: 10 GeVm-scale stages*
  - Fast reduced models (Envelope, Quasistatic, Lorentz boosted)
  - EM dispersion (laser v_{group})
  - Error accumulation control
  - Scaling
  - Hydro sim. of capilaries, jets

- 4: Scattering and radiation

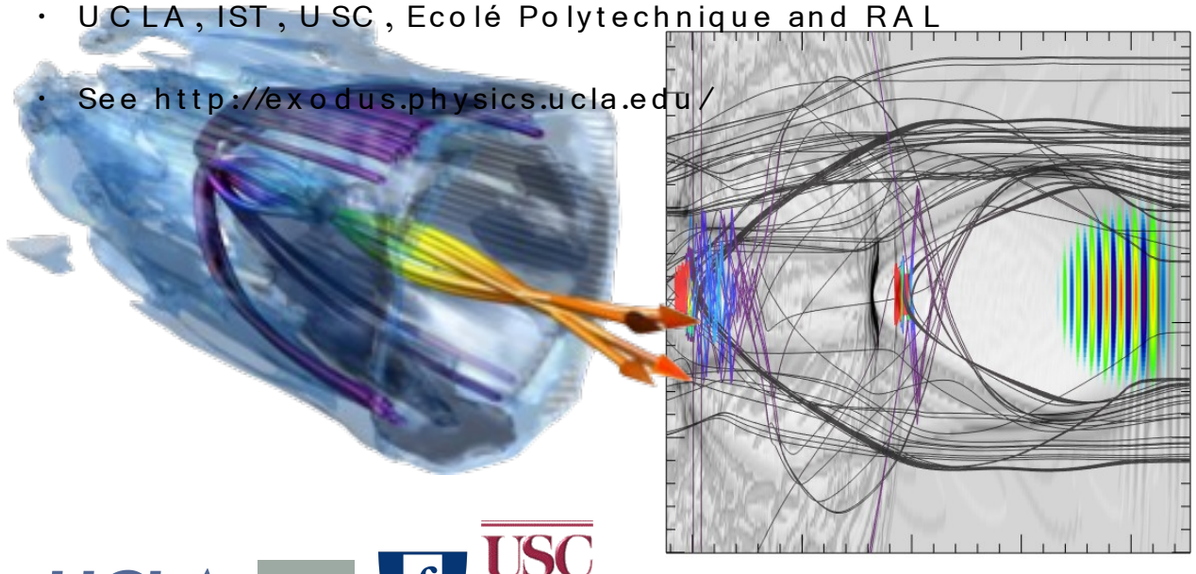
- 3: Staging*
  - Beam propagation
  - Plasma mirrors - explicit

*BELLA

Massively parallel PIC codes for large scale modeling

OSIRIS

* Fully Relativistic Electromagnetic PIC code
- Massively Parallel (scales well up to > 4096 cpus)
- Dynamic Load Balancing, Higher order particle shapes, Open EM boundary conditions, Ionization, Binary Collision Module, Parallel I/O
- Examples of applications
- Mangles et al., Nature 431 529 (2004).
- Tsung et al., Phys. Rev. Lett., 94 185002 (2004)
- Lu et al., Phys. Rev. ST: AB, 10, 061301 (2007)
- **Development institutions**
- UCLA, IST, USC, Ecolé Polytechnique and RAL
- See http://exodus.physics.ucla.edu/



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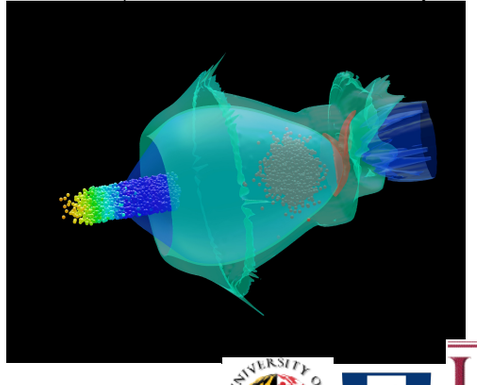
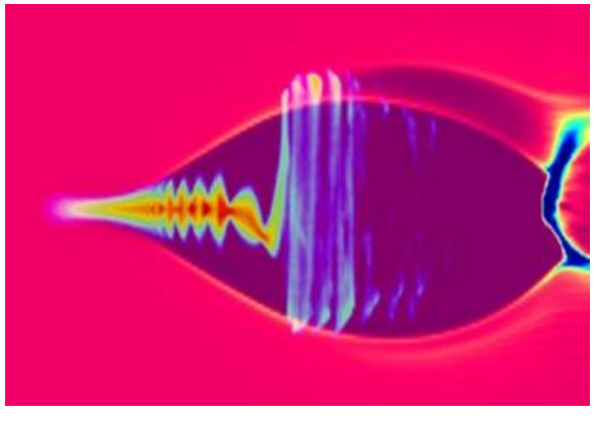
QuickPIC

* Quasistatic PIC + Ponderomotive guiding center + envelope model
- Can be 100+ times faster than conventional PIC with no loss in accuracy
- Scales to 1000's of processors
- Examples of applications
- Simulations for PWFA experiments, E157/162/164/164X/167 (Including Feb. 2007 Nature)
- Study of electron cloud effect in LHC.
- Plasma afterburner design up to TeV
- Beam loading study using laser/beam drivers
- **Development institutions**
- UCLA, IST and U. Maryland





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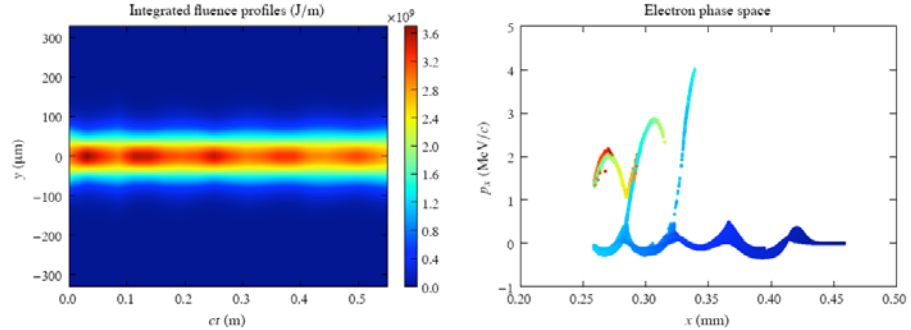
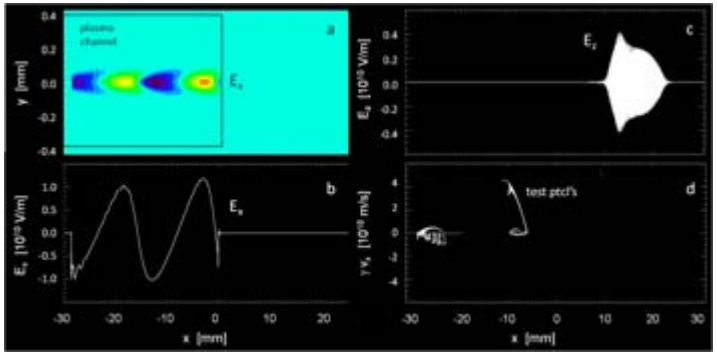
Designing TeV-scale LWFA concepts requires massively parallel PIC & more

