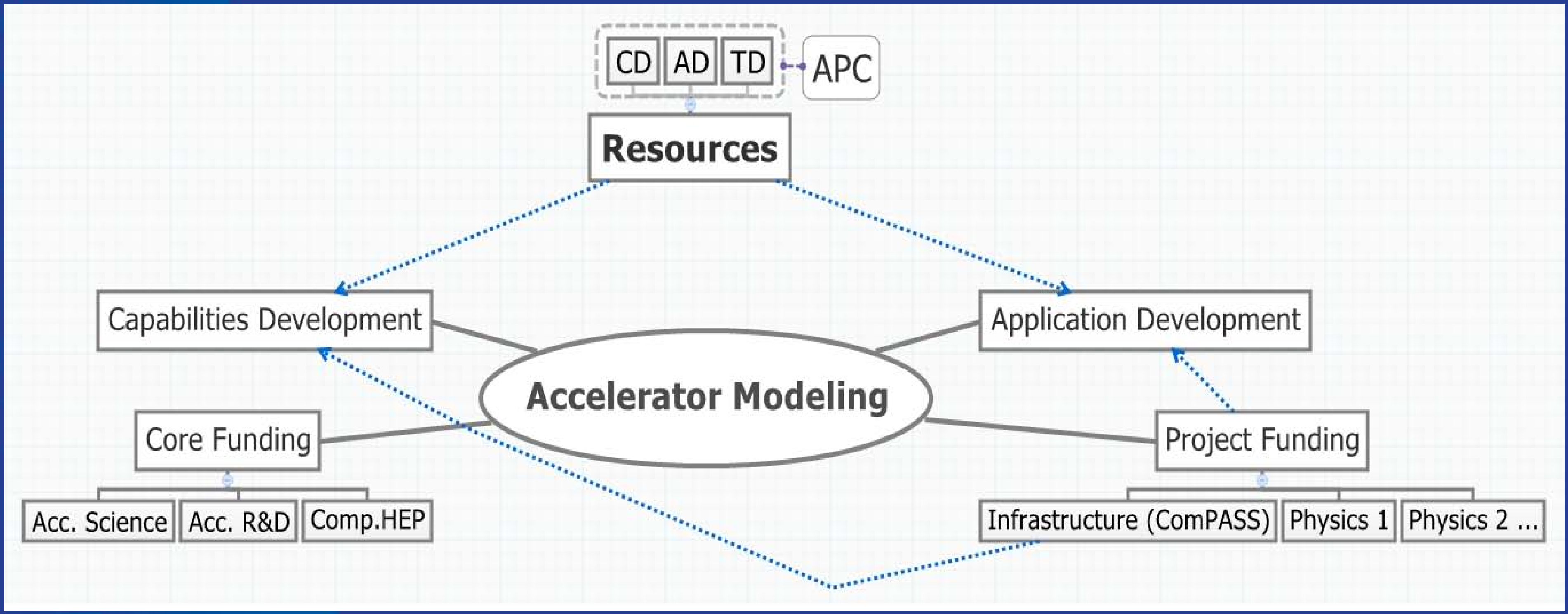
Accelerator & Detector Simulation

Panagiotis Spentzouris, CD/ADSS

ACCELERATOR MODELING

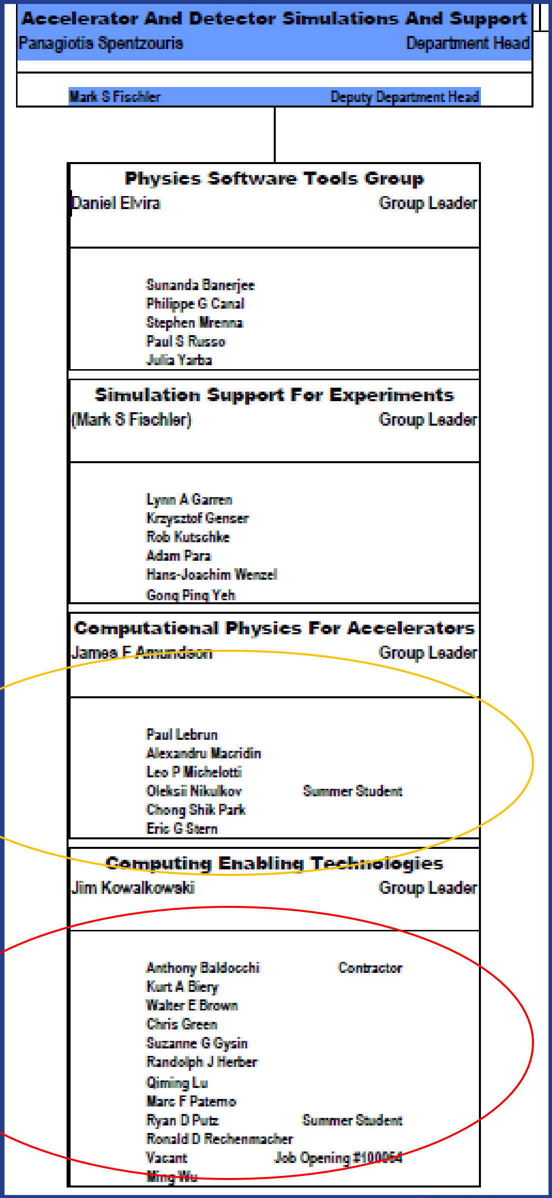
Accelerator Science Briefing - August 23, 2010

Accelerator Modeling Activity Highly Leveraged



Computational Accelerator Physics at FNAL: CD/APC resources

- Effort concentrated in CD/ADSS, but work closely with AD and TD personnel, in the context of the APC, to develop accelerator science applications
  - 4 FTE total in ADSS/CPA
    - Both core and project funds (~50/50 split): SciDAC, Project-X, Mu2e
  - Services and generic infrastructure development support (tools, new technologies) from ADS/CET



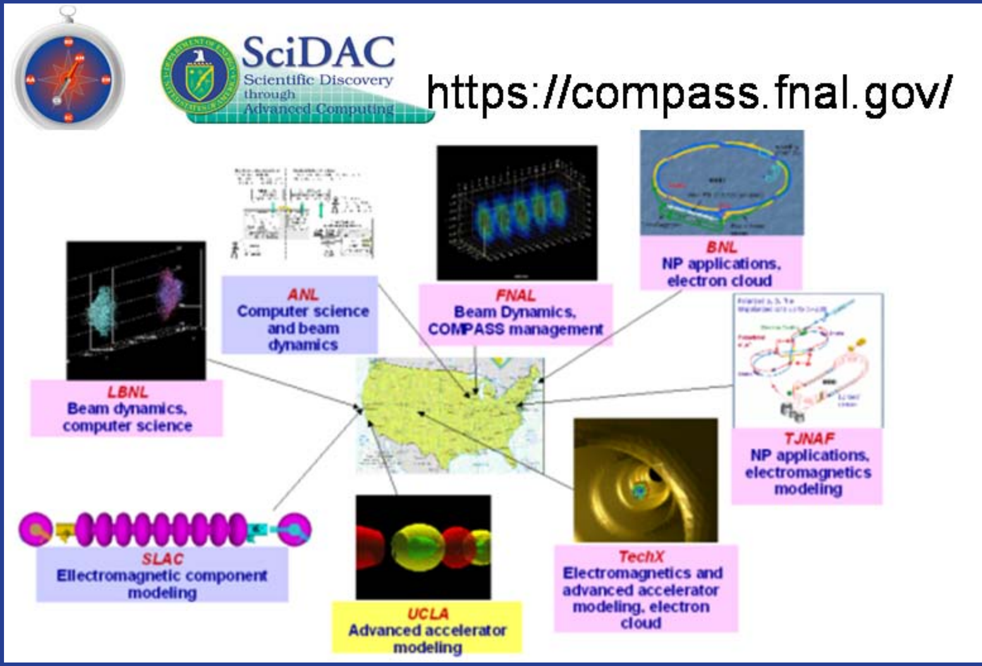
Rich capability and application development program

