Accelerator Modelling under SciDAC:

Meeting the Challenges of Next-Generation Accelerator Design, Analysis, and Optimization

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ICAP 2006

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Chamonix

SciDAC
Scientific Discovery through Advanced Computing

OUTLINE

- **SciDAC1: objectives and development approach**
- **SciDAC1 accomplishments: impact to present and future facilities**
- **SciDAC2: planning the future**

and BTW,

SciDAC: Scientific Development through Advanced Computing.

SciDAC1: 2001-2006

SciDAC2: 2007-2012 (?)

The SciDAC1 program

- **Develop scientific applications to *effectively* take advantage of terascale computing, by**
  - **— Creating a new generation of scientific simulation codes**
  - **— Creating the mathematical and computing systems software to enable these scientific simulation codes to use terascale computers**
  - **— Creating a distributed science software infrastructure to enable scientists to effectively utilize these codes.**

Accelerator modeling: emphasis on building teams of computer scientists, and computational and machine physicists

SciDAC Accelerator Science & Technology (AST) Project

Goals: Develop & apply an advanced, comprehensive, high-performance simulation environment to solve challenging problems and to enable new discoveries in accelerator science & technology

Participants:

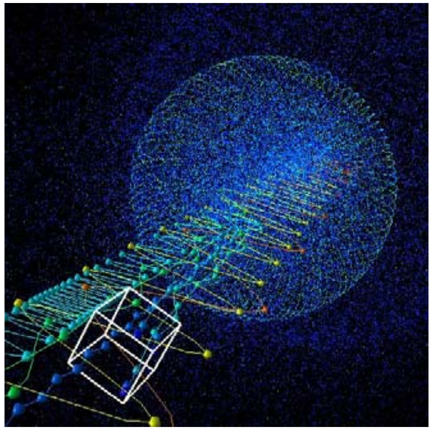
- Labs: LBNL, SLAC, FNAL, LANL, BNL, SNL
- Universities: Stanford, UCLA, USC, UCD, UMd
- Small business: Tech-X
- Collaborations w/ applied math and CS researchers

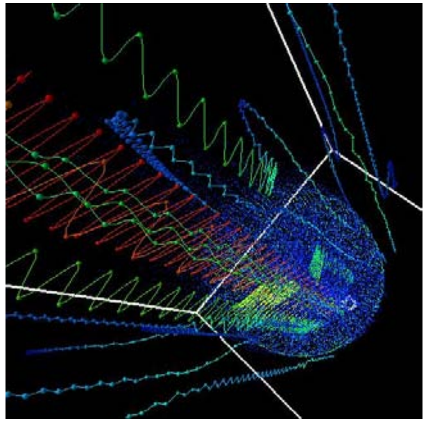
Sponsors: DOE/SC HEP (formerly HENP) in collaboration with ASCR

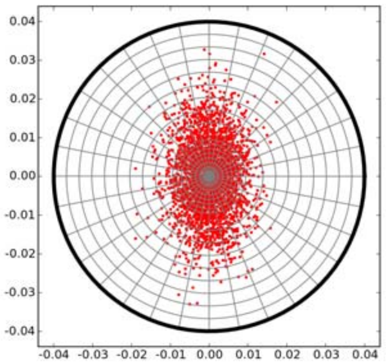
Collaborations w/ Applied Math & Comp. Sci

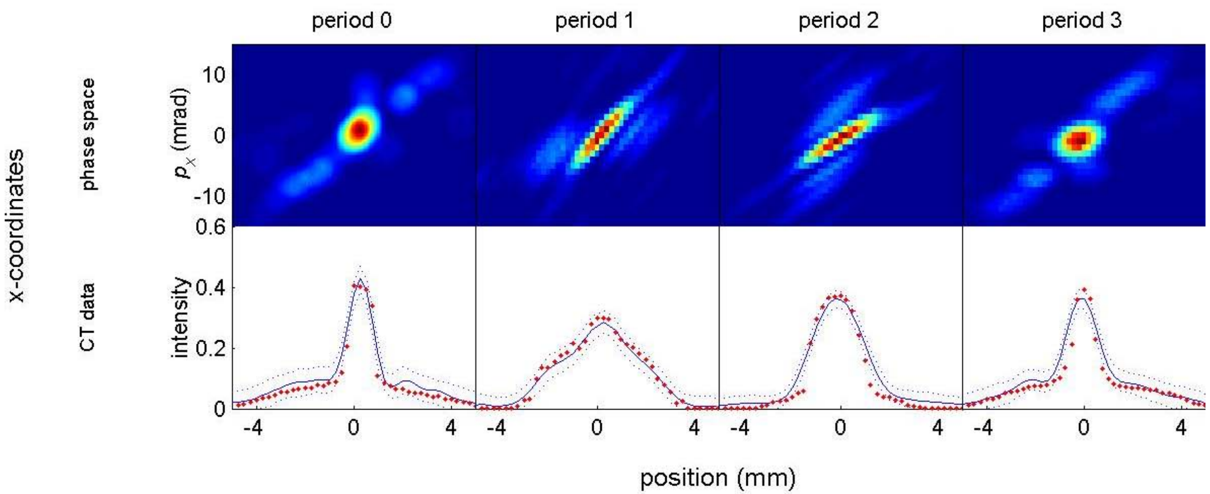
SciDAC **Integrated Software Infrastructure Centers**

- Linear solvers, eigensolvers
- Poisson solvers
- AMR
- Meshing
- Parallel PIC methods
- Performance optimization
- Statistical methods
- Visualization









AST Thrust Areas & Codes

Beam Dynamics (BD)
- BeamBeam3D, IMPACT-Z, IMPACT-T, ML/I, Synergia

Electromagnetics (EM)
- Omega3P, Tau3P, S3P, T3P, Track3P

Advanced Accelerators (AA)
- OSIRIS, VORPAL, QuickPIC, UPIC

Emphasis of this talk will be on BD and AA

SciDAC/AST codes have been applied to present & future projects

- ✓ Tevatron
- ✓ LHC
- ✓ NLC
- ✓ ILC
- ✓ PEP-II
- ✓ FNAL Booster
- ✓ FNAL Main Injector
- ✓ L'OASIS LWFA experiments
- ✓ SLAC PWFA experiments
- ✓ Plasma afterburner design
- ✓ RHIC
- ✓ RIA
- ✓ SNS
- ✓ LCLS
- ✓ Photoinjector design
- ✓ Advanced streak camera design
- ✓ CERN SPS
- ✓ JPARC commissioning
- ✓ FERMI design
- ✓ Int'l code benchmarking @ CERN PS

12 SciDAC project related talks in ICAP06!

J. Cary, “High Performance Self-Consistent EM modeling of beams”, **MOAPMP02**

J.-F. Ostiguy, “CHEF: A Framework for Accelerator Optics and Simulation”, **TUAPMP02**

R. Ryne, “Recent Progress on the MaryLie/IMPACT Beam Dynamics Code”, **TUAPMP03**

A. Candell, “Parallel Higher-Order Finite Element Method for Accurate Field Computations in Wakefield And PIC Simulations”, **WEMPMP03**

I. Pogorelov, “Recent Developments in IMPACT and Application for Future Light Sources”, **WEPPP01**

J. Qiang, “Recent Improvements to the IMPACT-T Parallel Particle Tracking Code”, **WEPPP02**

C. E. Mitchell, “Computation of Transfer Maps from Surface Data with Applications to Wigglers”, **WEPPP08**

D. L. Bruhwiler, “High-Order Algorithms for Simulation of Laser Wakefield Accelerators”, **WESEPP03**

“D. L. Bruhwiler Parallel Simulation of Coulomb Collisions for High-Energy Electron Cooling Systems”, **WEA1MP01**

J-L Vay, “Self-Consistent Simulations of High-Intensity Beams and E-Clouds with WARP/POSINST”, **WEA3MP02**

A. Kabel, “Accelerating Cavity Design for the International Linear Collider”, **WEA4IS01**

A. Adelmann, “H5Part: A Portable High Performance Parallel Data Interface for Electromagnetics Simulations”, **THM1MP01**

SciDAC2 codes

Codes used in SciDAC but effort not SciDAC funded

SciDAC codes

SciDAC AST codes: notable "firsts"

- First 100M strong-strong colliding beam simulation for LHC (BeamBeam3D; J. Qiang)

- First multi-bunch, multi-turn injection simulation from linac-to-booster w/ self-consistent 3D space charge (Synergia; J. Amundson and P. Spentzouris)

- First 100M simulation of a linac for an x-ray light source w/ self-consistent 3D space charge (IMPACT-Z; I. Pogorelov, J. Qiang)

- First self-consistent electromagnetic simulation of an intense beam in an ILC 'crab' cavity (VORPAL; J.R. Cary, C. Nieter & VORPAL team)

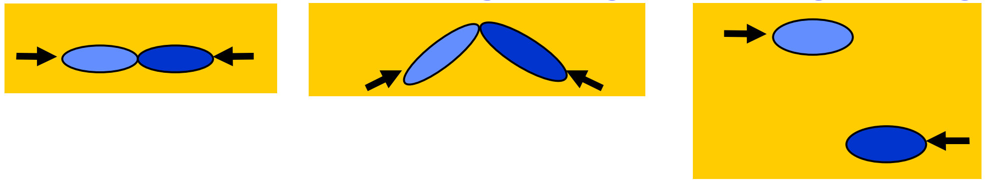
- First 3D simulation of a 1TeV Afterburner stage (QuickPIC; C.K.Huang et al.)
  - C.K. Huang received the 2007 Nicholas Metropolis award

- First 3D simulation of a GeV LWFA stage (OSIRIS; F.S.Tsung, W.Lu, M. Tzoufras et al.)

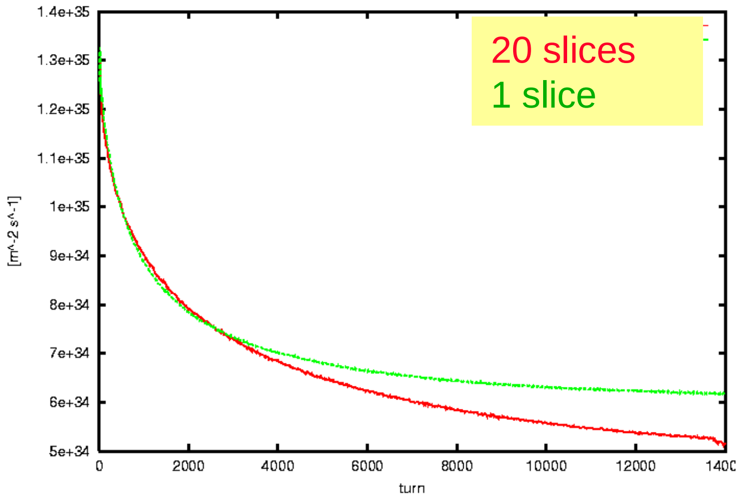
Selected AST project code descriptions and applications

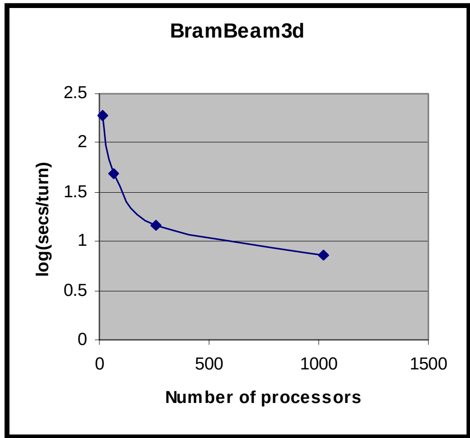
BeamBeam3D

- Multi-model parallel PIC code for simulating colliding beams (weak-strong,strong-strong,head-on,crossing angle, long range)
- Applied to Tevatron, LHC, PEP-II, RHIC



- Features: Integrated and non-uniform grid Green function, multi-slice/multi-bunch/multi-IP, impedance model