- VORPAL computational framework —
- Massively parallel electromagnetic PIC
  - Geddes *et al*, PRL **100**, 215004 (2008).
  - Nemeth *et al*., PRL **100**, 095002 (2008)
  - Bruhwiler *et al., J. Phys.: Conf. Series* ***46****, 215 (2006).*
  - Cary *et al*., Phys. Plasmas **12**, 056704 (2005).
  - Geddes *et al.,* Nature **431**, 538 (2004).
- Reduced models needed for m-scale ~10 GeV stages
  - Laser envelope model; ~100x speedup in 1D, 2D, 3D
    - also called "ponderomotive guiding center" (PGC) PIC
    - more accurate wake fields, laser group velocity than full PIC
    - Messmer & Bruhwiler, PRSTAB **9**, 031302 (2006).
    - Cowan *et al*, AAC Proceedings (2008), in press.
  - Lorentz boosted simulations in 1,2D
    - 10 GeV test case agrees with scaled PIC; >2,000x speedup
    - Bruhwiler *et al*, AAC Proceedings (2008), in press.
  - Cold, relativistic fluid model (and hybrid fluid-PIC)
    - Bruhwiler *et al*, AAC Proceedings (2008), in press.
- VORPAL has yet more capabilities relevant to SciDAC (EM, EC)

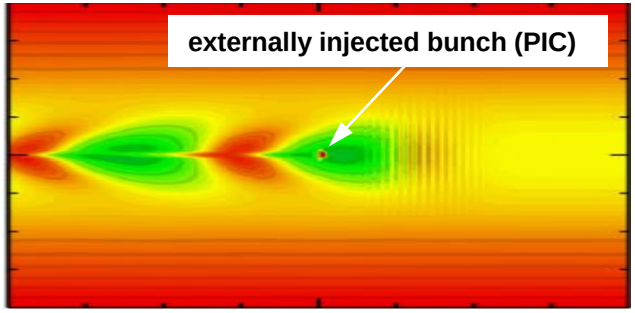


Laser envelope model; downramp injection & acceleration



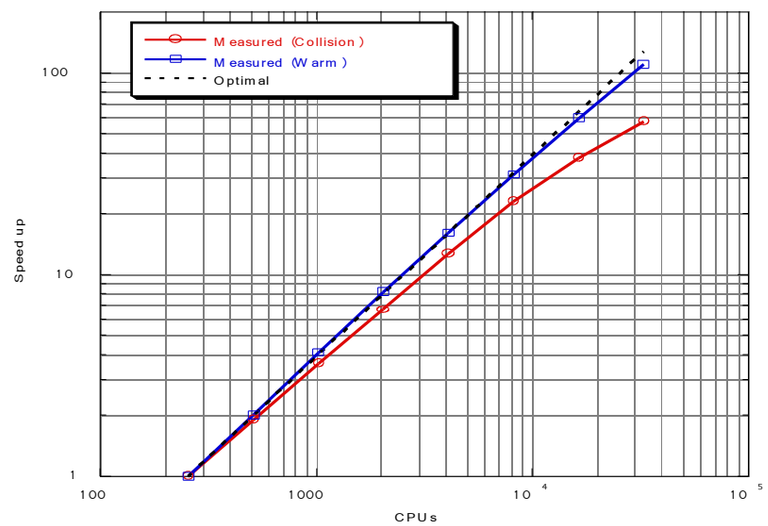
Explicit PIC in boosted frame; >2,000x speedup

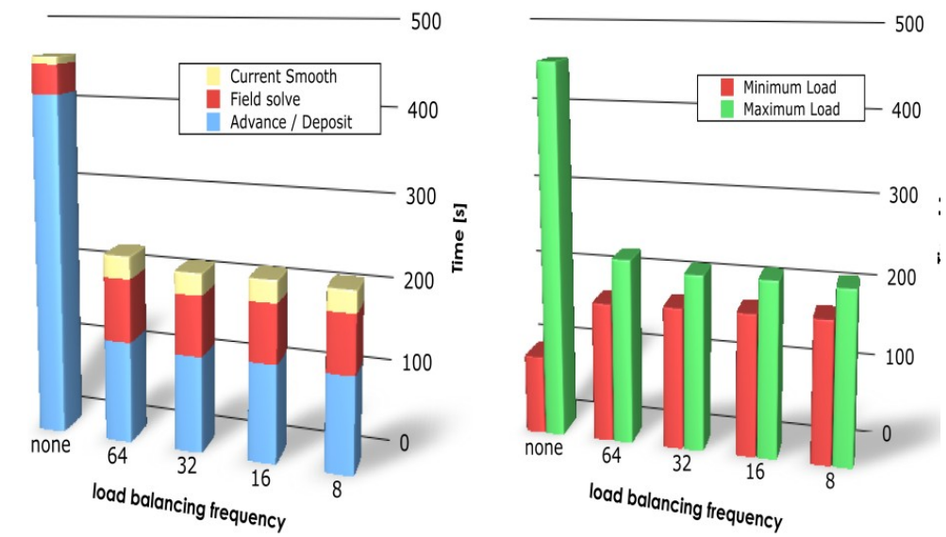
- Future simulation needs
  - improve boosted-frame & laser envelope modes
  - beam propagation between stages
  - laser-plasma modeling of liquid mirrors
  - hydrodynamic evolution of capillary discharge plasma channels
  - mesh refinement, improved load balancing, perfect dispersion
  - Coulomb scattering, radiation, positron production
  - code coupling