Highlights

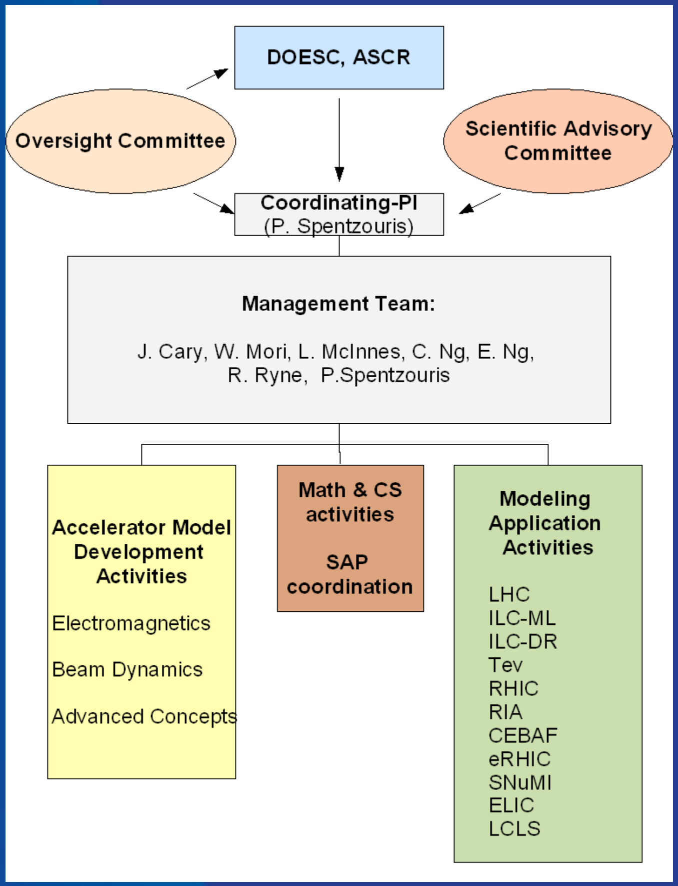
Capabilities	Application	Code
Accelerator design	All	CHEF, MICCD, LLSC, HELIX
Beam Beam	Tevatron LHC (LARP) μ collider	BeamBeam3D, BBSIM, Lifetrac
e-cloud	Project-X ILC R&D	Posinst, VORPAL ORBIT
Space-charge & impedance	Run II Project-X μ2e	Synergia ORBIT
Beam shaping: crystal collimation, hollow beams	LARP R&D	STRUCT, MARS, WARP, Lifetrac

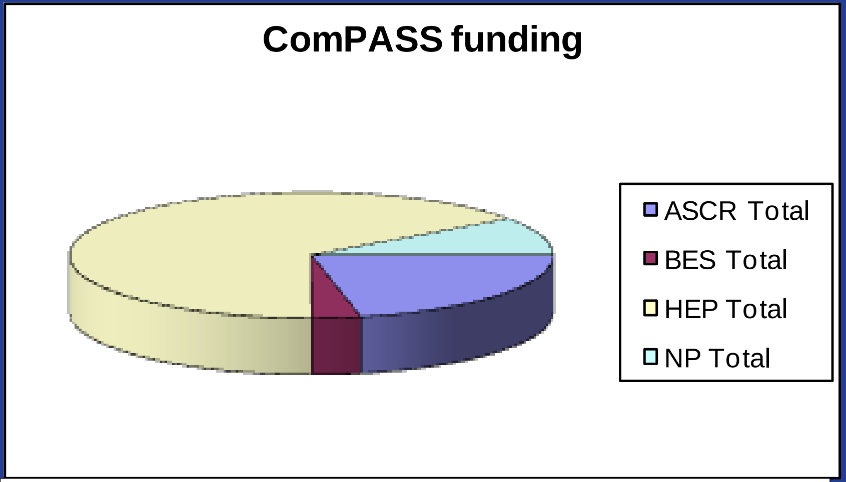
Accelerator Modeling Project: ComPASS

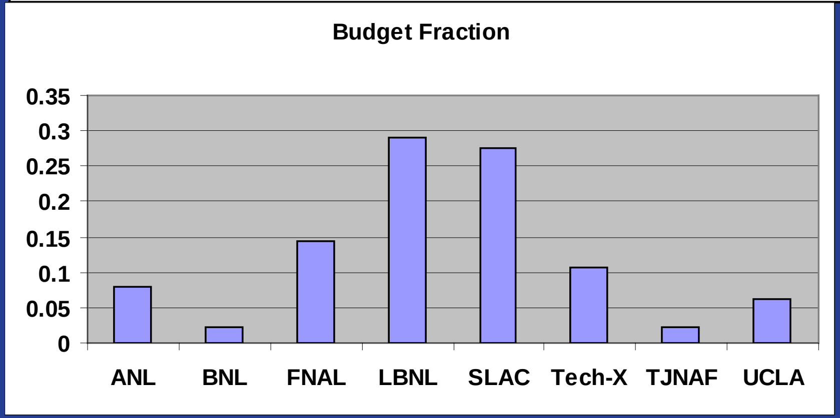
- We lead the SciDAC2 ComPASS project. The collaboration aims to develop HPC accelerator modeling tools for
  - Multi-physics, multi-scale for beam dynamics; "*virtual accelerator*"
  - Thermal, mechanical, and electromagnetic; "*virtual prototyping*"
- The Fermilab team focuses on beam dynamics capabilities and application development



ComPASS







- Total funding ~3.0 ($M)/year, for 5 years (FY07-FY11)
  - FNAL receives funding for 2.2 FTE (~500 ($k)/year)
- Submitted (lead institution) proposal for exascale co-design

Exascale co-design center proposal

Exascale Co-Design Center for Accelerator Modeling

Lead Institution: Fermi National Laboratory
Principal Investigator: Panagiotis Spentzouris
M.S. 203, P.O. Box 500, Batavia, IL 60510
phone: (630) 840-4342; email: `spentz@fnal.gov`

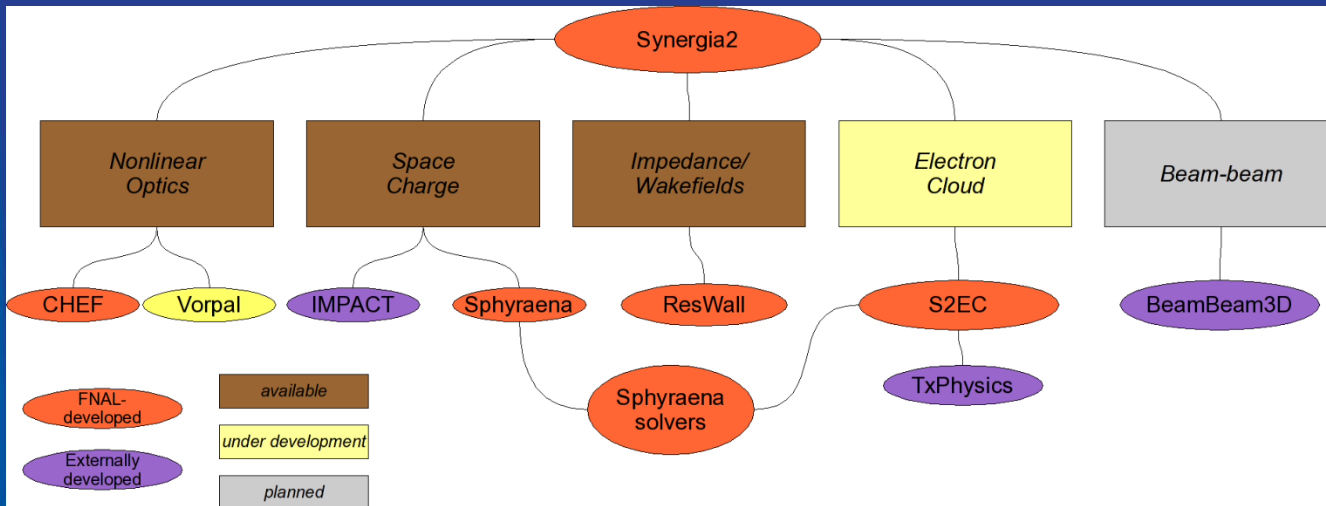
Co-PIs: C. Janssen (Sandia), B.Norris (ANL), D. Quinlan (LLNL), J. Shalf (LBNL)

Senior Researchers: L. McInnes (ANL), J. Amundson, C. Green, M. Paterno (FNAL), H. Childs, A. Shoshani, S. Williams, K. Wu (LBNL), H. Adalsteinsson (Sandia), J. Cary, P. Messmer (TechX), W. Mori, G. Reinman, C. Anderson, V. Decyk (UCLA)

Project Summary

Particle accelerators are critical to scientific discovery in the DOE program in America and, indeed, the world. The development and optimization of accelerators are essential for advancing our understanding of the fundamental properties of matter, energy, space and time. In the past ten years, high-performance-computing (HPC) accelerator modeling tools have been employed to tackle some of the most difficult accelerator science problems, using codes developed under the SciDAC program. These codes obtain good scalability and parallel performance efficiency on many hundreds to a few thousand processors on current supercomputers. In order to continue supporting accelerator science advances it is imperative that we utilize emerging extreme scale computing plat-

Accelerator modeling tools development: Synergia



- Beam Dynamics framework with fully 3D PIC capabilities
  - Utilizes both native and external physics modules/algorithms
  - Includes space-charge & impedance (single and multi-bunch)
  - Single-particle physics from CHEF
- Runs on desktops, clusters and supercomputers
- Flexible framework allows for fully dynamic simulations including ramping, feedback, etc
- Development and support , ongoing activity
  - Capabilities, portability, user interface

Recent Synergia development: implement careful treatment of impedance of laminated structures

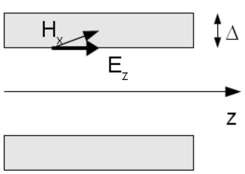
Literature calculations in frequency domain involving different regimes don't trivially translate to a "simulation ready" wake function.