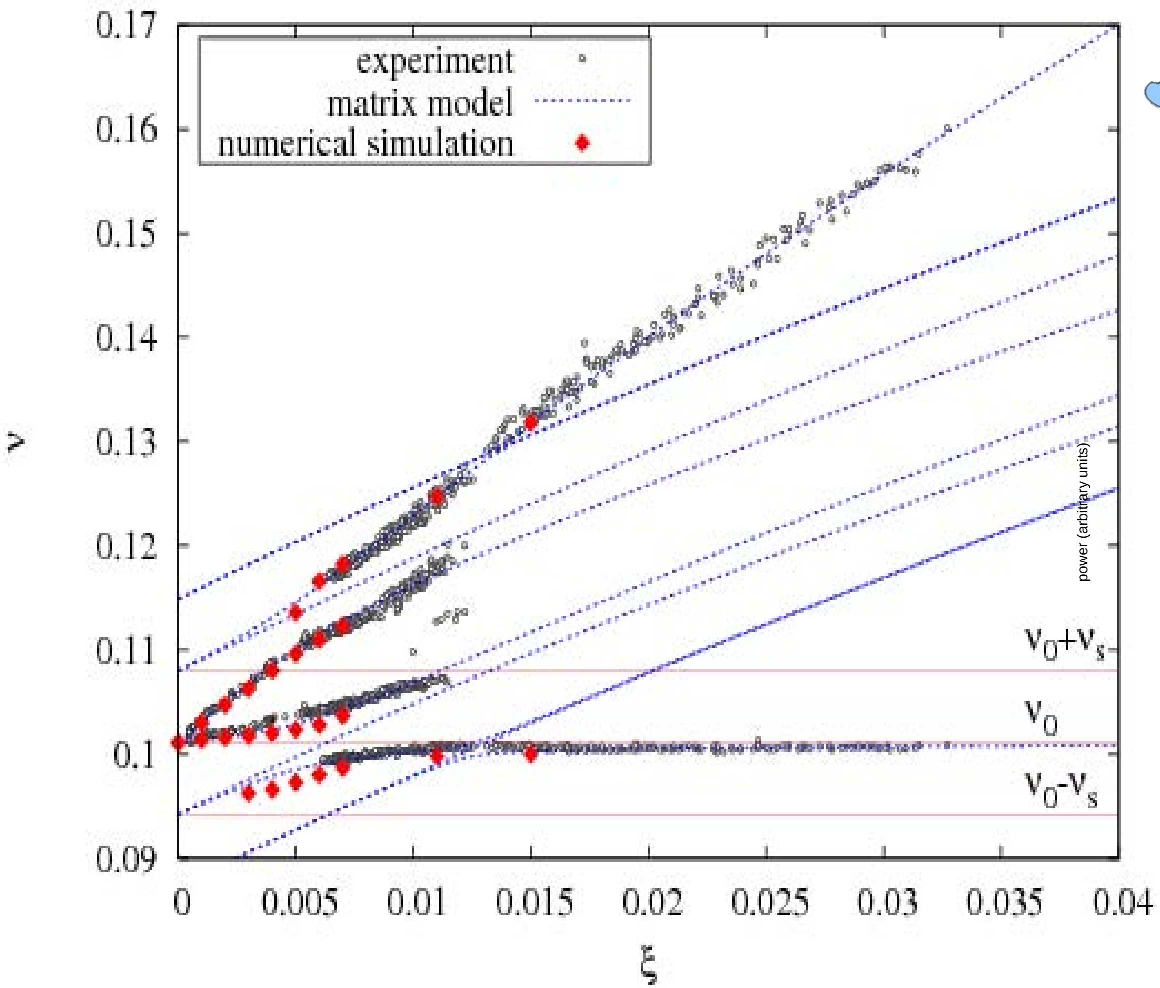


# of procs	Execution time/turn (sec)
16	188
64	49
256	14.77
1024	7.18

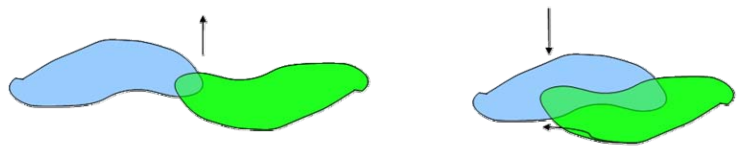
PEP-II simulations show need for multi-slice modeling for accurate luminosity calculation. (J. Qiang/LBNL, Y. Cai/SLAC, K. Ohmi/KEK)

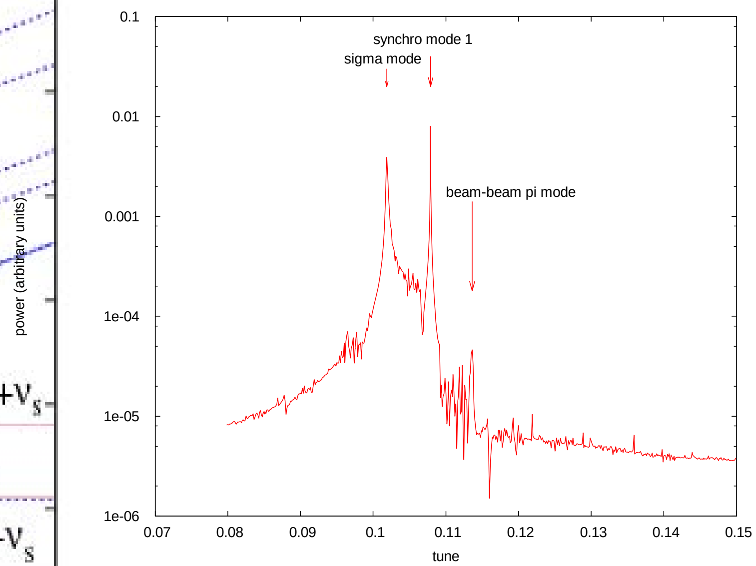
Scaling at NERSC SP3: weak-strong model (100Mp, 512x512x32 grid, 4 slices)

Simulation of beam-beam effects in VEPP-II: Comparing matrix model, BeamBeam3D, expt



Beam-beam code validation comparing with VEPP-II data





2-bunch coherent spectrum for $\xi=0.008$. Shown are the beam-beam σ and π modes and one synchro-mode.

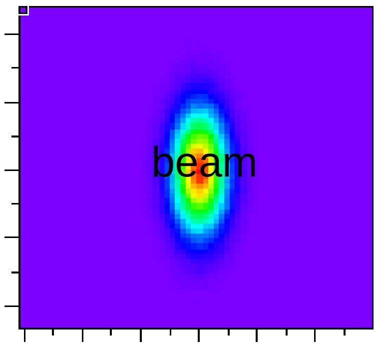
E. Stern, A. Valisev (FNAL), J. Qiang (LBNL)

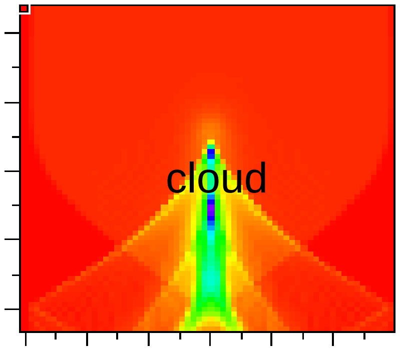
Application of QuickPIC to Electron-Cloud :

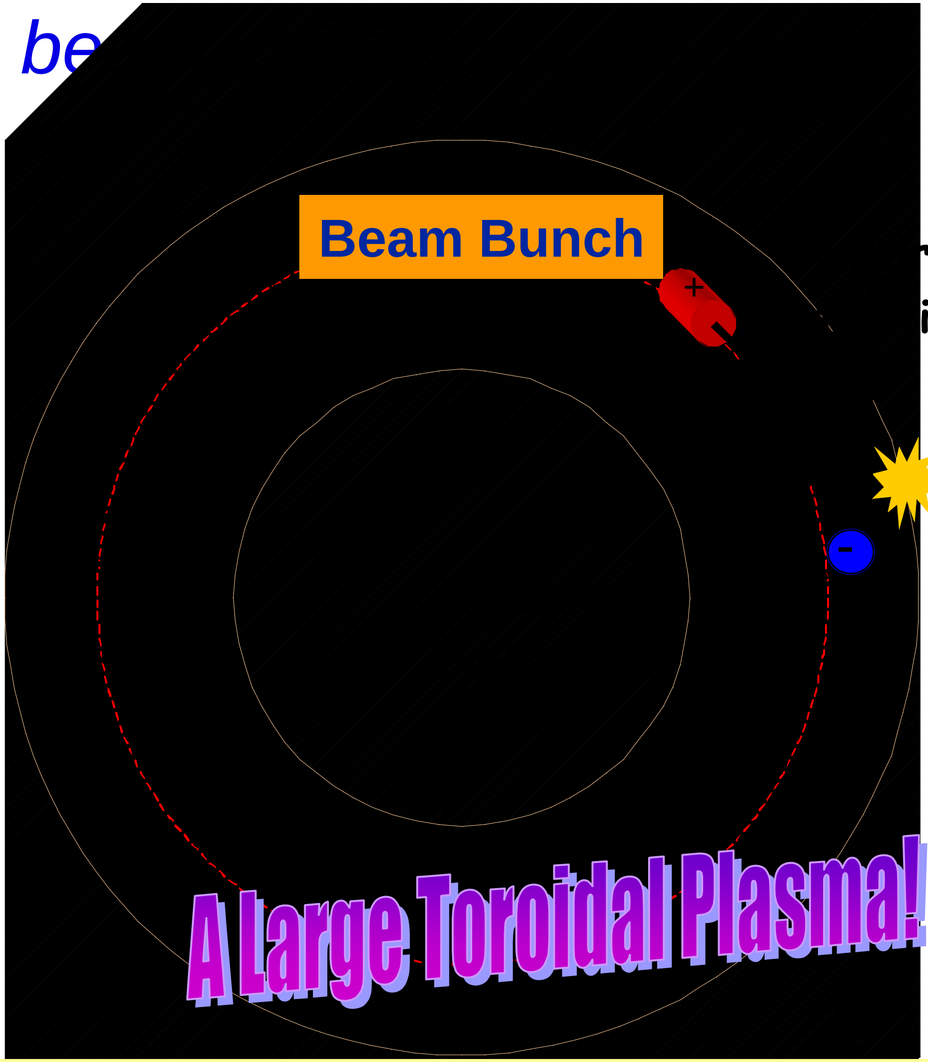
A few 10000's km be

QuickPIC adapted to circular problem
- Magnetic field
- Non-neutral plasma
- Lattice effects

•Can now model 100 msecs



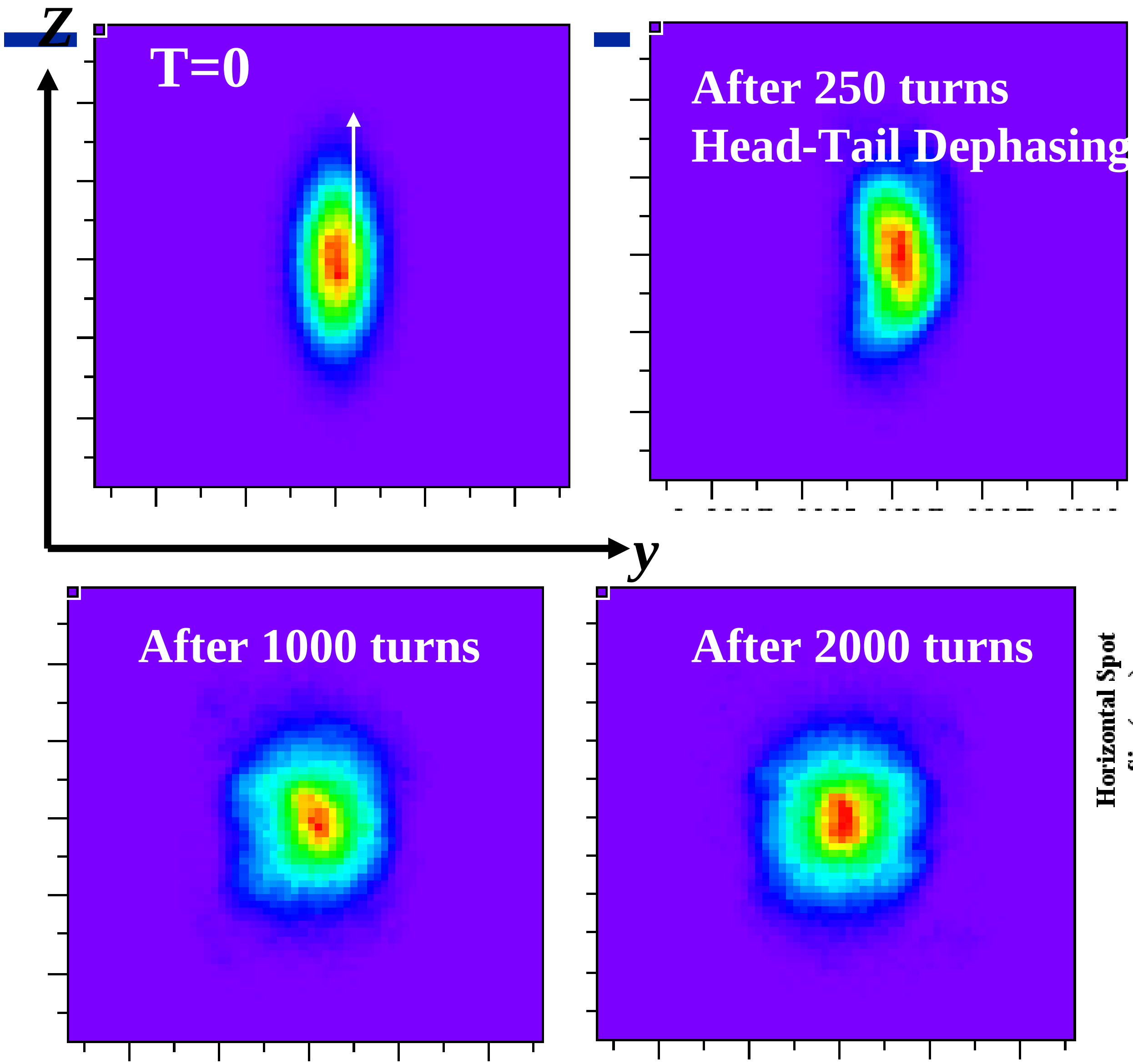


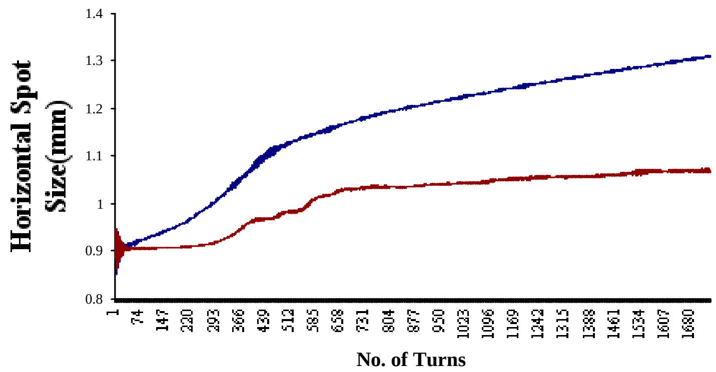


Illustrates how multidisciplinary collaboration can lead to unexpected benefits: A laser/plasma code applied to LHC and FNAL MI.