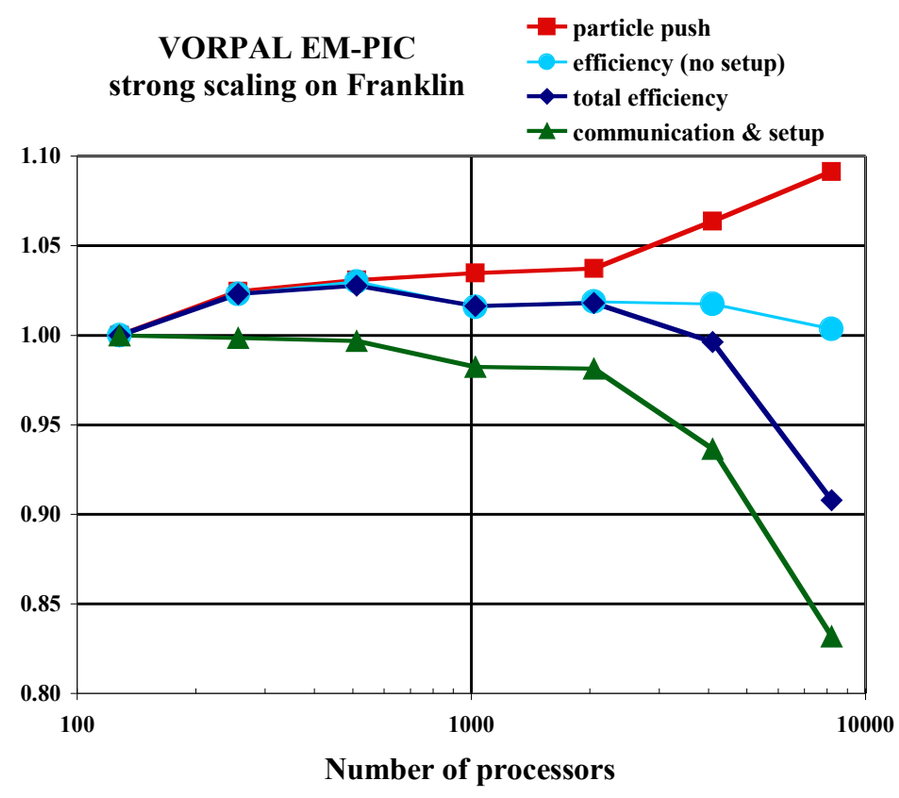
Hybrid fluid-PIC; no particle noise in plasma

SciDAC codes scale well on a variety of platforms





SIRIS is shown on up to 32,768 processors on the
sults when the particle push and field solve are



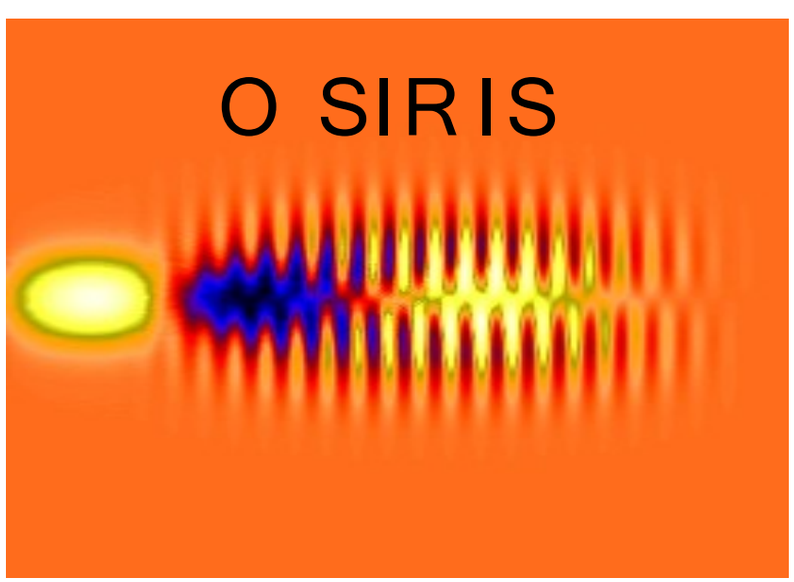
* thermal plasma plus relativistic beam; electromagnetic PIC
  – 512 x 256 x 512 = 67 x 10^6 cells; ~1x10^9 particles
* efficiency ~100% out to 8,192 proc's, for long simulations
  – particle push (dominates run time) speeds up by 10%
  – approx. balanced by communication overhead
  – for >4,096 proc's, set up time becomes significant