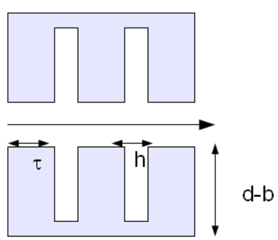
➢Capability required for FNAL Booster modeling

Longitudinal impedance

$$E_z = -X(\omega) H_x$$

$$Z^{\parallel}(\omega) \approx \frac{X(\omega)}{2\pi b}$$





$$X_{RW}(\omega) = \frac{1+i}{\delta\sigma}$$ infinite wall

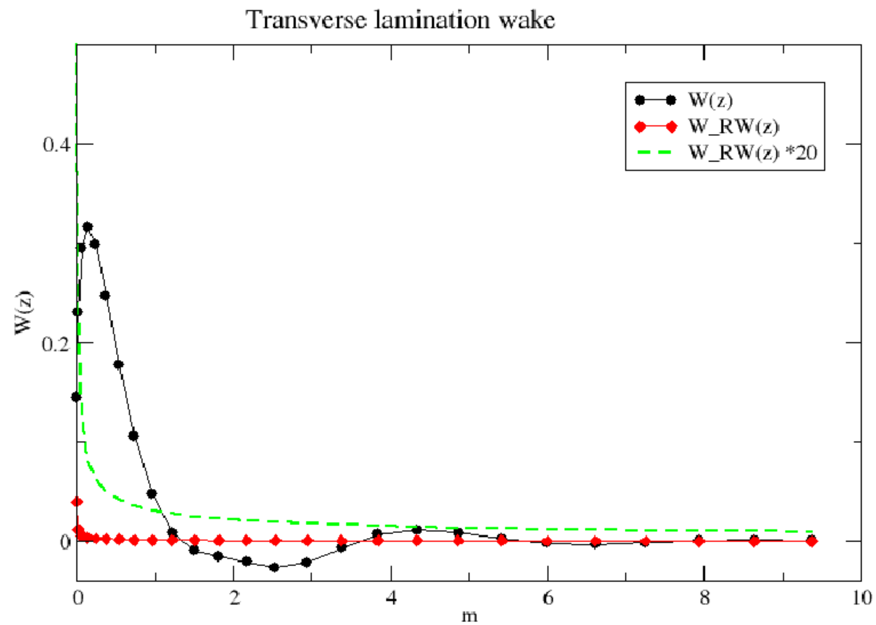
$$\delta = \sqrt{\frac{2}{\omega\mu\sigma}}$$

$$X(\omega) = \frac{(\tau X_l + h X_c)}{\tau + h}$$

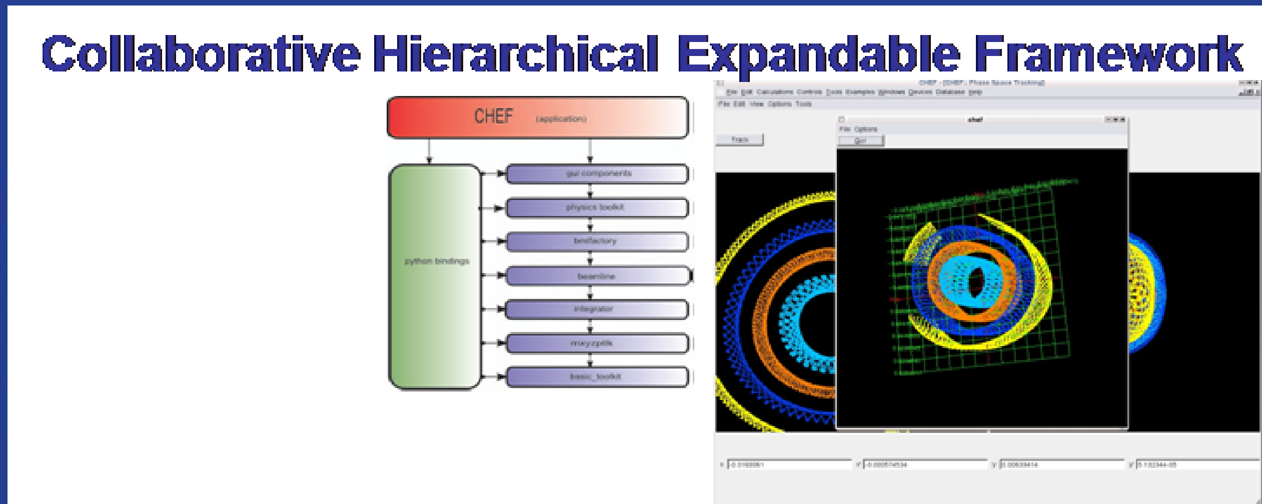
$$Z^{\parallel}(\omega) \approx \frac{X(\omega)}{2\pi b}\frac{1+\eta}{1-\eta}$$ finite thickness

$$\eta = e^{-2(1+i)\frac{\Delta}{\delta}}$$

Low ω $X_c = 2\frac{d-b}{h} X_{RW} \approx 400 X_{RW}$

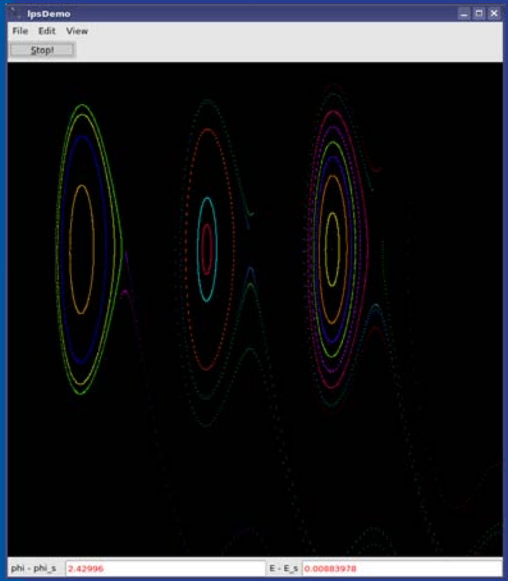


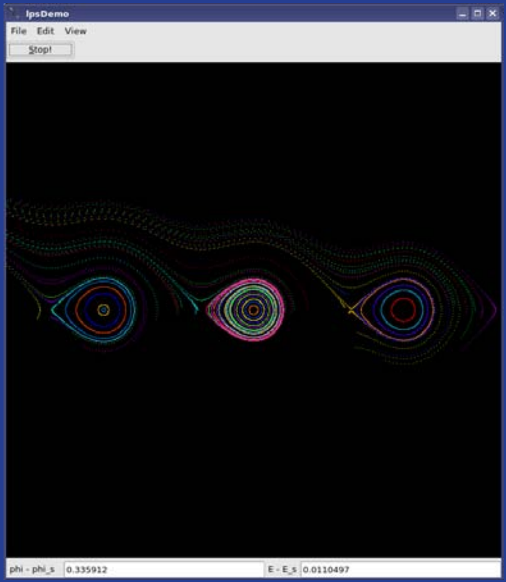
Tools development, continued: CHEF



- CHEF originally developed at Fermilab starting in the early 90’s
- Single-particle optics with full dynamics
- Can be reduced to arbitrary-order maps
  - We have done demonstration calculations in Synergia to 15th order
- Supports customizable propagators (fully extendable)
- MAD and XSIF parsers
  - Internal representation not limited by MAD parameters
- Development and support, ongoing activity