Ali Ghalam, B. Feng, T. Katsouleas (USC); W. B. Mori, C. Huang, V. Decyk, (UCLA); G. Rumolo, F. Zimmermann, E. Benedetto (CERN); P. Spentzouris (FNAL)

QuickPIC LHC modeling: Snap shots of Beam Evolution





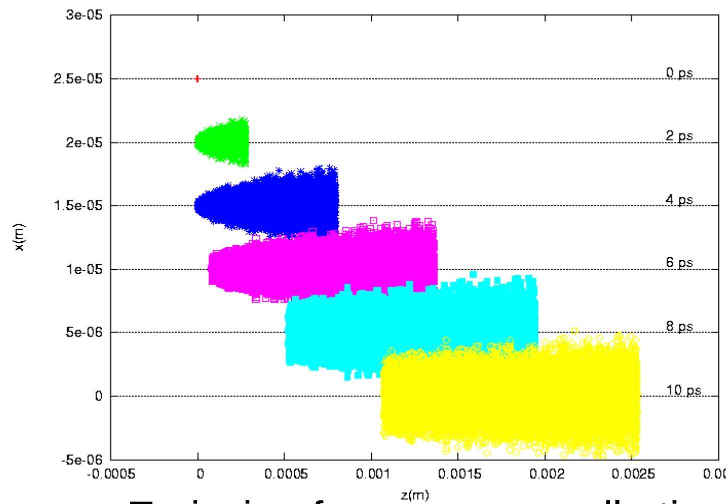
Single kick not suffcicient: A. Z. Ghalam, T. Katsouleas(USC)

G. Rumolo, F.Zimmermann(CERN)

C. Huang, V. Decyk, W.Mori(UCLA)

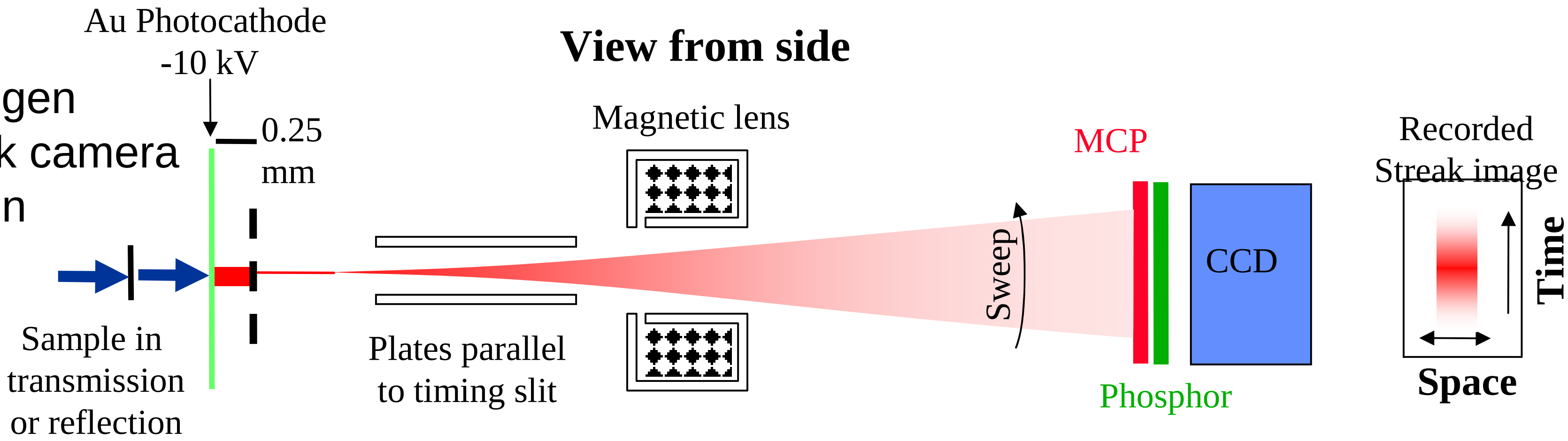
IMPACT: Integrated-Map & Particle Accelerator Tracking

- Code suite includes IMPACT-Z, IMPACT-T parallel PIC codes
- Originally for ion linacs; major enhancements under SciDAC for electron linacs, photoinjectors, …
- Recent enhancements
  - —high aspect ratio Poisson solver
  - —binning for large energy spread
  - —multi-charge state (RIA)
  - —wakes, 1D CSR

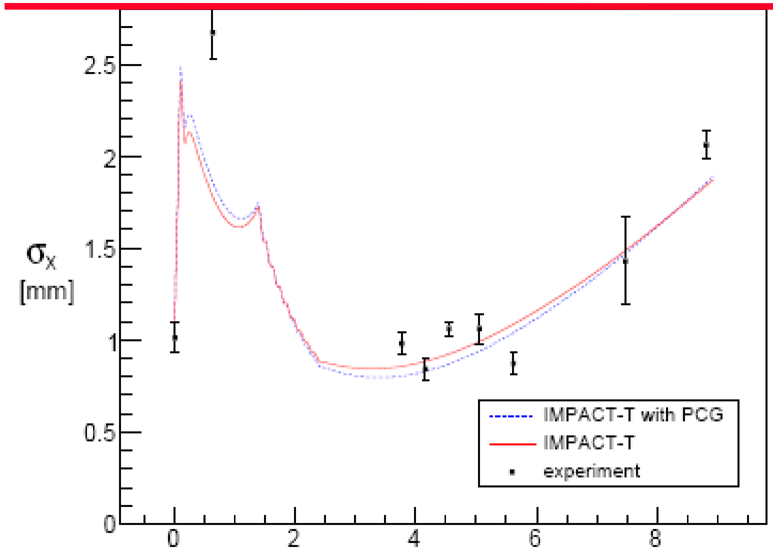


Emission from nano-needle tip

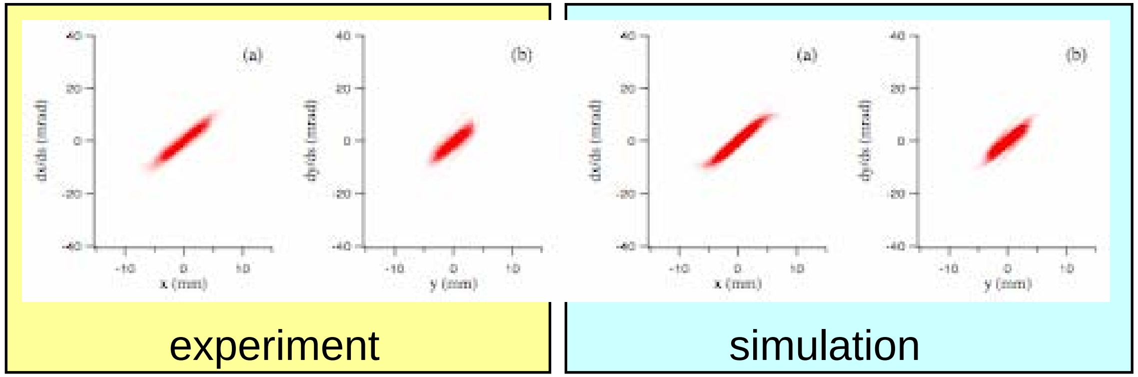
- Applied to SNS, RIA, JPARC, Fermi@Elettra
- photoinjectors @ ANL, BNL, Cornell, FNAL/NIU, JLAB, LBNL, SLAC/LCLS
- Next-gen streak camera design



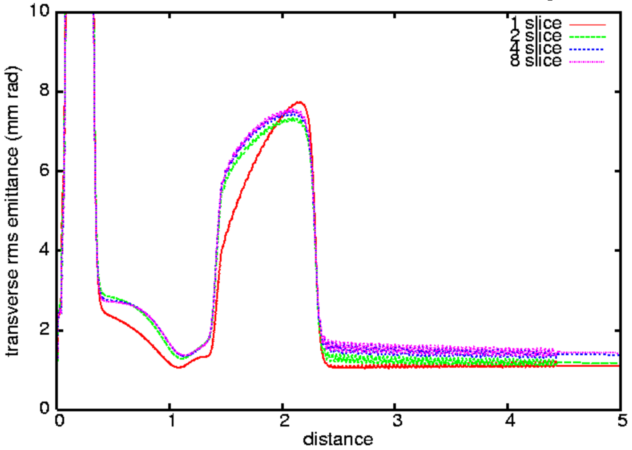
Example IMPACT applications: HEP, NP, BES



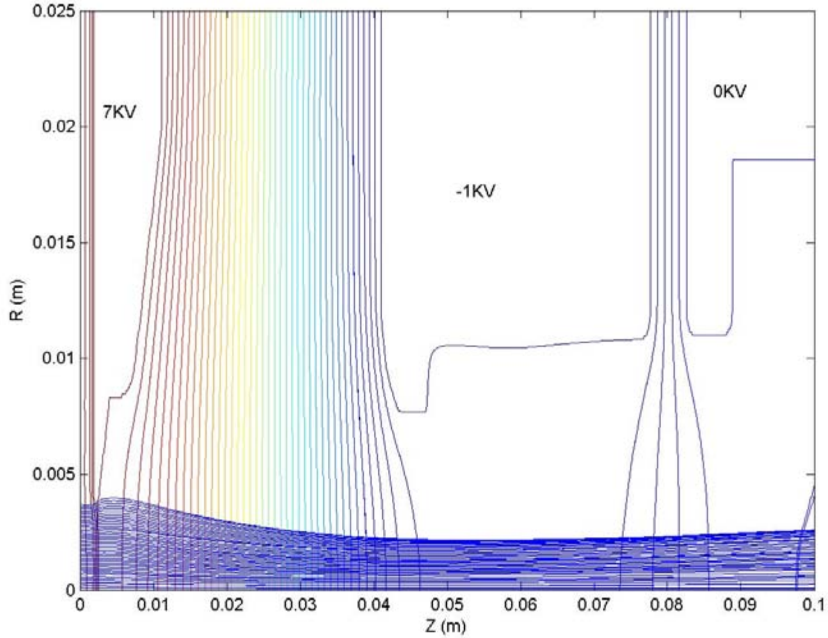
Beam size vs z in the FNAL/NICADD photoinjector: simulation & experiment (C. Bohn/NIU, F. Piot/FNAL)



JPARC commissioning, horizontal phase space, simulation vs. expt (M. Ikegami/KEK)