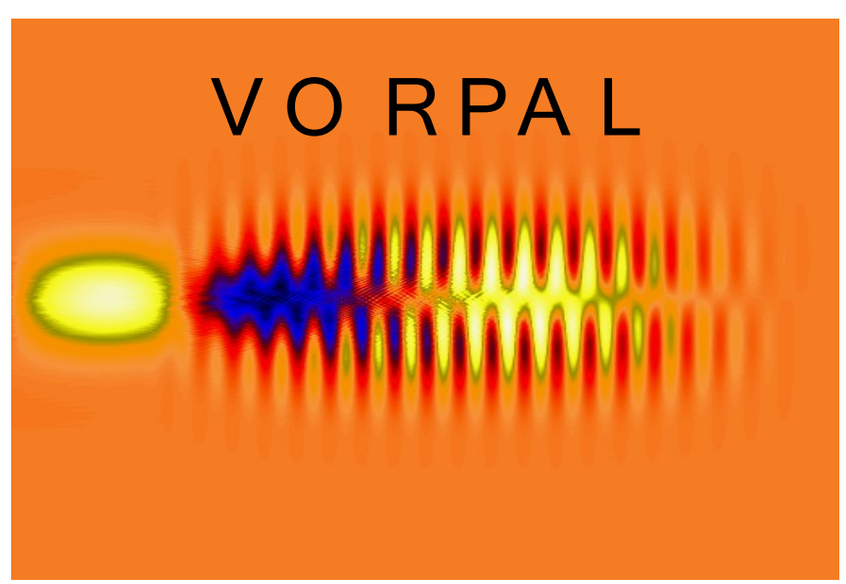
Code and Model Verification

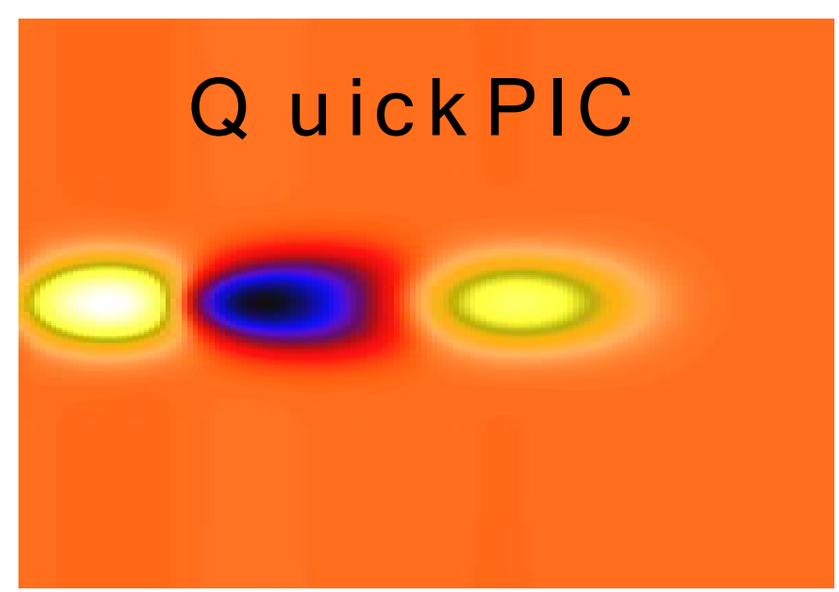
- Code verification is important especially for regime with no analytical results.
- Understanding of different numerical models, algorithms and implementations through benchmarking.

Benchmark Parameters

- $\lambda_0 = 0.8\ \mu m$, $I_{peak} \sim 10^{18}$ W cm^{-2}, $\tau_{fwhm} = 30$ fs
  $n_e = 1.38 \times 10^{19}$ cm^{-3}
- $80 \times 80 \times 20\ \mu m^3$ box, rectangular mesh of $512 \times 512 \times 512$ cells
- 8 particle/cell for full PIC