Recent CHEF development

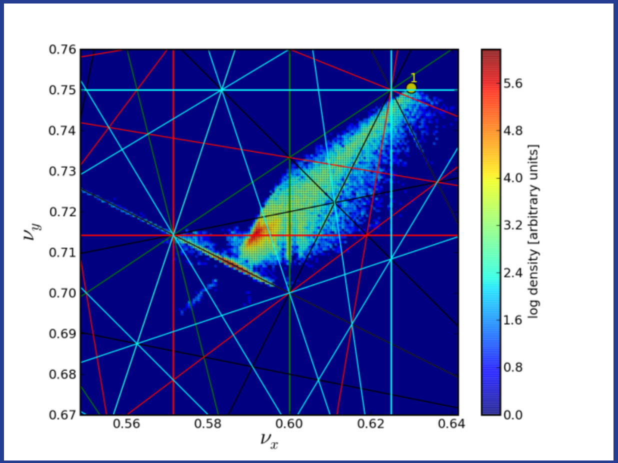


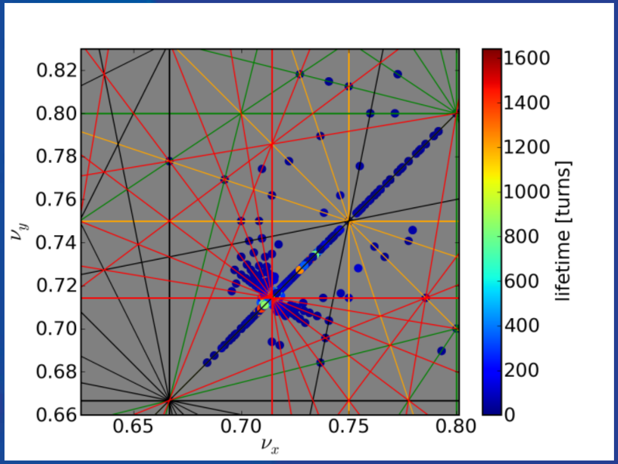


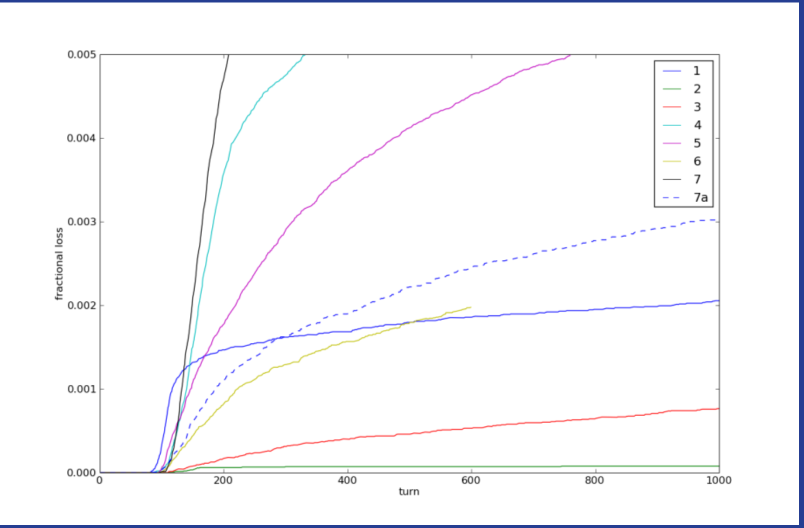
- Implement matching and beam generation using normal form coordinates

Recent Synergia application: Mu2e extraction design

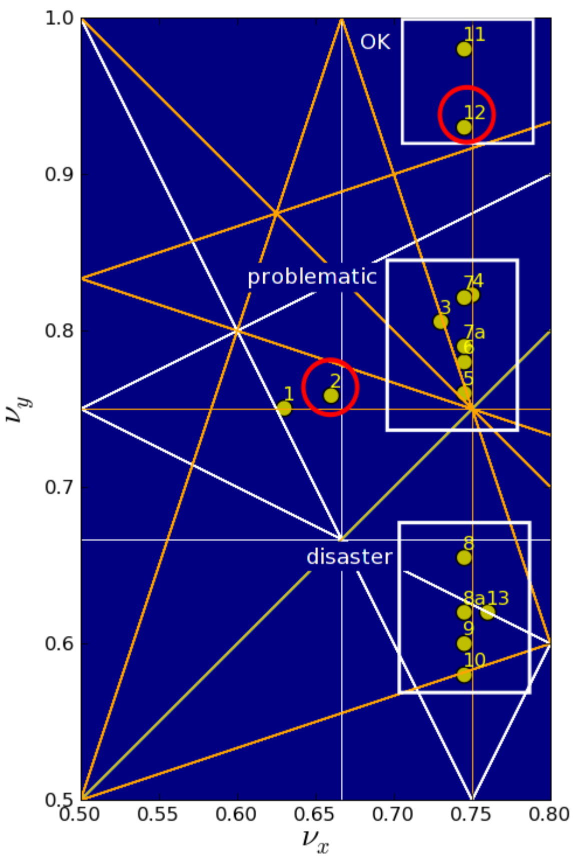
- Model resonant extraction including space-charge at the Debuncher : Mu2e requires 10^5 more particles than current operations!
  - Optimize tune and resonant extraction parameters to minimize losses

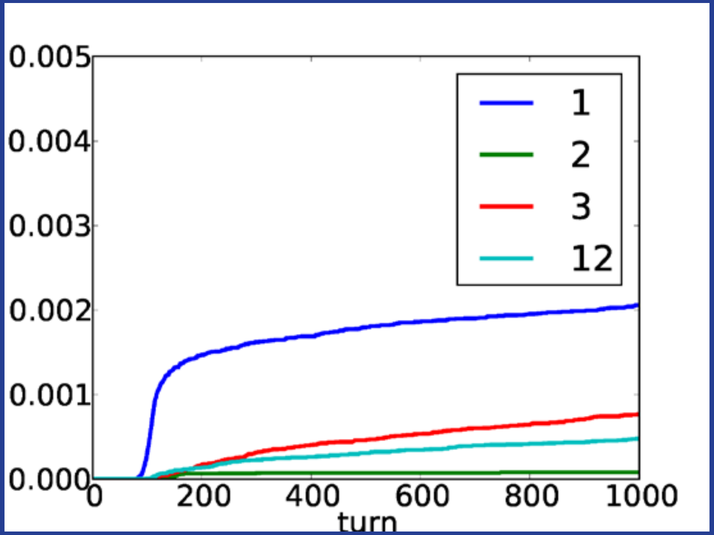






Mu2e design parameter scans

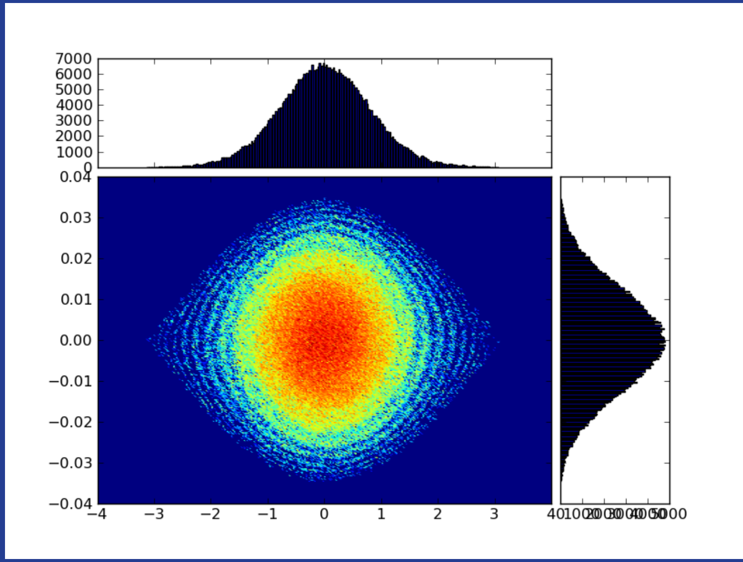


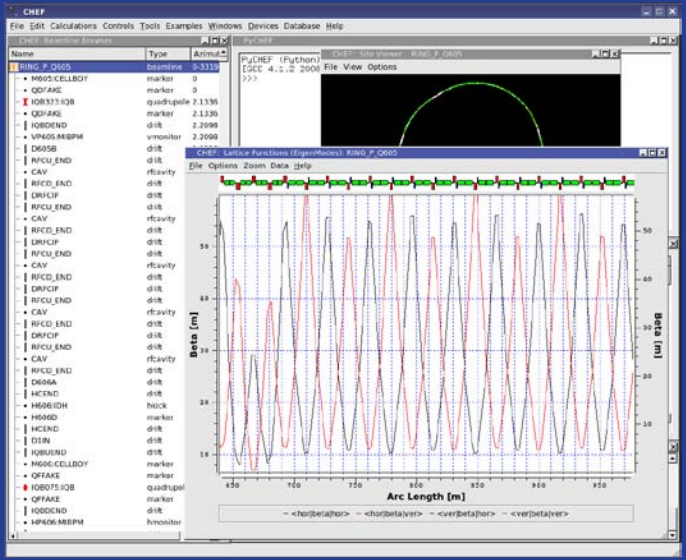


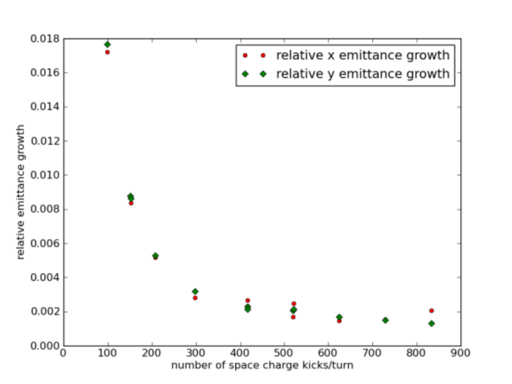
Even the most optimal case has unacceptable losses, so our studies resulted in changing the design (lower intensity), which we are currently studying with CHEF and Synergia.