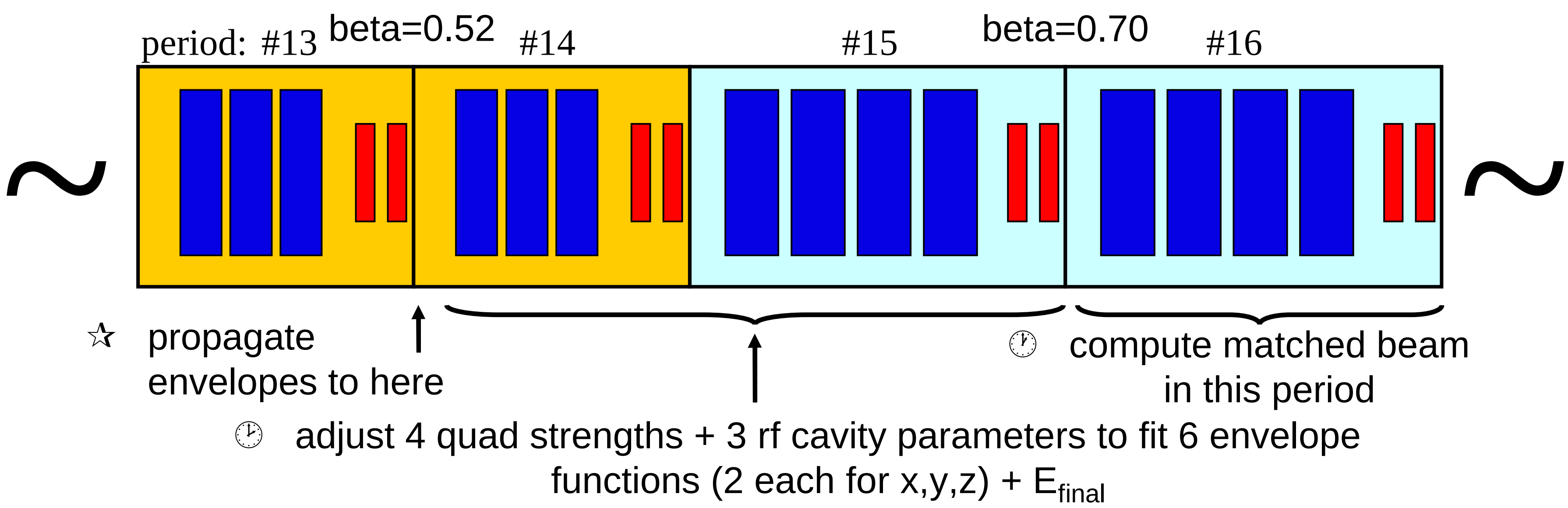
LCLS photoinjector emittance evolution (J. Qiang/LBNL, C. Limbourg/SLAC)



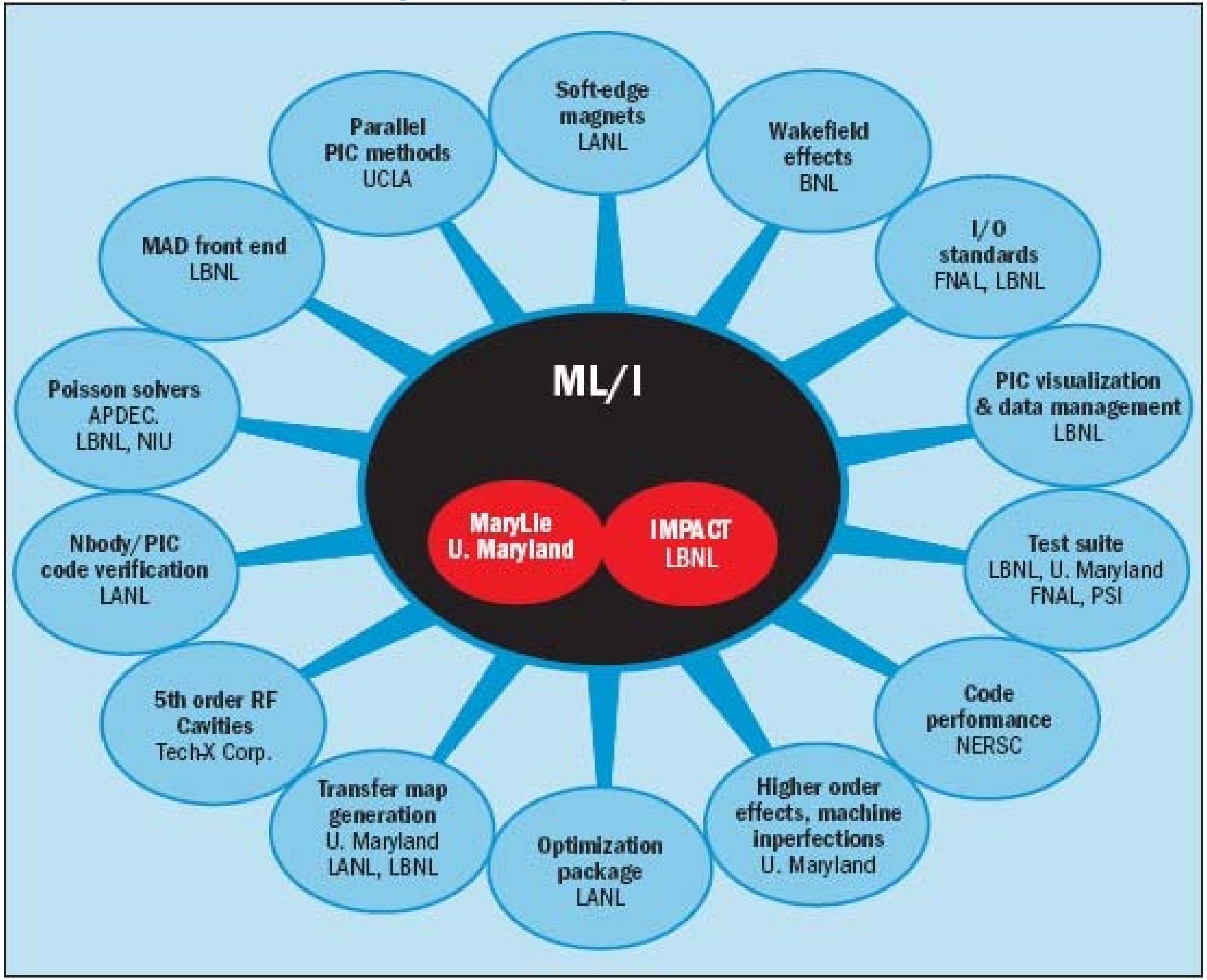
Ion beam formation & transport from RIA ECR ion source (J. Qiang)

MaryLie/IMPACT (ML/I)

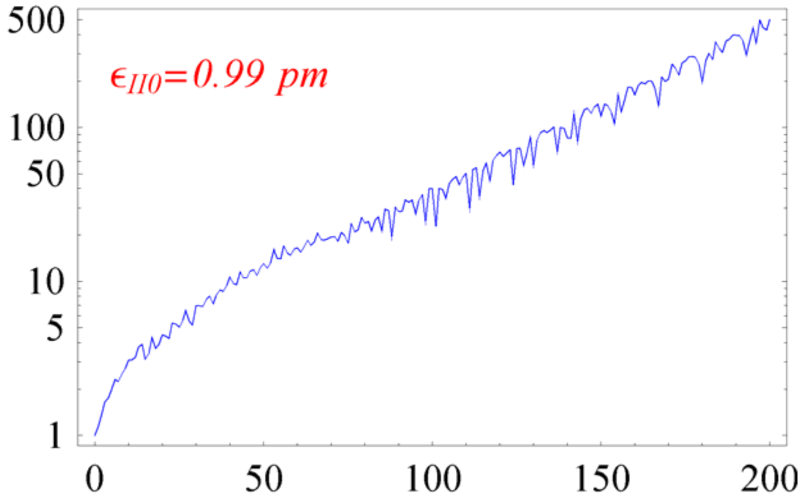
- **ML/I: hybrid code combining MaryLie 5th order magnetic optics with IMPACT parallel PIC + new capabilities**
  - —Embeds operator splitting for all thick elements
  - —New modules (wakefields, soft-edge magnet models, …)
- **Multiple-physics, multi-purpose**
  - —Particle tracking, envelope tracking, map production/analysis
  - —Fitting/optimizing, e.g. zeroing 3rd order while minimizing 5th
  - —Designing matching sections, e.g. superconducting linacs

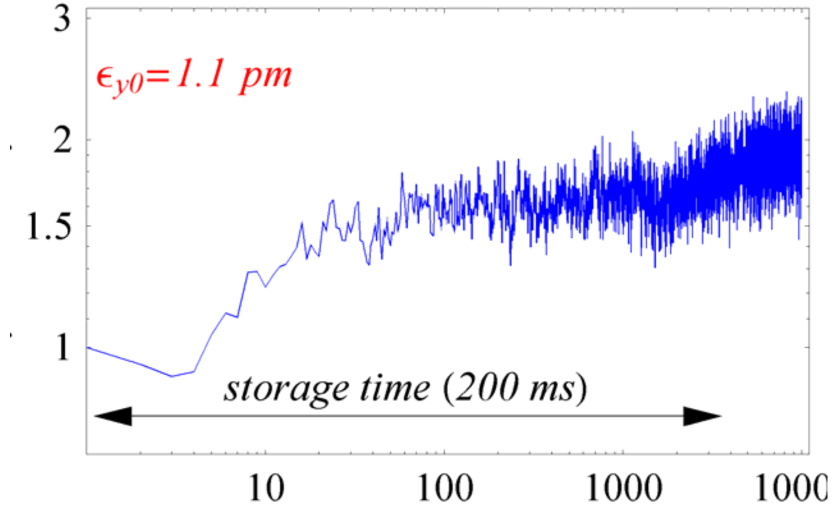


Following the SciDAC model, AST codes are developed by large, multi-disciplinary teams
Example: MaryLie/IMPACT



ML/I applications

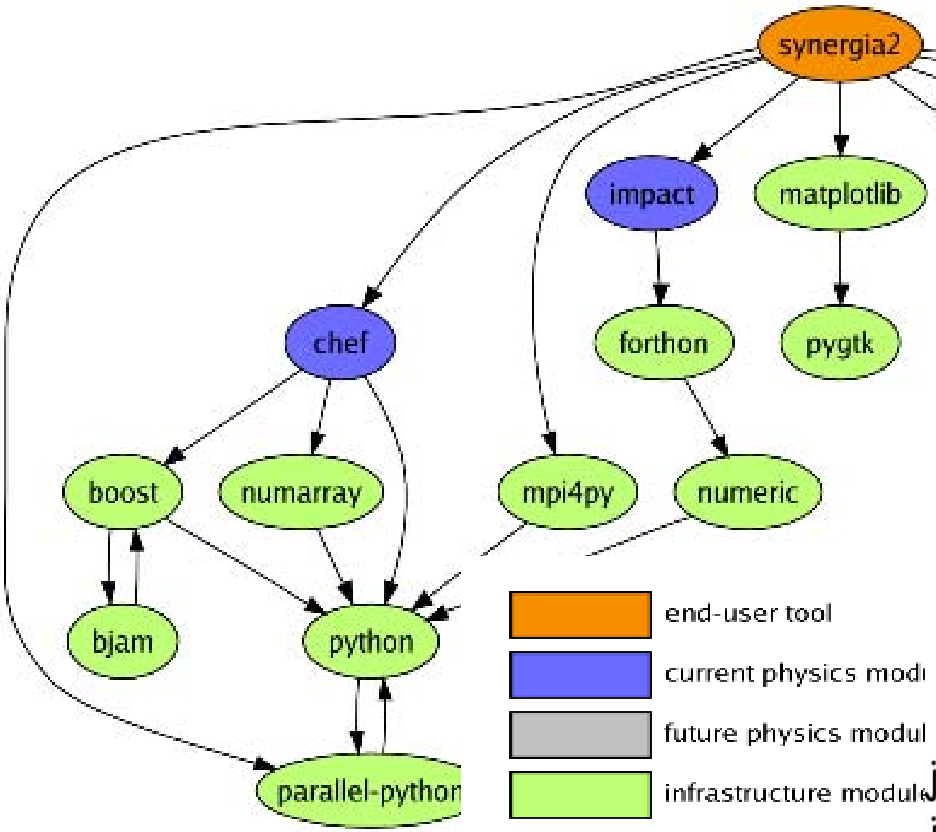




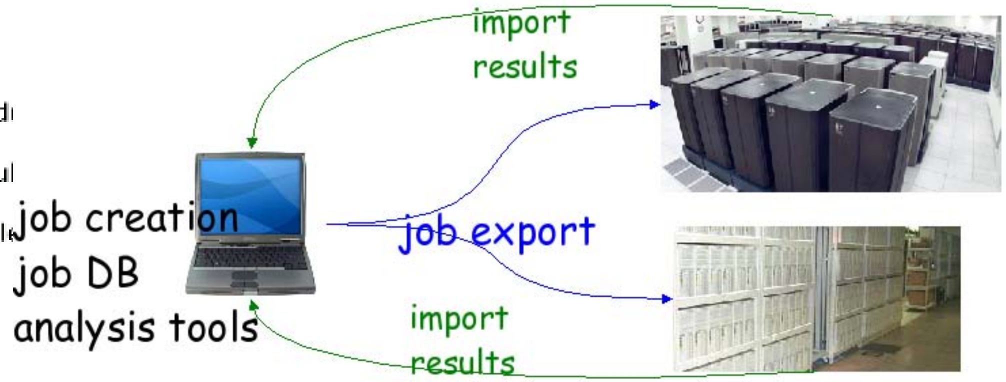
ILC damping ring simulations showing emittance growth w/ linear (left), nonlinear (right) space-charge models. M. Venturini, LBNL. These simulations contributed to the ILC-DR design selection.