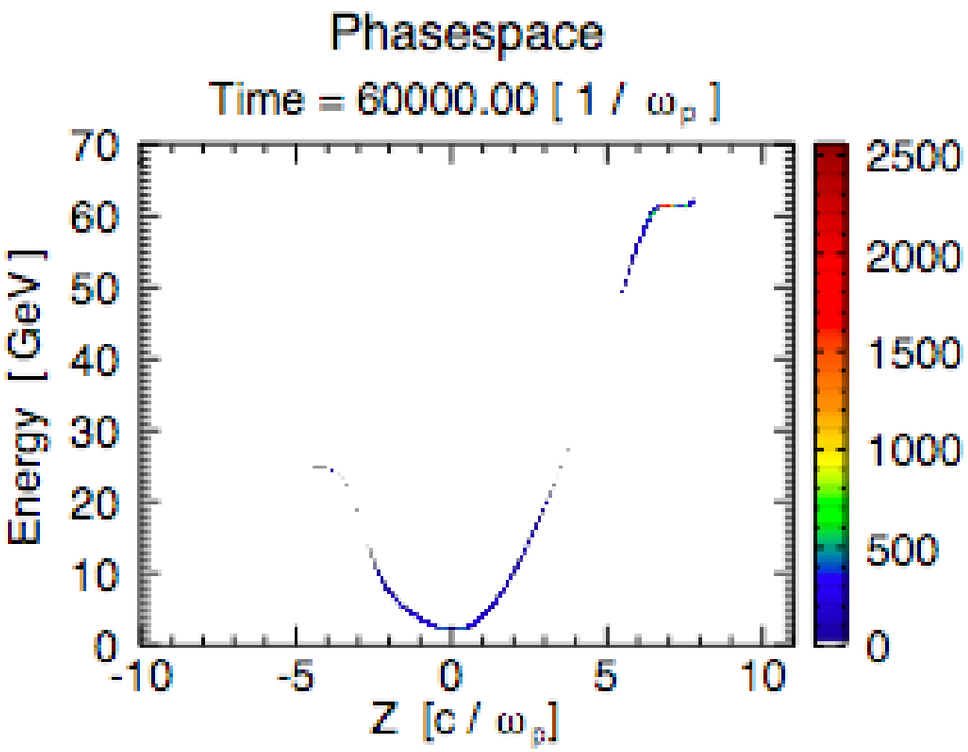


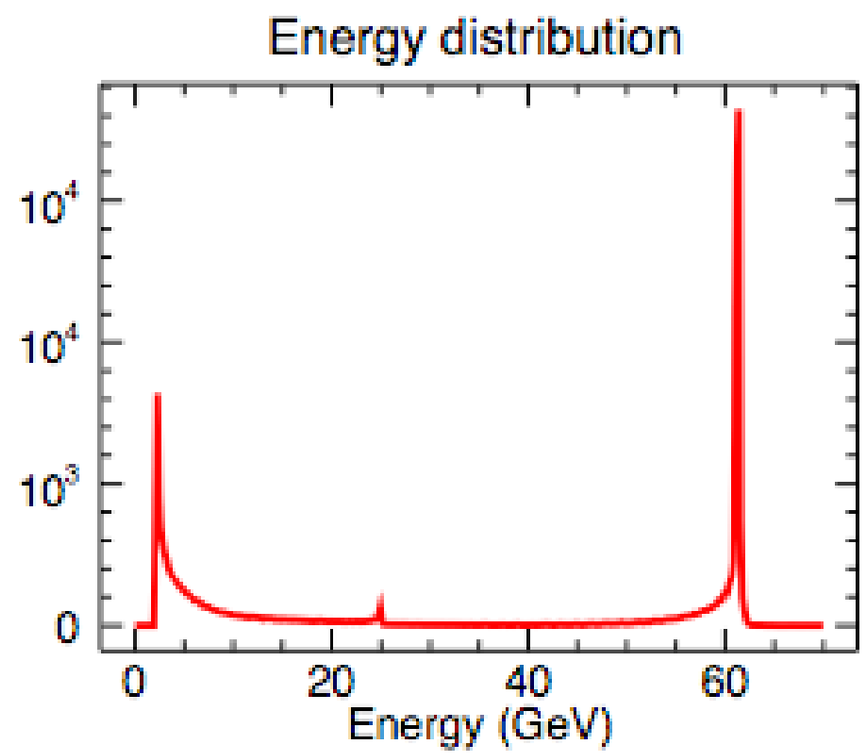


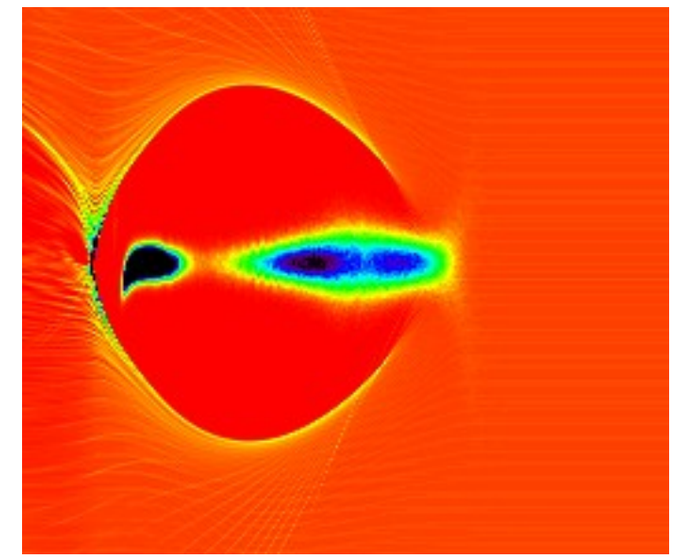


Nominal 25 GeV PWFA stage using QuickPIC

Preionized







n_p= $1\times10^{17}cm^{-3}$

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

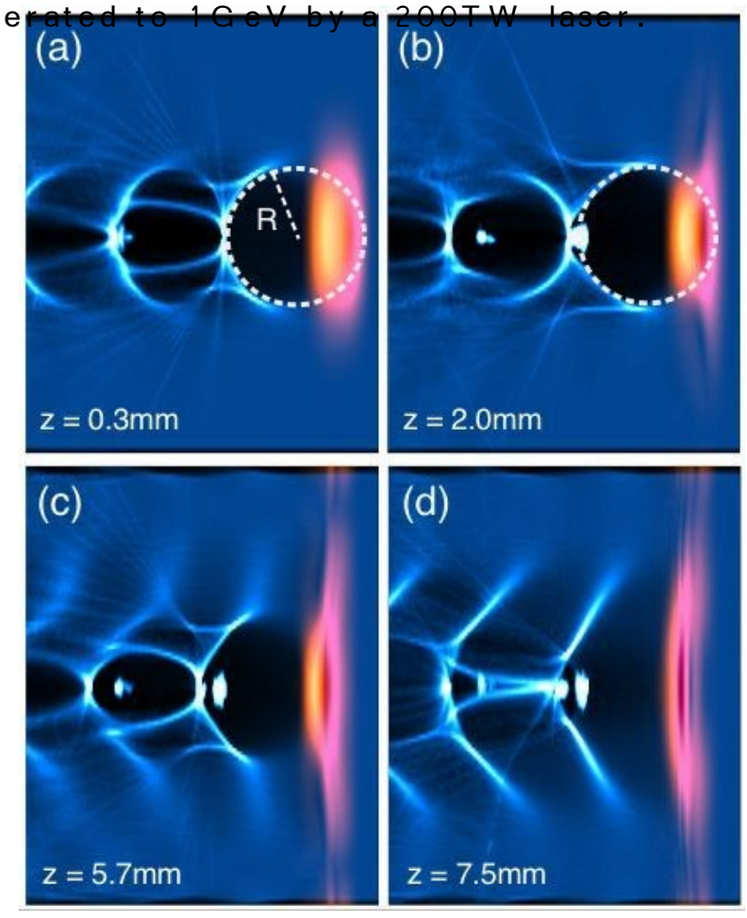
Efficiency from drive to trailing bunch ~48%!

SLAC Duke UNIVERSITY UCLA USC

Large scale modeling is being used to unravel the physics of LW FA in the Bubble or blowout regime

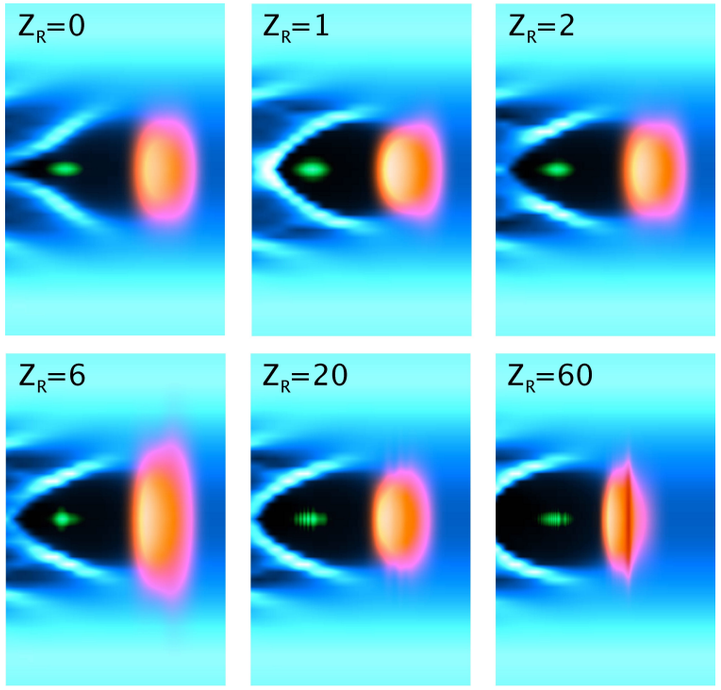
OSIRIS

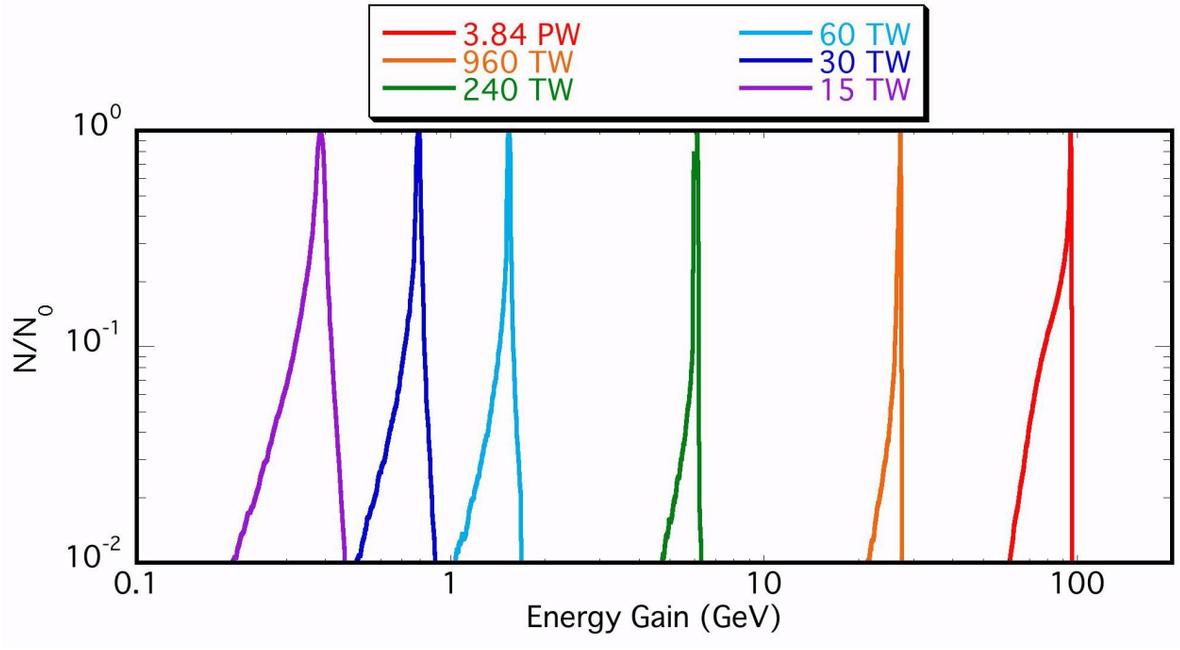
* **3D simulation**
  - Typical simulation with 4000·256·256 grids, and 4·10^5 time-steps.
  - **Theoretical framework (Lu et al.)**
  - Simulations lead to a theoretical framework.
  - It allows us to choose the parameters for stable high-quality accelerators. Below, 0.3nC were accelerated to 1GeV by a 200TW laser.