Accelerator Science Applications: MI space-charge (Synergia)

- Begin modeling space charge effects and mitigation techniques for Main Injector with Project-X beam parameters
- Objective is to extend the model to include realistic apertures and fringe fields and study losses and mitigation (such as 2nd harmonic rf, etc) if necessary

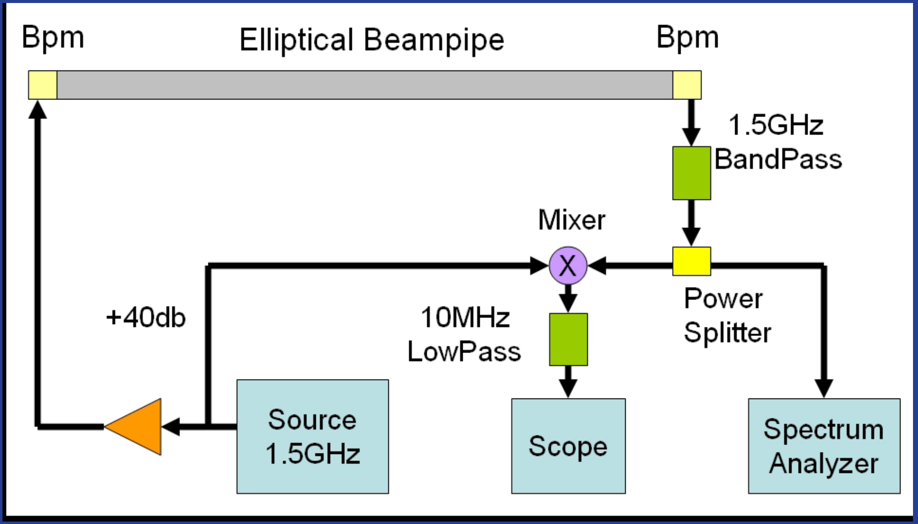


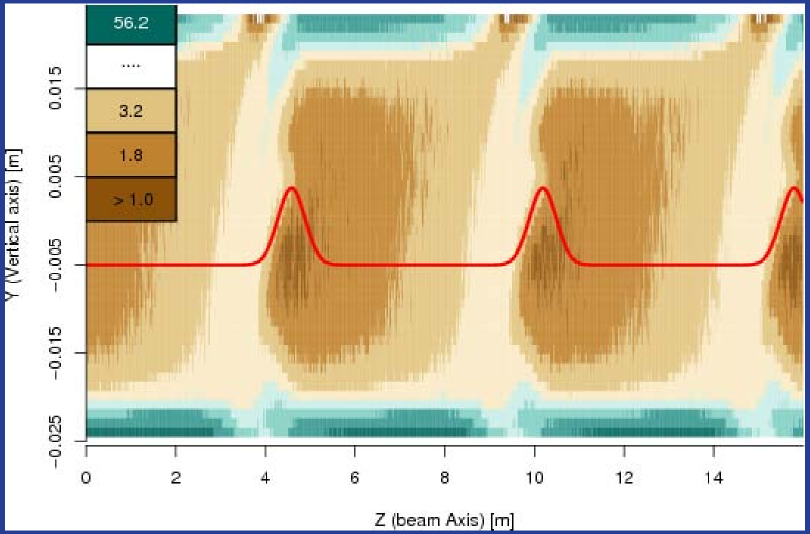




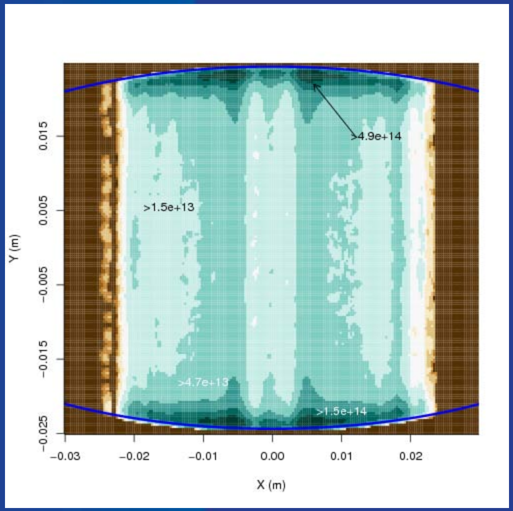
Accelerator Science Applications: Project-X ecloud generation/detection in the MI

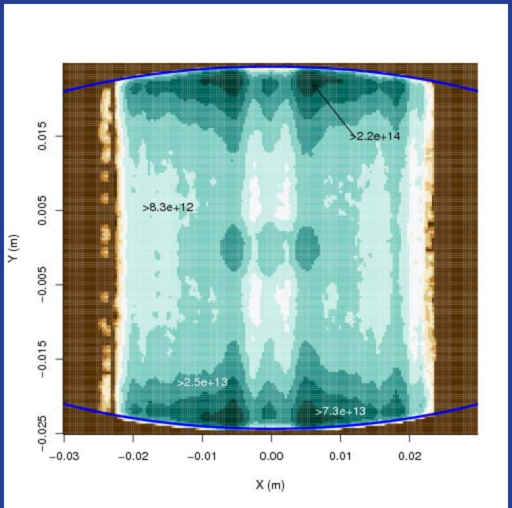
- Simulation of microwave transmission properties through an e-cloud at the Main Injector with VORPAL
  - Essential for utilizing e-cloud detector based on microwave propagation
  - Multi-scale, multi-physics problem
- Model MI beam line: either short (0.25 m) in a dipole or long (12.6m) to fully simulate the microwave absorption experiment, which includes dipoles and a quadrupole

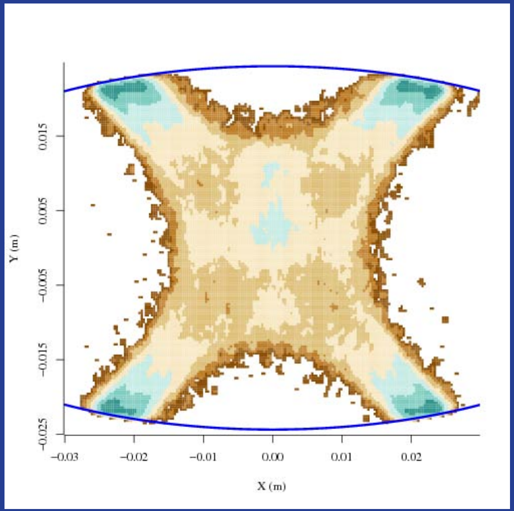




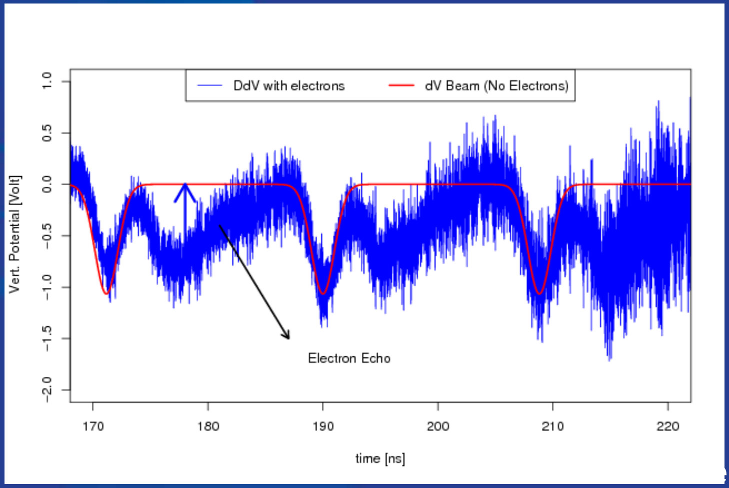
Intrinsically 3D multi-scale problem







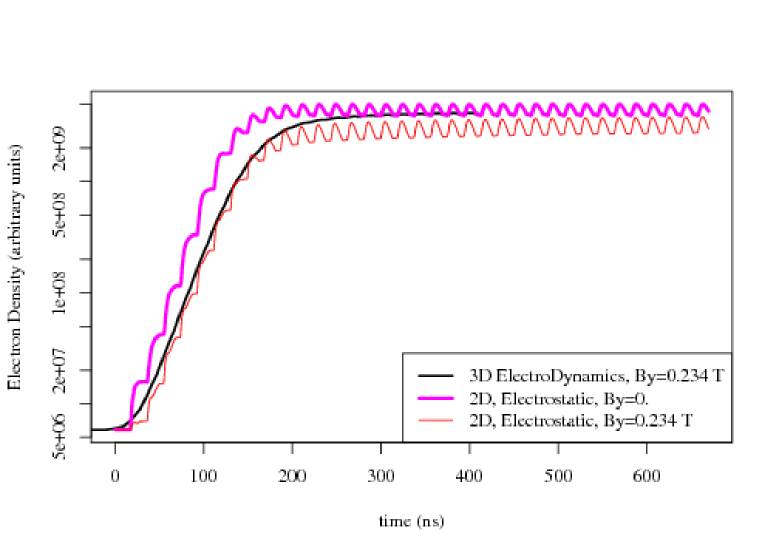
- Spatial distributions of the cloud has been studied in details, during the pinch (acceleration phase) and the relaxation phase, in between proton bunches, where the electrons drift along magnetic field lines towards the wall.

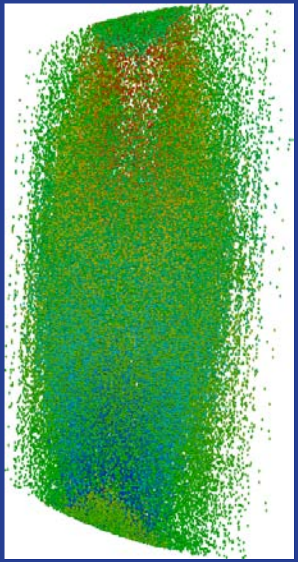


BPM response showing the beam signal and the noise from the EC, for a short BPM (~5 to 10 cm) located in a dipole.