Synergia

- Multi-language, extensible, parallel framework
- Incorporates multi-physics; state-of-the-art numerical libraries, solvers, physics modules

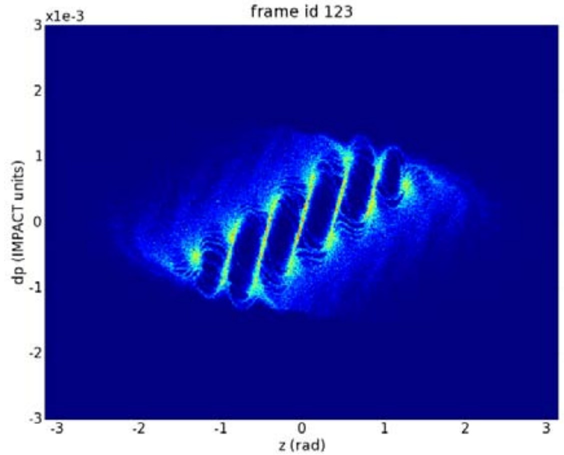


3D space-charge, impedance, arbitrary order lie maps, …

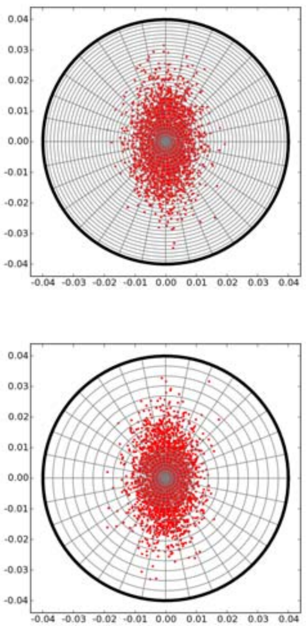


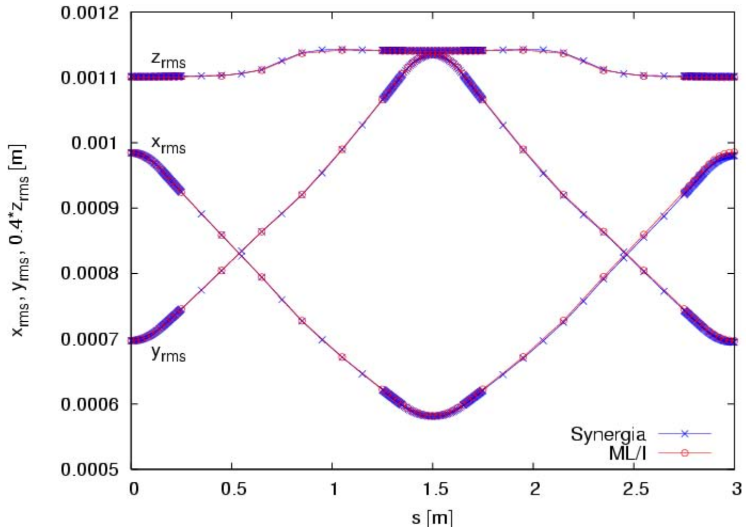
Unique capabilities for synchrotrons, boosters, and storage rings

- Multi-bunch capability
- Multiple Poisson solvers
  - IMPACT, multigrid (PETSc)
- Multi-turn injection
- Ramping rf and magnet modeling
- Active feedback modeling

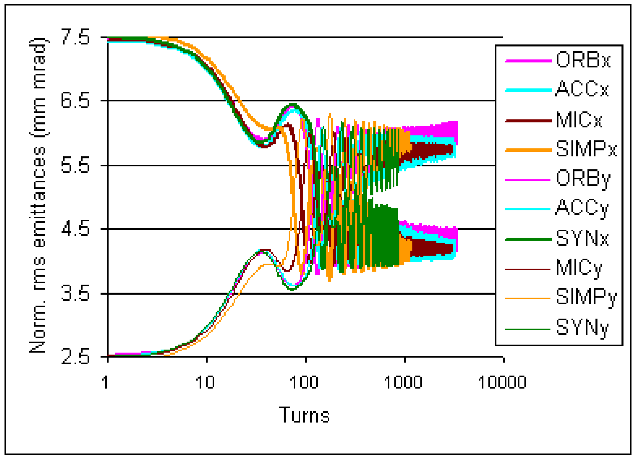


Longitudinal phase space shows halo & space-charge “drag” during bunch merge



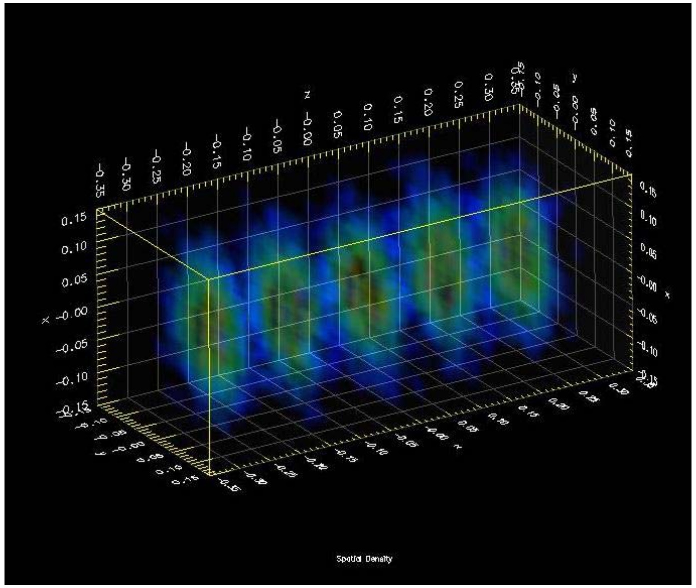


From test suite: comparison w/ analytical result (J. Comp. Phys, **211**,1, 2005)



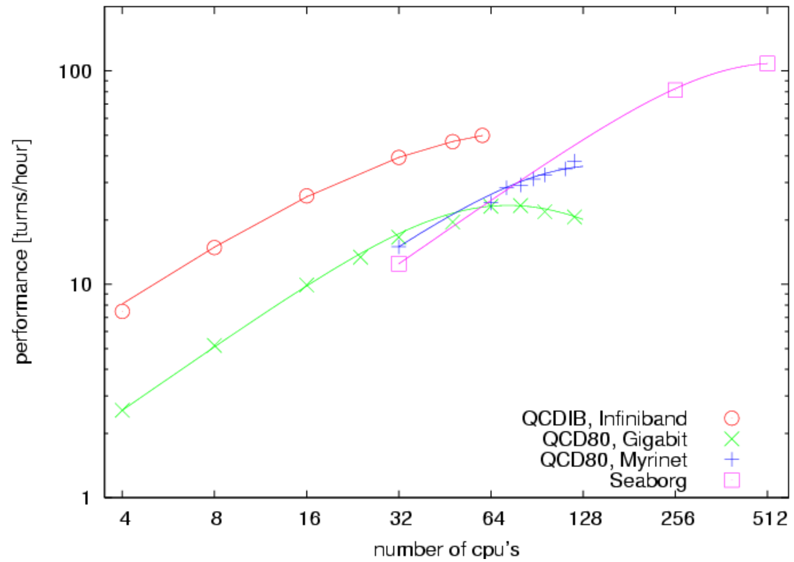
Synergia used in international space charge benchmark effort lead by I.Hofmann (PAC'05)

Synergia simulation of the Fermilab booster: Multi-bunch modeling in 3D



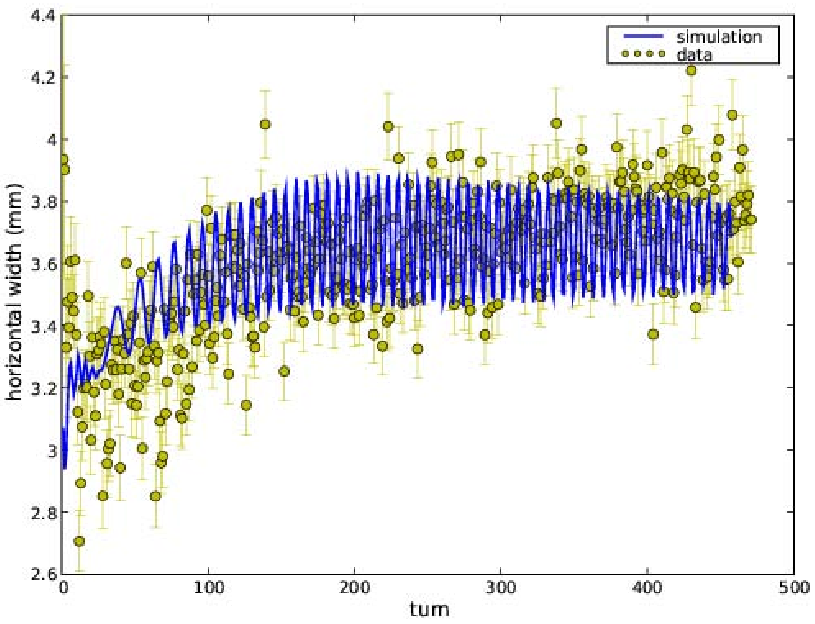
Merging of 5 linac microbunches in the FNAL booster (J. Amundson, P. Spentzouris)

- Self-consistent 3D space-charge model
- 2nd order maps (arbitrary order possible)
- Use 33x33x257 grid and ~ 5,000,000 particles
- Multi-turn injection