QuickPIC

* **LW FA stages designed and simulated for energy gain up to 100GeV.**
* **Simulations confirmed theoretical predictions, used to refine framework**
* **100GeV simulation:**
  - $2^{11}\cdot2^{7}\cdot2^{7}$ grids and 7,200 3D time-steps (240 Rayleigh lengths).





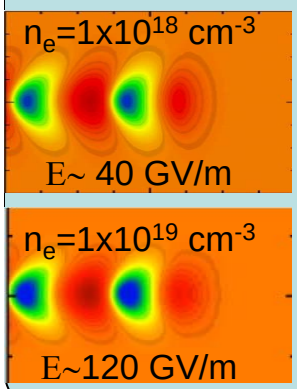
Simulating BELLA 10 GeV experiments
Stages for a Laser Plasma Collider

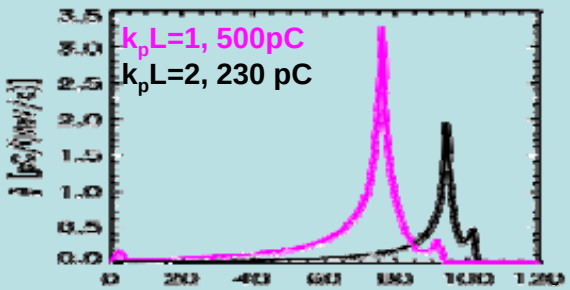
- LBNL BELLA proposal – 40 J PW laser for 10 GeV, staging, controlled injection
- SciDAC simulations supporting design

Scaled simulations

Wake scales with n_e

Predict efficient 10 GeV low ΔE stages at 40J, 1m

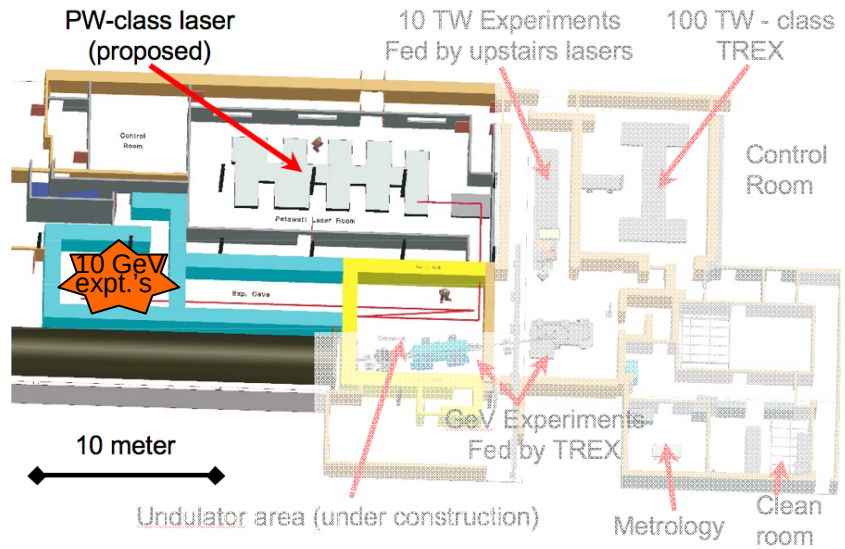




Px [MeV at 10^{19}]
[x100 MeV at 10^{17}]

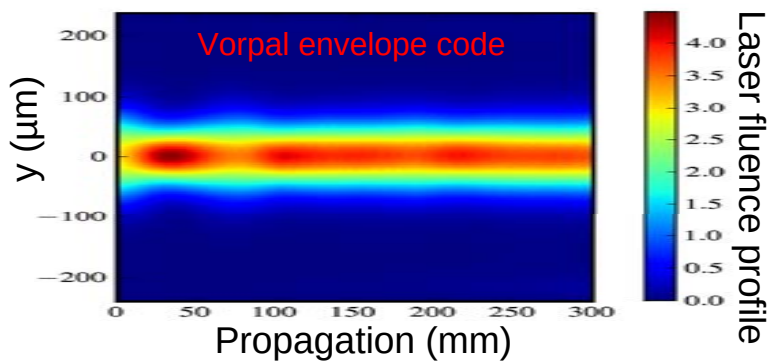
E. Cormier-Michel, et al,Proc AAC 2008

BELLA laser



Full simulation - fast reduced codes

(Envelope* and Lorentz§)



- **Injector**– coupled explicit, reduced simulation
- **Staging** – plasma mirrors, beam transport
- **Low emittance**– momentum accuracy**
  – resolve µm scale bunch
- **Accelerator structure** – hydro modeling

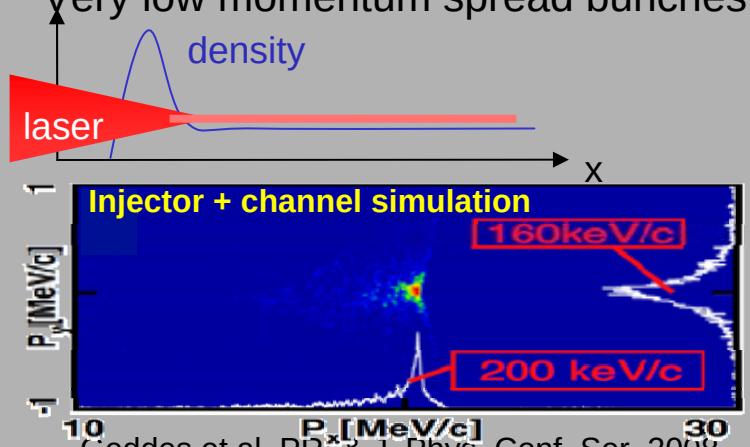
*B.Cowan, et al,Proc AAC 2008, § D. Bruhwiler, AAC 2008,
** E. Cormier-Michel PRE 2008

Controlled injection & GeV experiments
Designing controlled laser driven accelerators

Controlled of electron injection sets phase in wake for beam quality, stability

Plasma density down-ramp exp+sim.