Full 3D treatment necessary

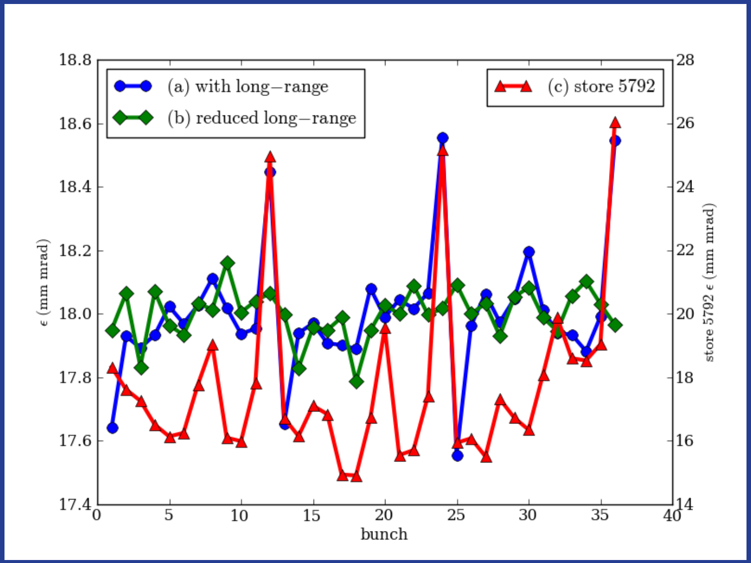
- Earlier analysis modeled EM fields using 2D approximation
- Our recent results comparing full VORPAL (3D) to VORPAL 3D and POSINST (ran at FNAL and LBNL) show that prediction for saturation of e-density is affected (factor ~2.5) by such approximation

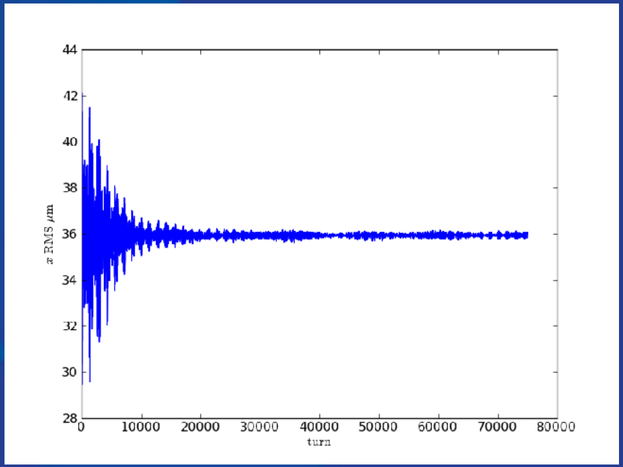


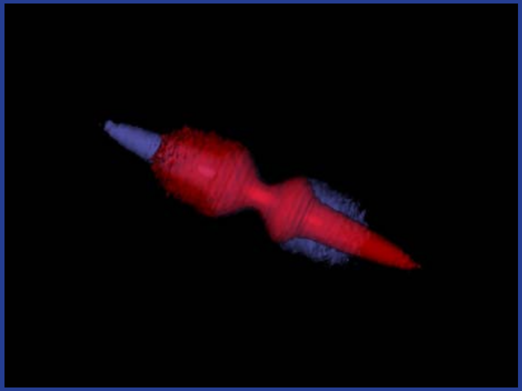


Accelerator Science Applications: Tevatron

- Model strong-strong beam-beam & impedance effects with 36 on 36 bunches at the Tevatron (BeamBeam3D)
  - Results used to optimize chromaticity settings at the squeeze, resulting in reduced losses

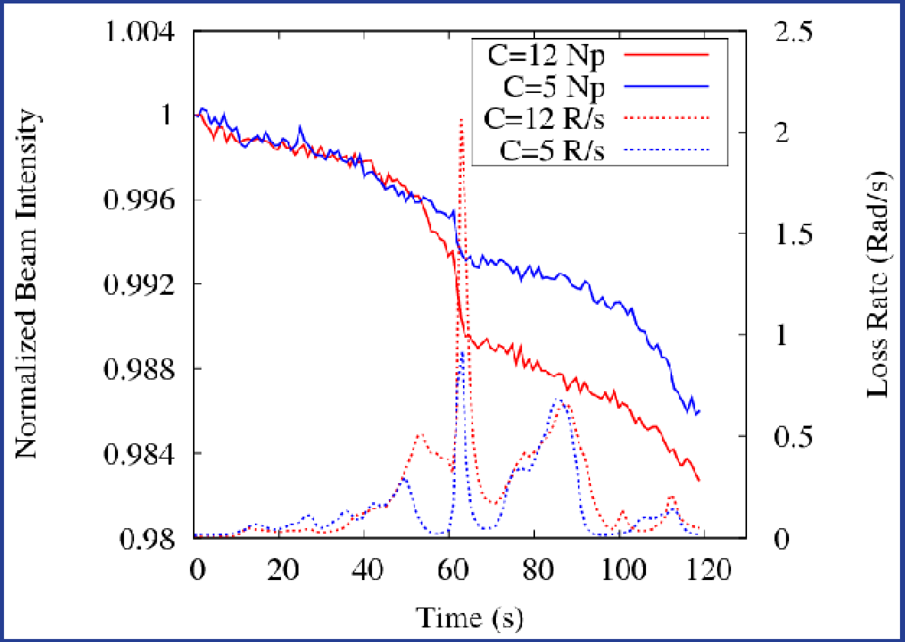






Tevatron, continued

- Success! Simulations support the use of lower chromaticity during injection!
  - A. Valishev, PAC2009, “Recent Tevatron Operational Experience”
  - Stern et al, “Fully 3D multiple beam dynamics processes simulation for the Fermilab Tevatron”, published in PRSTAB 2010.
  - Included in the highlights of the accomplishments of seven years of SciDAC



Issues

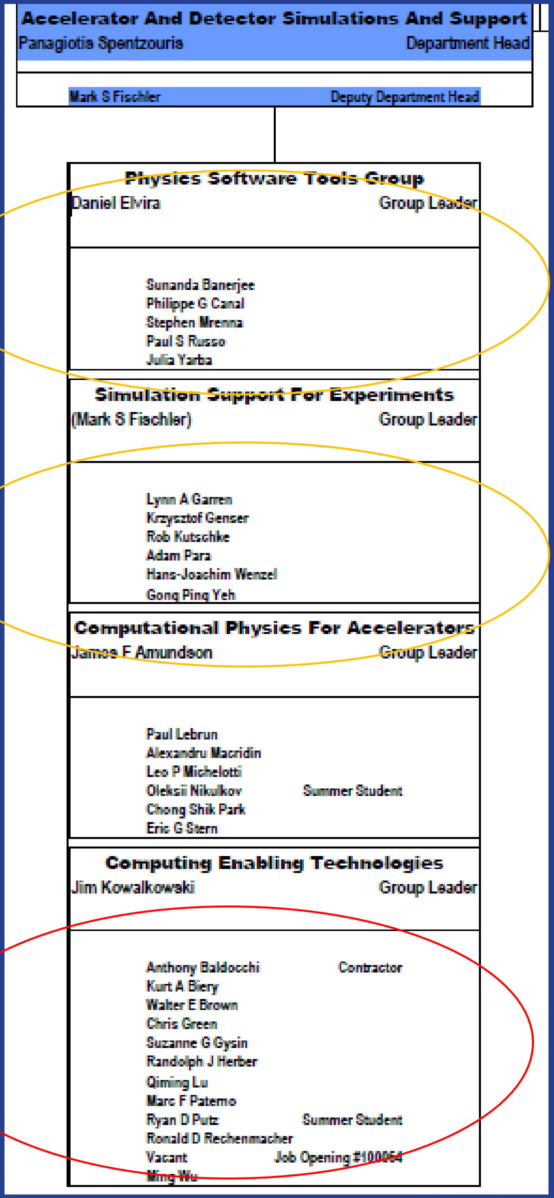
- Highly leveraged activity
  - Negative changes to any of the funding sources very disruptive
- Currently, we can execute our plan on development (SciDAC) and support of activities (physics project funds) with core funding providing the flexibility (buffer) to quickly respond to high priority requests in either front
  - Such flexibility quickly degrades with any loss of effort
- ComPASS has been a successful project, but SciDAC2 funding ends after FY11
  - Uncertainty on size and structure of SciDAC3
  - Uncertainty on relation of SciDAC3 to the co-design centers
- We are confident that we will be able to successfully compete in either program, but we will need to work with OHEP to define our strategy

Detectors, generators, and infrastructure

HEP EXPERIMENT

Highly leveraged activity

- Capability and applications development in areas that are synergistic with our LHC (CMS, LPC) and IF program (Mu2e, neutrinos) activities
- Provide general user support (at the application level)
- Services and generic infrastructure development support (tools, new technologies)