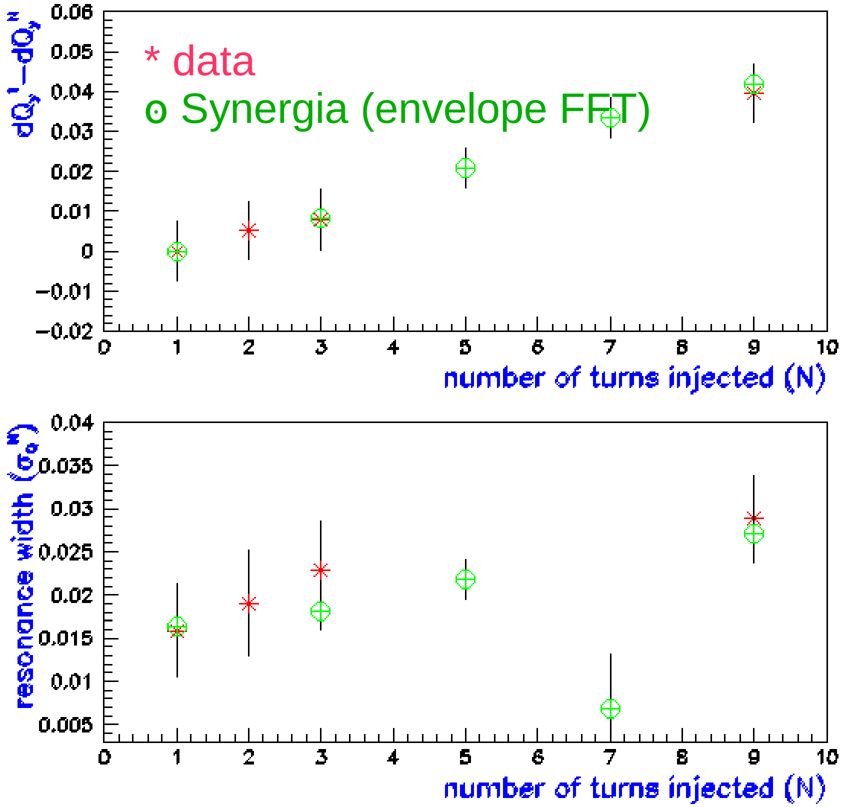


- Machine ramping with position feedback
- 6-D phase space beam matching

Booster simulations compared with experiment

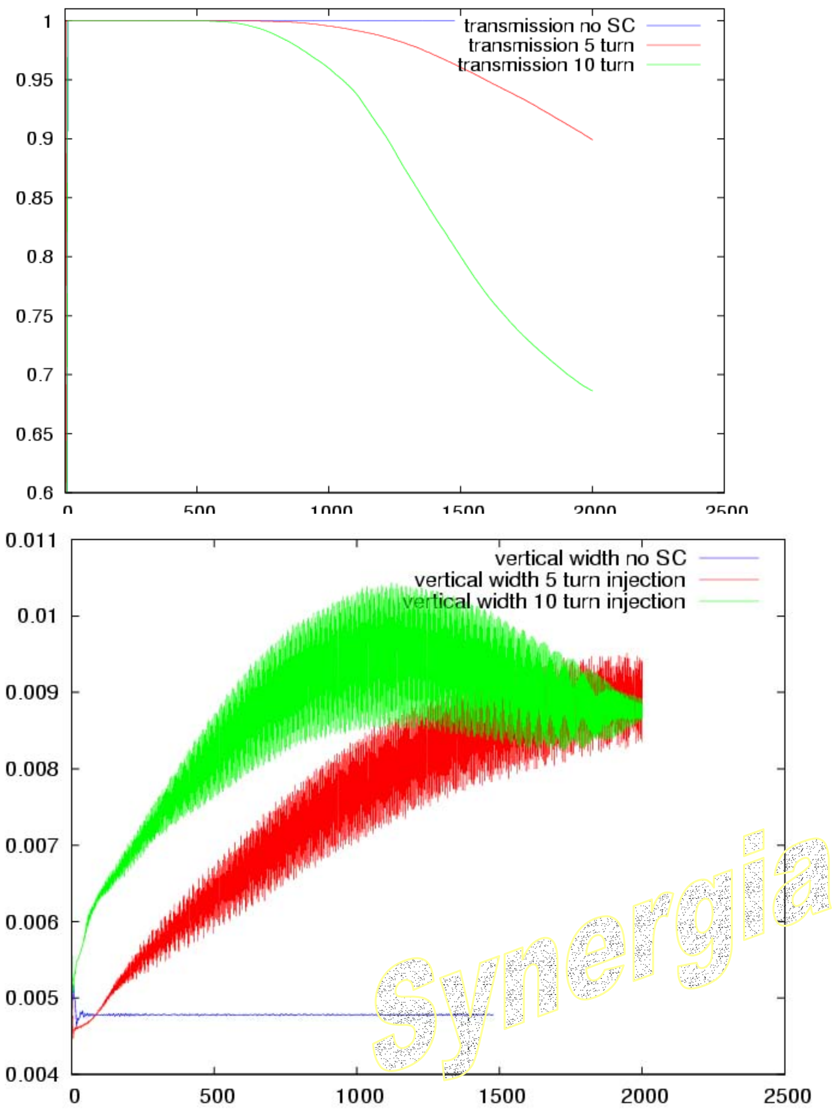


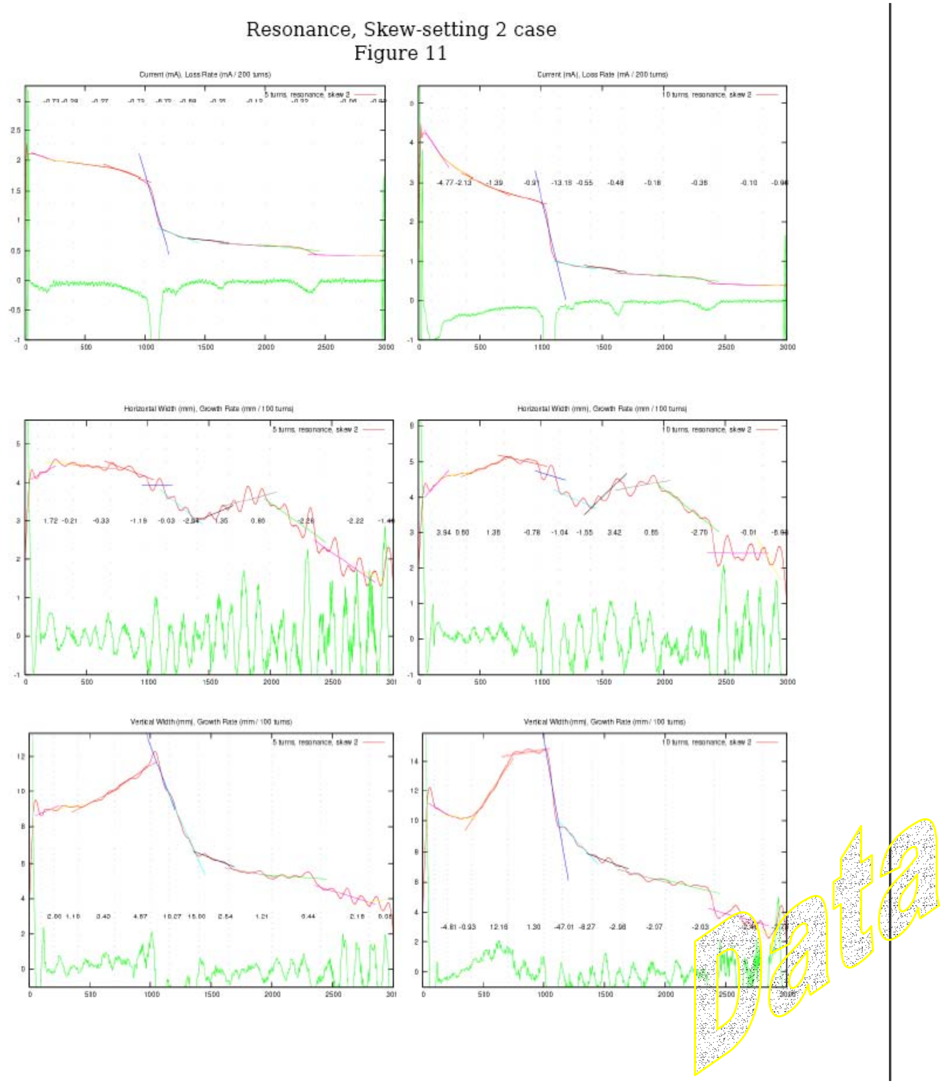
3D Booster simulation including injection, rf ramping, etc. Comparison with experimental data



Space charge tune shift using a coasting beam and scanning the half integer resonance

Qualitative beam loss prediction





Booster close to sum resonance

Significant progress in laser/plasma based accelerator concepts

- **3 Key breakthroughs**
  - **Observation of low-energy spread bunches from LWFA**
  - **Production of 1 GeV beam from LWFA**
  - **Doubling of a 28.5 GeV beam in a PWFA**

The physics behind these breakthroughs has been understood (in some cases predicted) through large-scale PIC codes including SciDAC codes (OSIRIS, VORPAL,QuickPIC)

Plasma-Based Acceleration

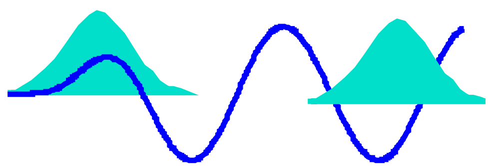
<u>Conventional Accelerators</u>

- Limited by peak power and breakdown
- 20-100 MeV/m

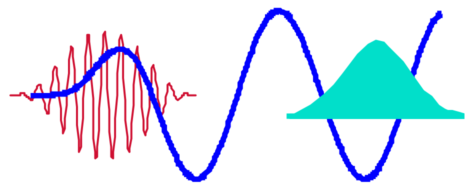
<u>Plasma</u>

- No breakdown limit
- 10-100 GeV/m

- Plasma Wake Field Accelerator (PWFA)
  A high energy electron bunch

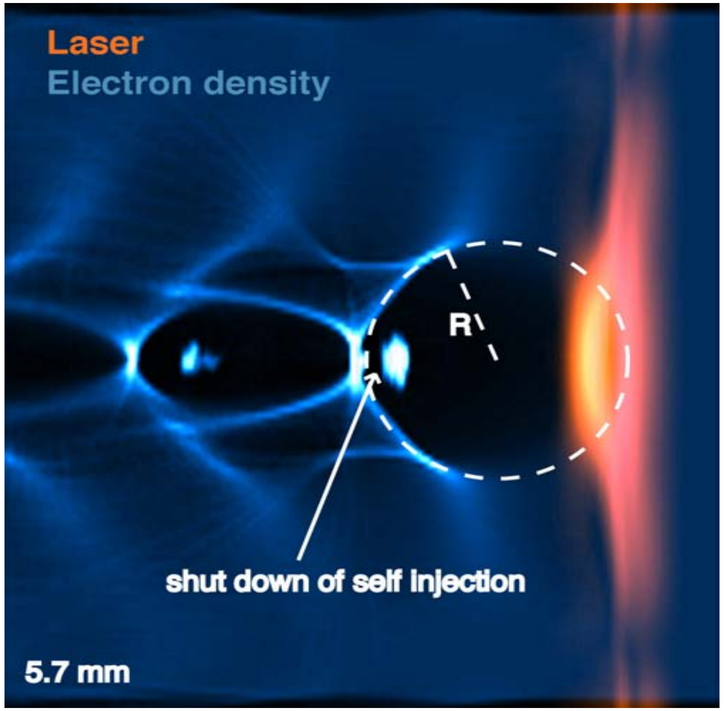


- Laser Wake Field Accelerator (LWFA)
  A single short-pulse of photons



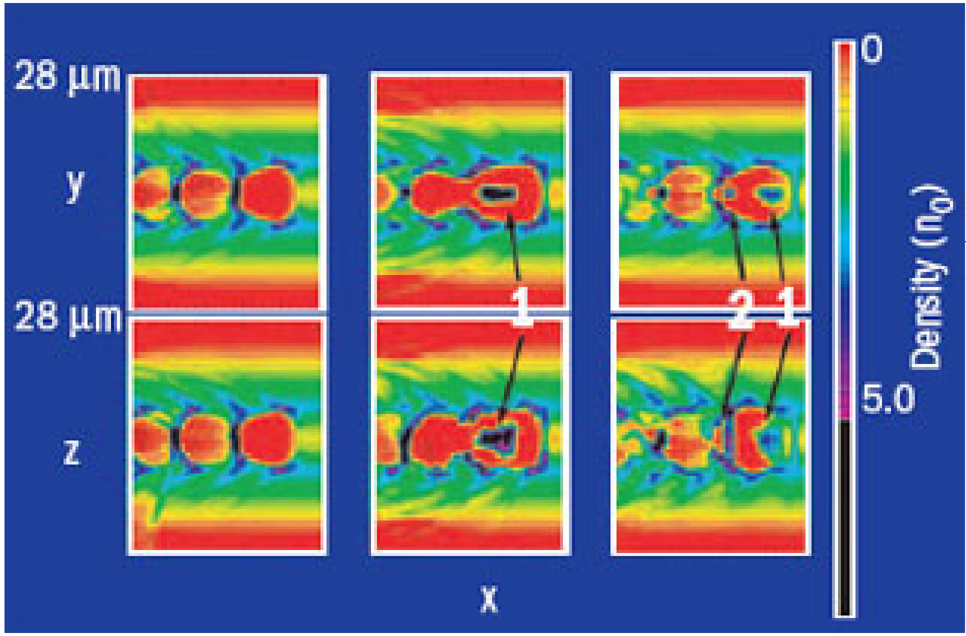
Breakthrough: Production of low energy spread beams from a LWFA

SciDAC codes used to successfully model LWFA experiments (VORPAL simulation, J. Cary/TechX)



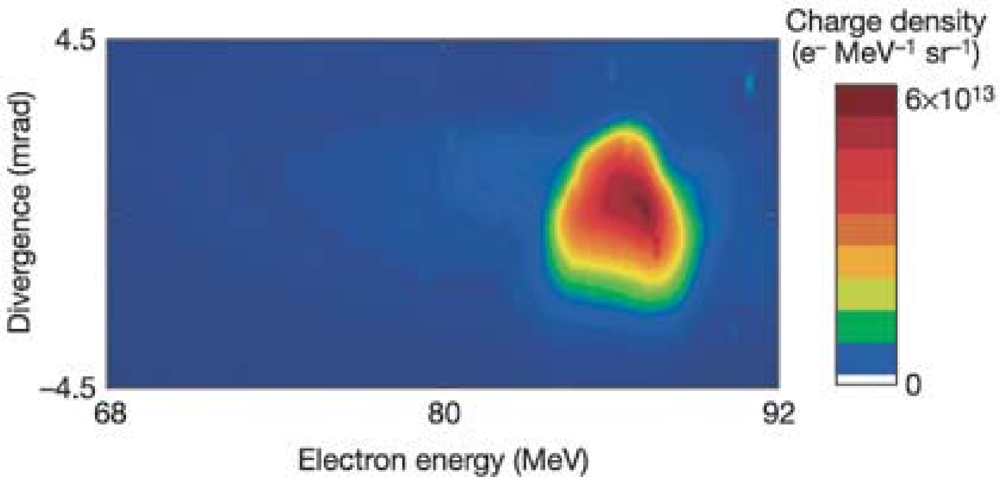
SciDAC codes used to explore and discover paths to 1 GeV and beyond (W. Mori, OSIRIS simulation)