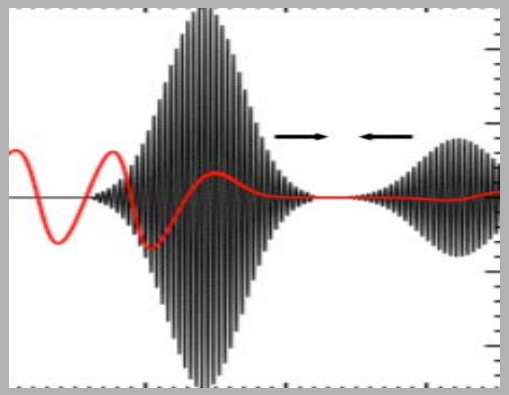
Very low momentum spread bunches*



Geddes et al, PRL& J. Phys. Conf. Ser. 2008.

Colliding laser pulses

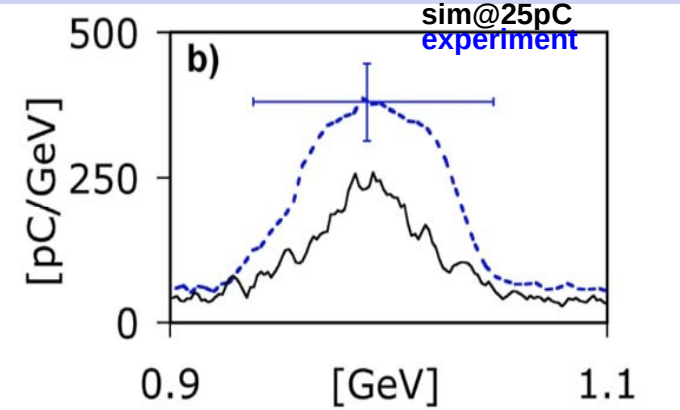
Detailed phase space control



Concept: Esarey et al, PRL 1997

GeV Experiments

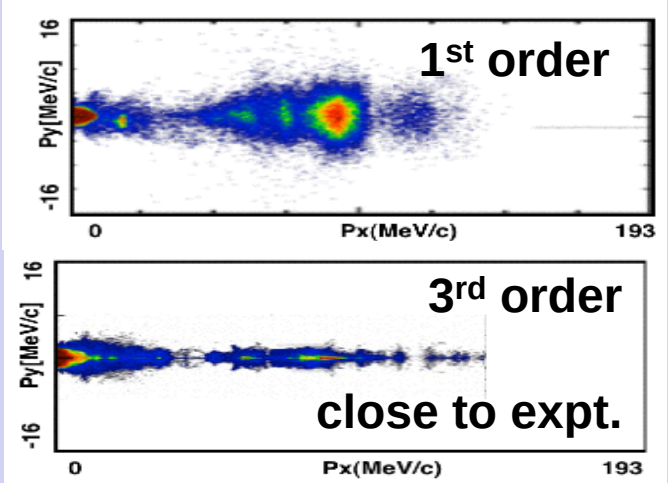
Simulations validated to experiment physics/scaling of self-trapped stages



Leemans et al, Nature Physics 2006; Gonsalves et al PAC 2007

Momentum accuracy: high order weight *

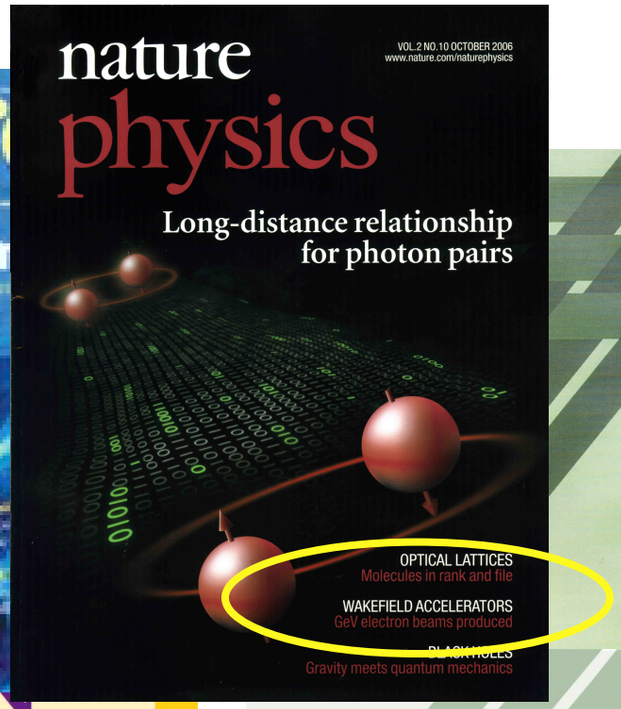
Accurate plasma temperature, bunch divergence