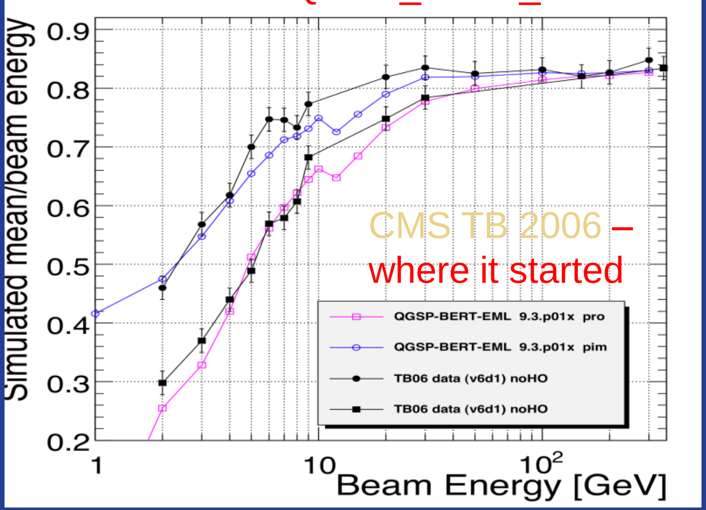
Fermilab

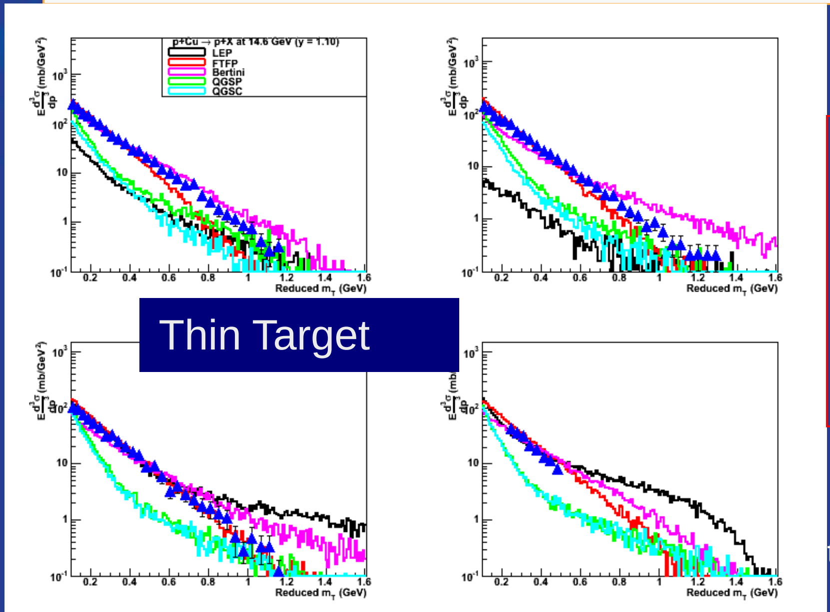
Hadronic Physics in G4

S. Banerjee, D. Elvira, J. Yarba

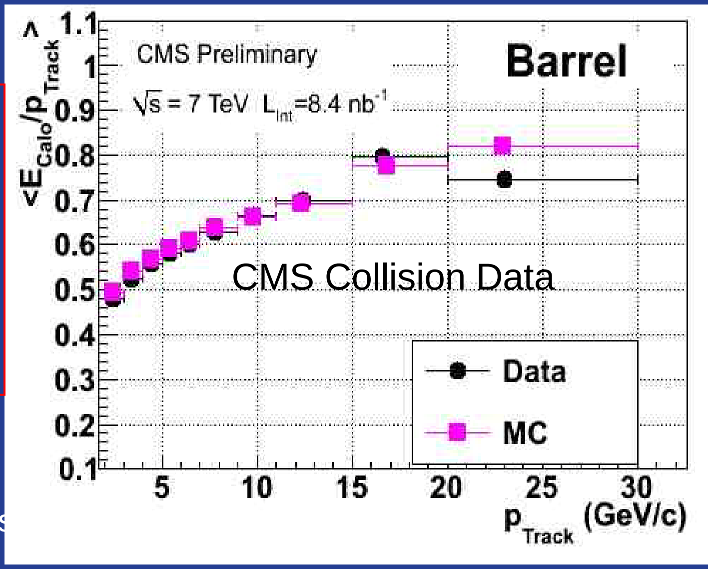
- **Focus on:**
  - Models Validation vs Data
  - Models Development/Evolution
  - Overall Comparison
- **Data Sets:**
  - Thin Target Data (1.4-14.6GeV/c)
  - CMS TestBeam Data
  - Isolated Particles in CMS Collision Data

Evolution QGSP_BERT_EML





CMS: Mean energy of p, π agree to <3% for beam energy >2 GeV

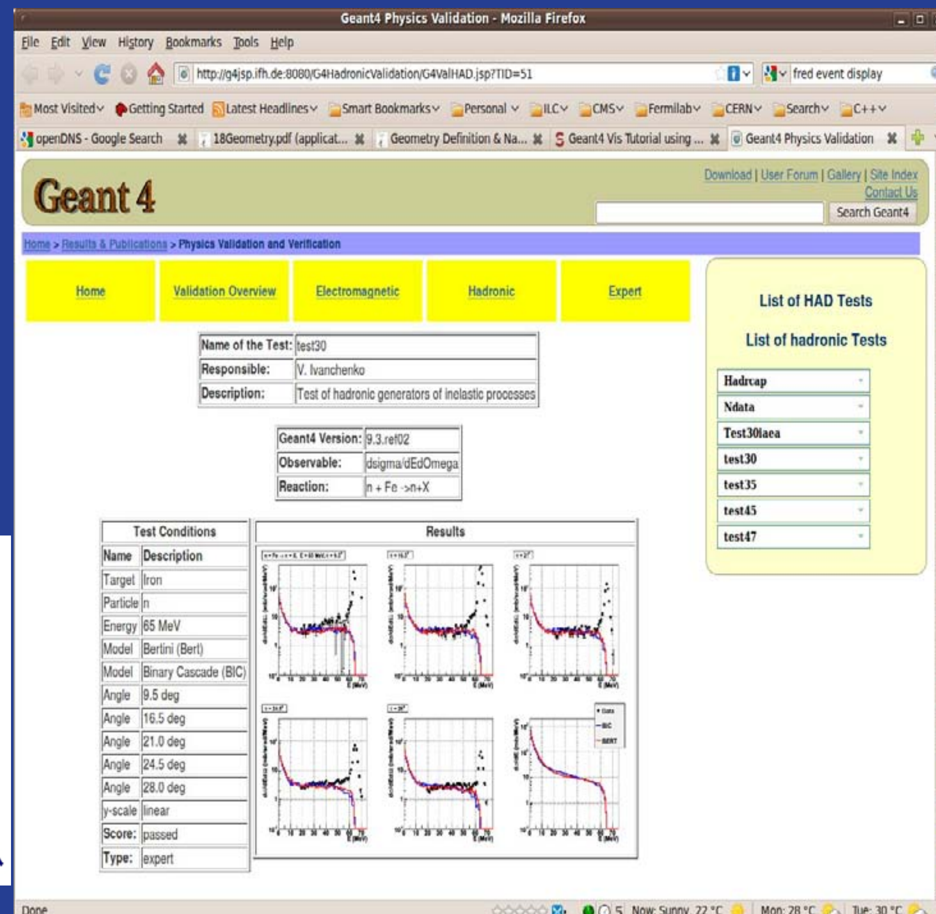


Framework for G4 Hadronic & EM Physics

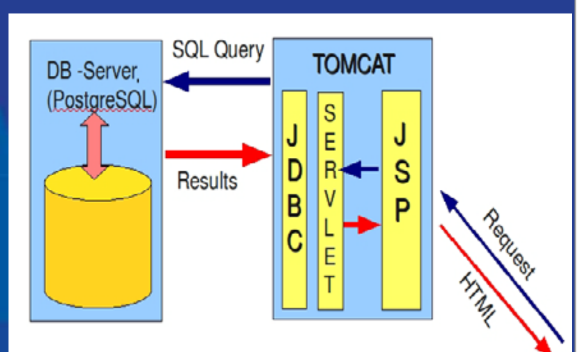
S. Banerjee, D. Elvira, H. Wenzel, J. Yarba in collab. with A. Schaelicke (DESY)

- Motivation:
  - Standardize testing among model developers
- Benefits:
  - Improve consistency
  - Quality assurance of test procedures
  - Access at central location
  - Share the tools and resources
  - Share the comparison reference
  - Track history

Deployed at:
http://g4jsp.ifh.de:8080/G4HadronicValidation/



Web Application:
Store the results and tests
Publish the results



G4 Computing Performance

D. Elvira (leader of G4CPT), K. Genser, J. Kowalkowski, M. Paterno

Geant4 Computing Performance Task

Contact Person

- Daniel Elvira

Mission

The G4CPT is not a task force but rather an open ended effort with the following objectives:

a. Profiling to identify bottlenecks in Geant4 based on main stream applications. We need to discuss profiling tools, what we want to measure, metrics. EM, Geometry and hadronics are the areas more involved in CPU usage.
b. Code reviews geared towards improving computing performance and coding practices.
c. Establish computing performance activities with the High Energy Physics, Medical and Space G4 communities.
d. Identify issues in multi-core, multi-thread G4.