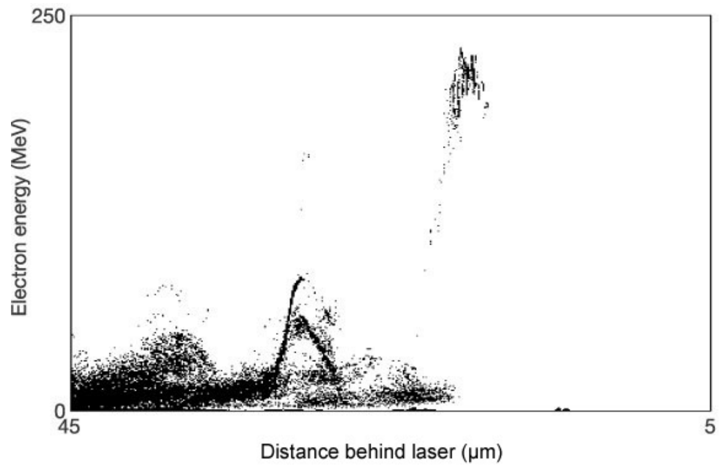
LWFA: prediction, experiment, verification



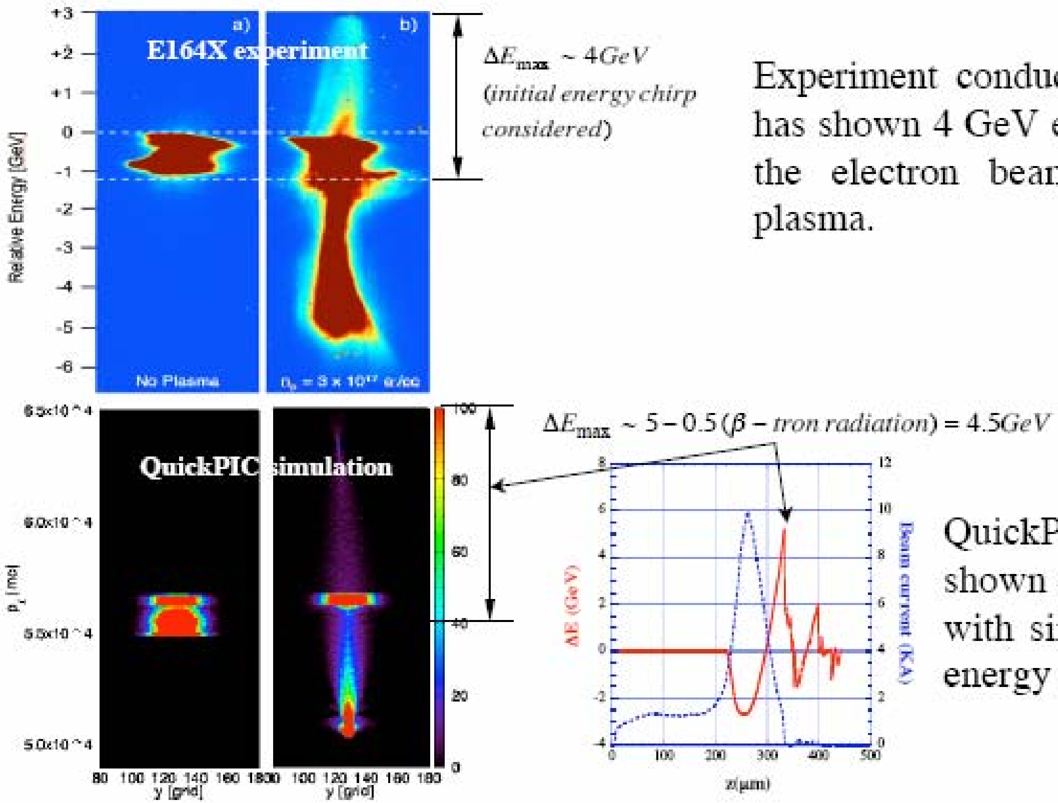
OSIRIS simulation predicting short electron bunch if acceleration path matched to de-phasing length.

Experimental measurement and VORPAL simulation



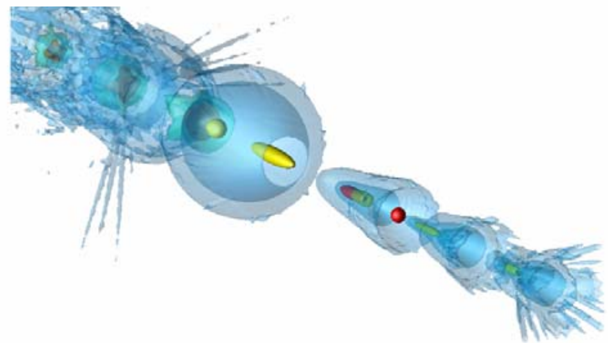


Breakthrough: Energy ~doubling in a PWFA:
Modeling afterburner-related experiments (E167) w/ QuickPIC



Experiment conducted at SLAC has shown 4 GeV energy gain of the electron beam in 30 cm plasma.

QuickPIC simulation has shown 4.5 GeV energy gain with similar features in the energy diagnostics.



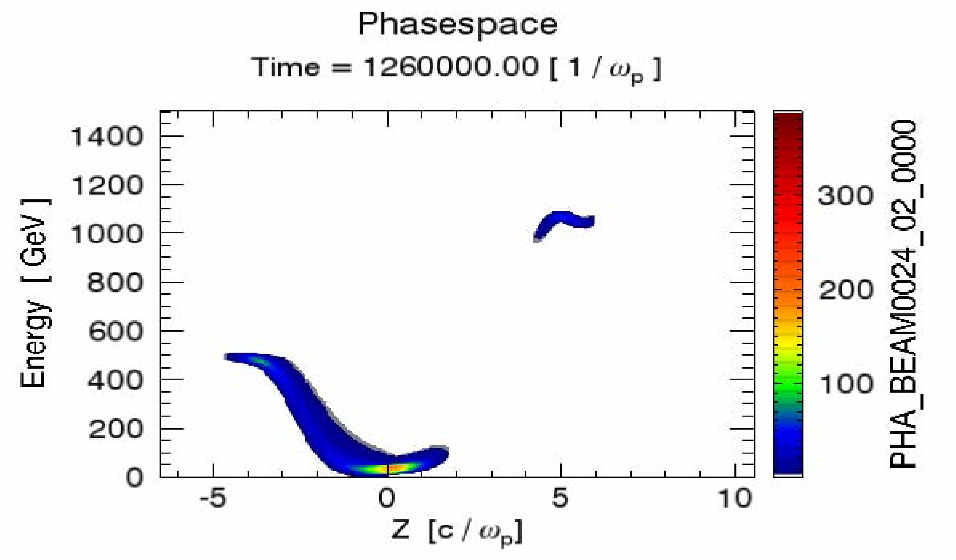
In the most recent energy doubling experiment, the observed results (e.g. the final energy spectrum) agreed very well with QuickPIC predictions.

The simulations played an important role in elucidate the underlying physical mechanism (e.g. beam head erosion) for experimental observations.

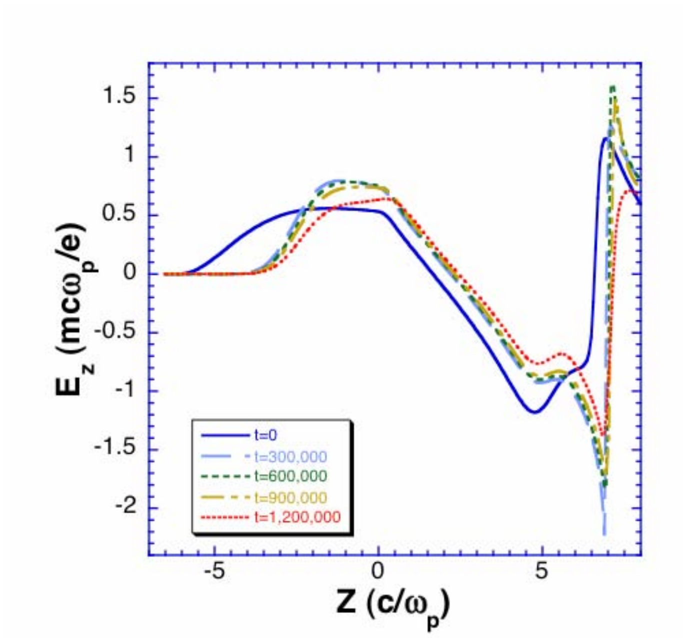
Virtual demonstration of a TeV afterburner

- Energy of 500GeV beam is doubled in only 25 meters
- Despite some hosing wake structure remains stable
- 1TeV energy with 5% energy spread

Energy of drive and trailing beam after s = 25 m



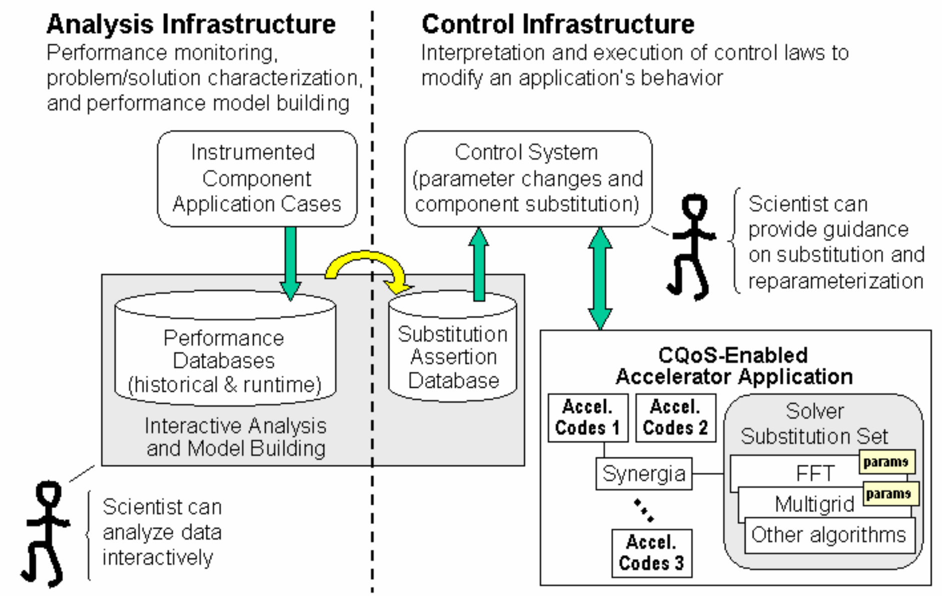
Accelerating field remains stable



Future: SciDAC2 impact of petascale computing

- **Under SciDAC2 we will take advantage of the extraordinary opportunities of petascale computing**
- **Develop a comprehensive accelerator modeling framework capable of multi-physics simulation necessary for end-to-end modeling**
- **Develop common interfaces for code interoperation**

Using SciDAC2 applied math and computer science tools, integrate algorithm optimization into the simulation environment, at the *user level*

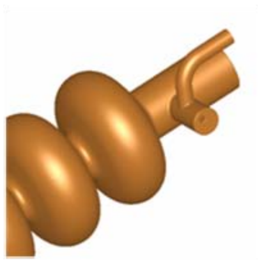


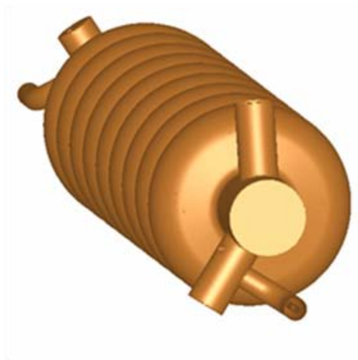
Explore new synergies

Utilize fully self consistent EM+particle PIC codes (VORPAL) for EM design:

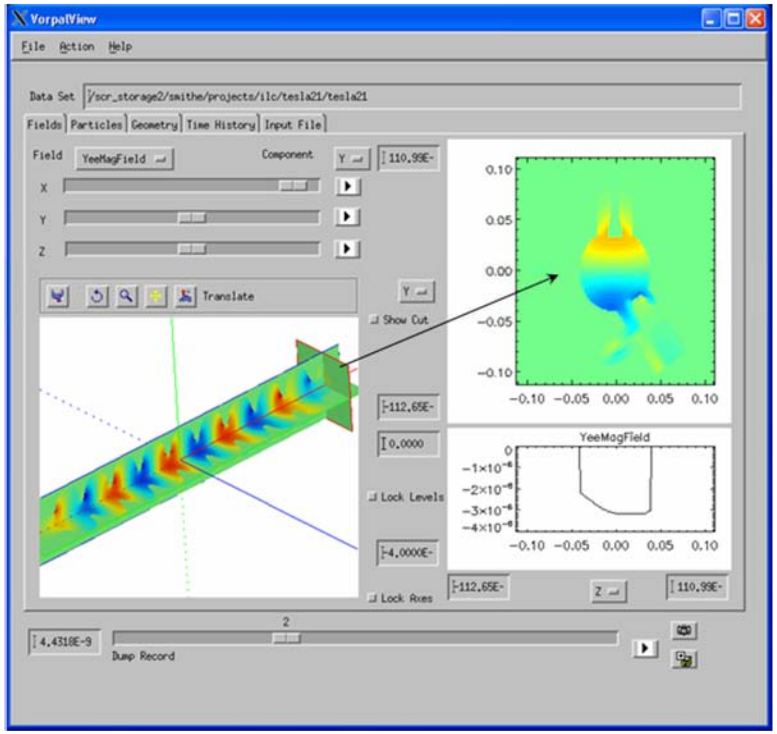
self-consistent propagation in loaded cavities