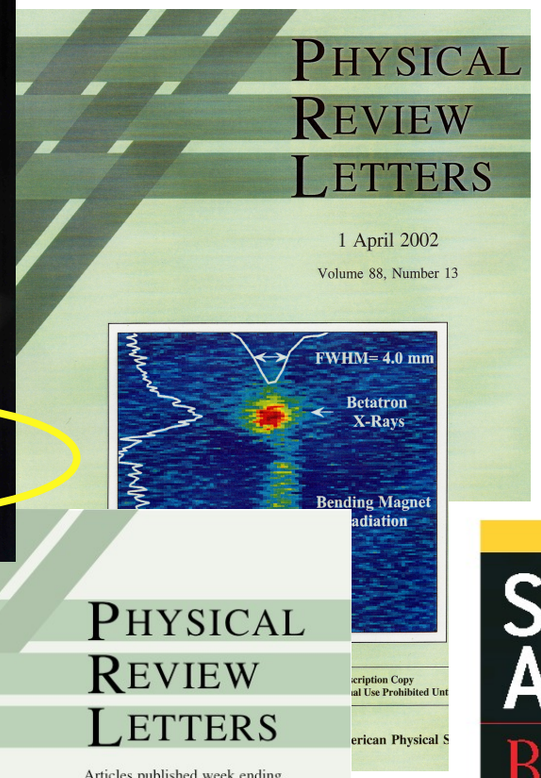


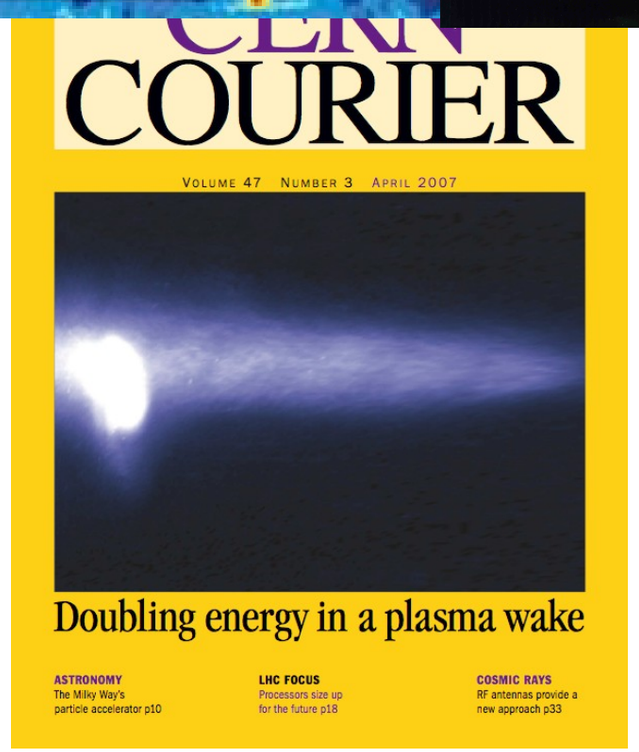
MIchel et al, PRE 2008; Geddes et al, AAC 2008

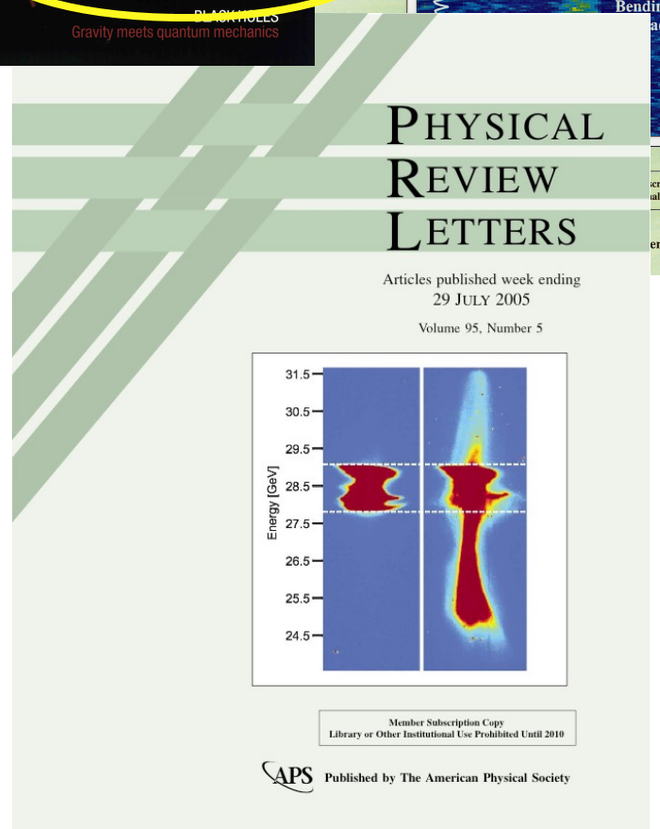
Recent progress has put plasma-based acceleration at the Forefront of Science:

SciDAC codes directly impacted this progress!



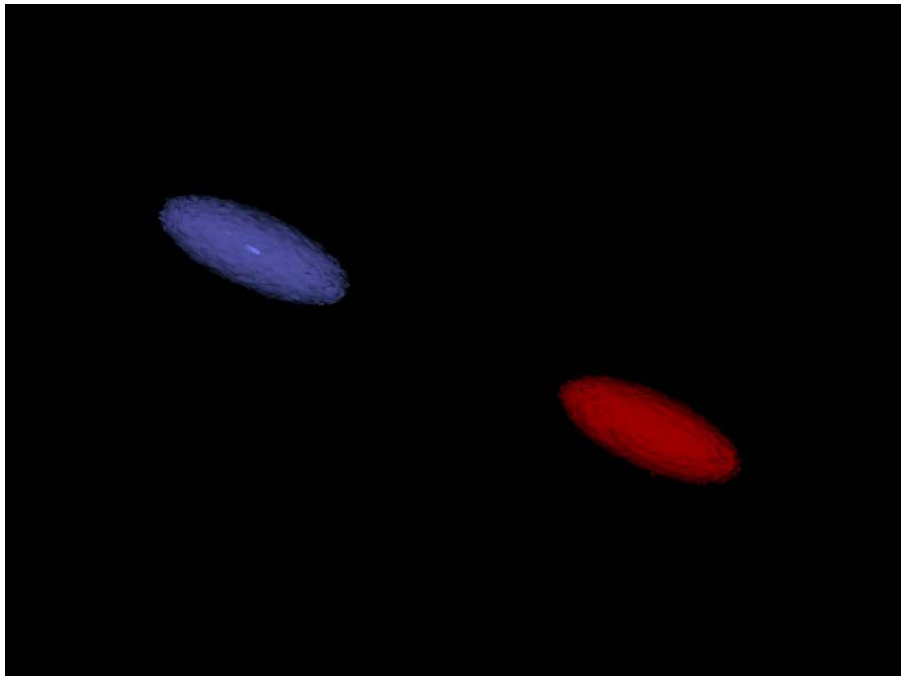






Summary

- Accelerators are complex instruments with a wide spectrum of design requirements depending on the application
  - Multi-scale, multi-physics modeling requirements
- To help maximize performance and minimize cost, ComPASS is developing the new generation of HPC accelerator modeling tools, aiming to
  - Provide integrated multi-physics capabilities
  - Utilize petascale capable solvers and algorithms
- The ComPASS target applications are well aligned with the accelerator science priorities of HEP, NP, and BES
- The success of the program relies on the success and effectiveness of the collaboration of ComPASS with the SciDAC CET and Institutes.

Questions

- And a movie