- secondary emission from cavities
- feedback systems
- beam diagnostics
- mode and wakefield calculations

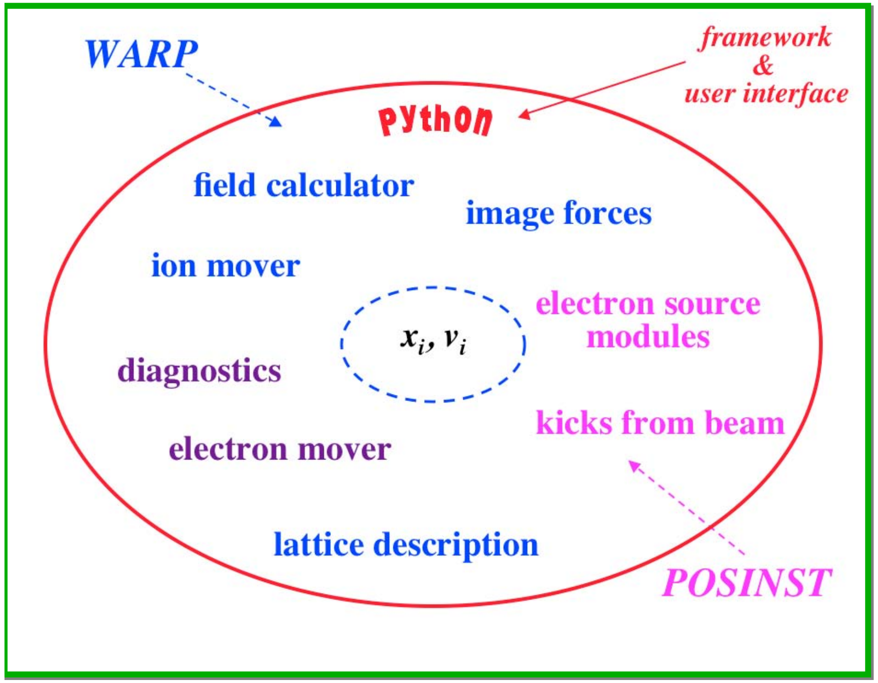




Fully 3D Tesla cavity
VORPAL simulation



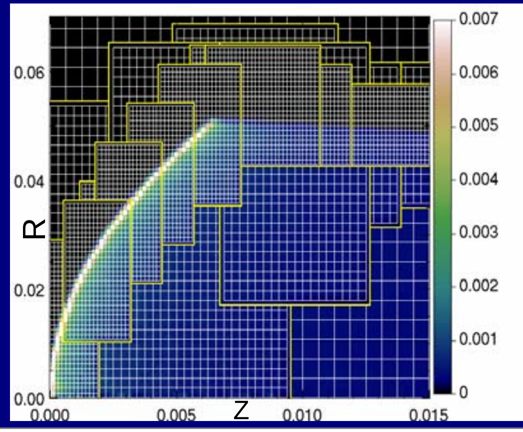
WARP-POSINST hybrid code



+ Adaptive Mesh Refinement

concentrates resolution only where it is needed

Speed-up x10-10^4

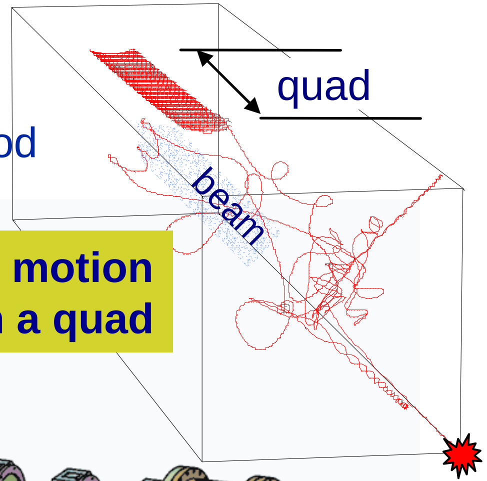


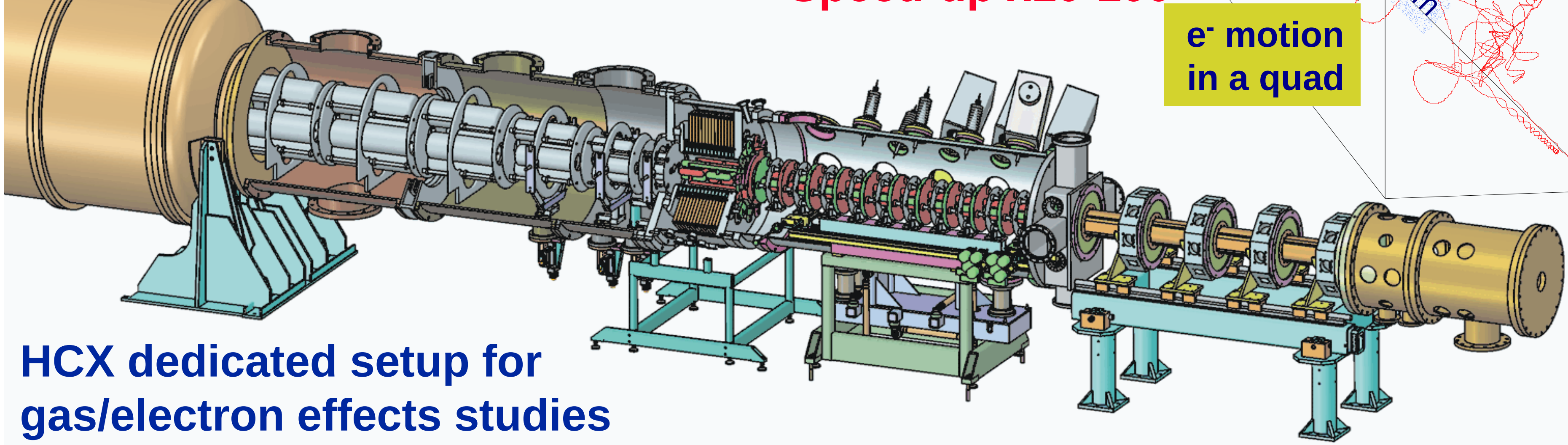
New e^- mover

Allows large time step greater than cyclotron period

Speed-up x10-100

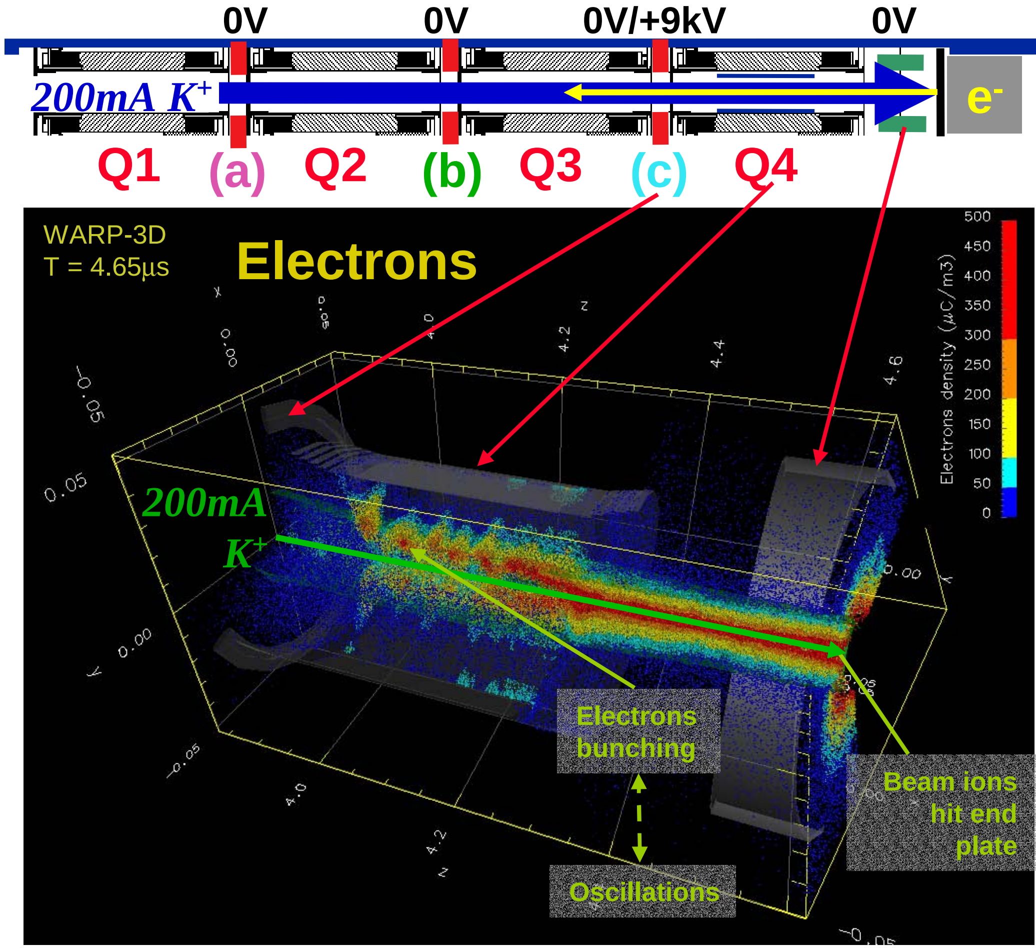
e^- motion in a quad



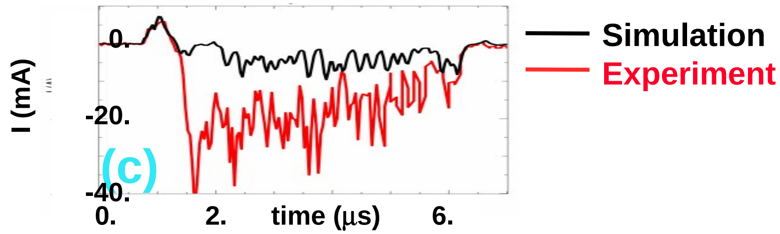


HCX dedicated setup for gas/electron effects studies

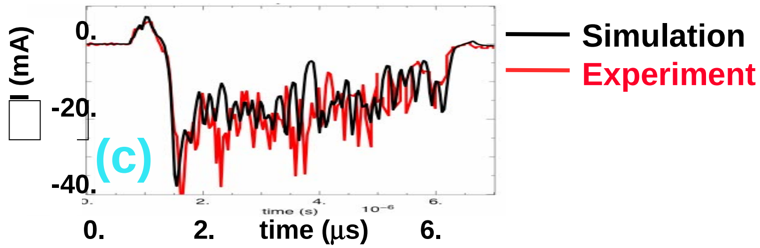
6 MHz signal in clearing electrode: simulation & expt



- **Good test of secondary module**
  - secondary electron emission turned off:



- **run time ~3 days,**
  - without new electron mover and MR, run time would be ~1-2 months!



Excellent agreement with Secondary emission model turned on

M. Furman, J.-L. Vay (LBNL); A. Friedman, R. Cowan (LLNL); P. Stoltz (Tech-X); P. Colella (LBNL)

Illustrates the benefits of collaboration in computational accelerator physics: An OFES code (WARP), combined w/ a OHEP code (POSINST) into a unique parallel capability that will serve both communities.

Application Focus

- **Accelerator design and optimization**
  - **HEP: ILC, LHC, Tevatron, PEP-II, proton drivers**
  - **NP: RHIC, RIA, CEBAF**
  - **BES: SNS, 4th generation light sources**
    - ➔ **emphasis on problems which require large scale (parallel) computing**
    - ➔ **work closely with machine designers and operators to apply the tools**

Application Focus

- **Push the energy frontier in advanced accelerators**
  - **—Explore TeV scale afterburners with high fidelity**
  - **—Explore 10 GeV+ LWFA systems**
- **Provide the tools for near real-time feedback to accelerator control rooms and beam-based experiments**

SciDAC2 collaboration: J. Cary (Tech-X), K. Ko (SLAC), W. Mori (UCLA), R. Ryne (LBNL), P. Spentzouris (FNAL)