Generators

S. Mrenna, J. Yarba

- Pythia is the workhorse of Run2 **and** LHC experiments. (S. Mrenna co-author.)

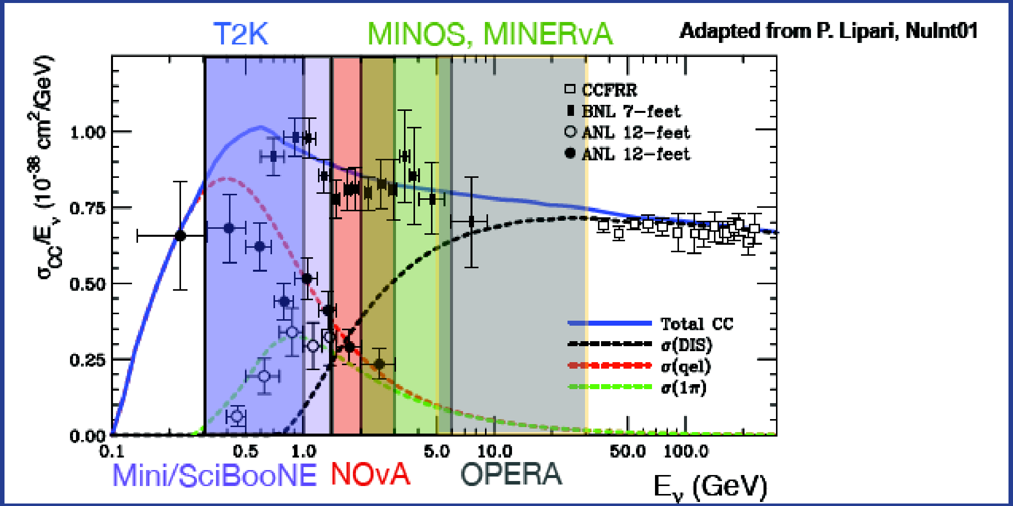
Development with particular focus on physics validation, numerical stability, performance, and flexibility of the new C++ version. Approximately 3 releases per year.

- Generator tuning based on LHC collider data. (S. Mrenna in the context of the CMS Collaboration.)

- CMS core generator activities, including code development and dataset generation strategies (S. Mrenna, J. Yarba). Theory and Generator liaison (S. Mrenna.)

- Muon Collider phenomenology. Producing a fast generator/detector simulation code that incorporates machine backgrounds. (S. Mrenna.)

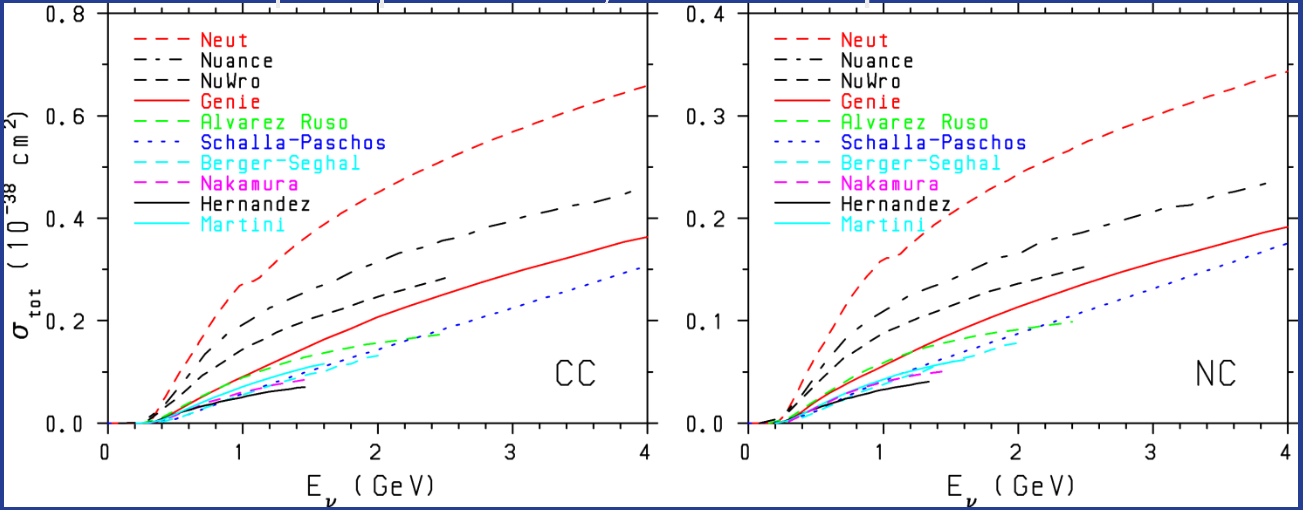
Neutrino Generators



- Modeling neutrino interactions in the 1 GeV energy region is important because this energy domain is typical for many FNAL experiments such as MiniBooNE, Sci-BooNE, MINOS, MINERvA, NOvA, micro-BooNE, (LAr in general), water Č in general
- Currently supporting MINOS switch to the GENIE framework (and participate in GENIE development effort)
    - GENIE is based on C++/Root (geometry, etc) and is developed/maintained by a large collaboration

Neutrino Generators

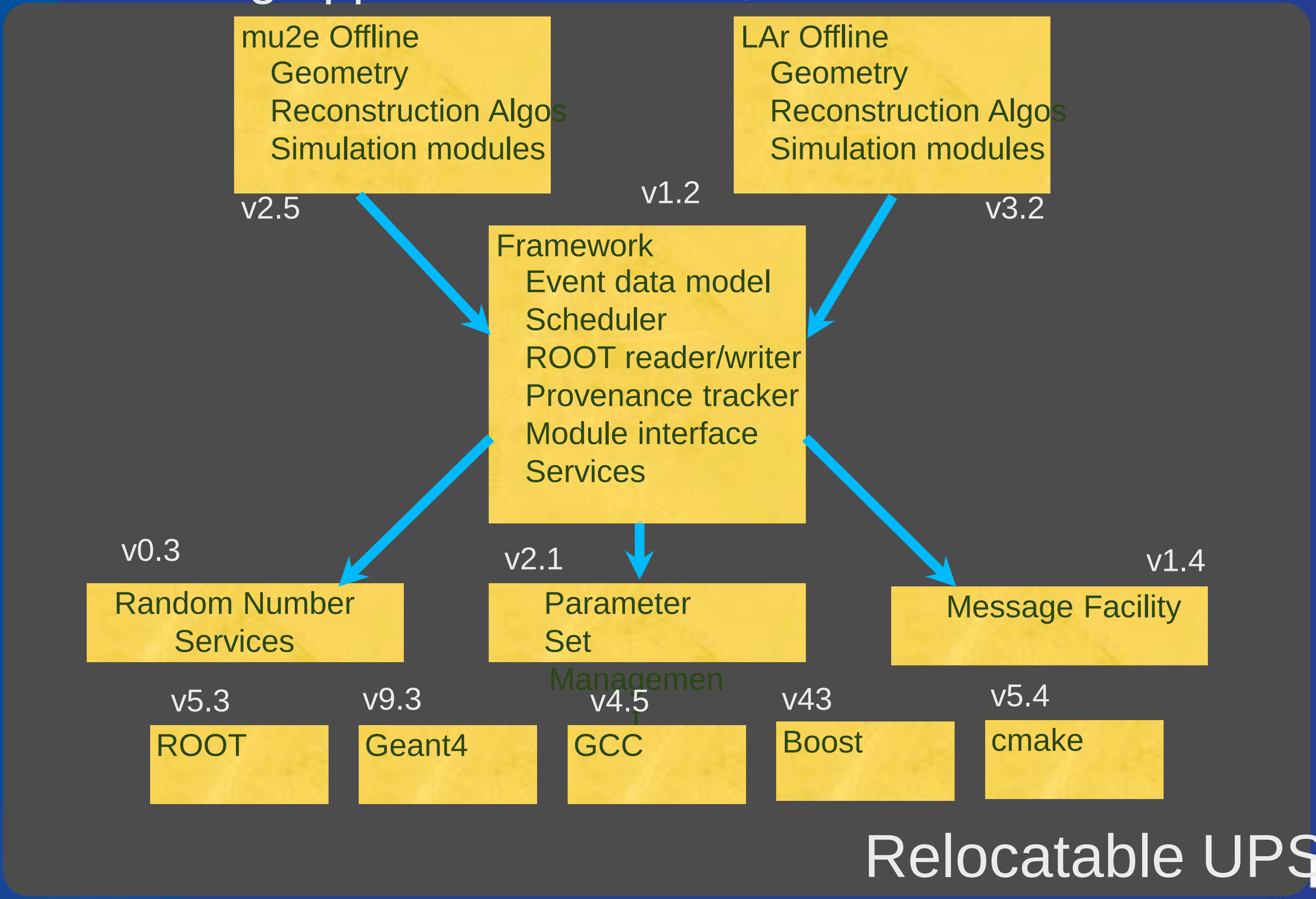
Coherent pion production, model comparison from NuInt09



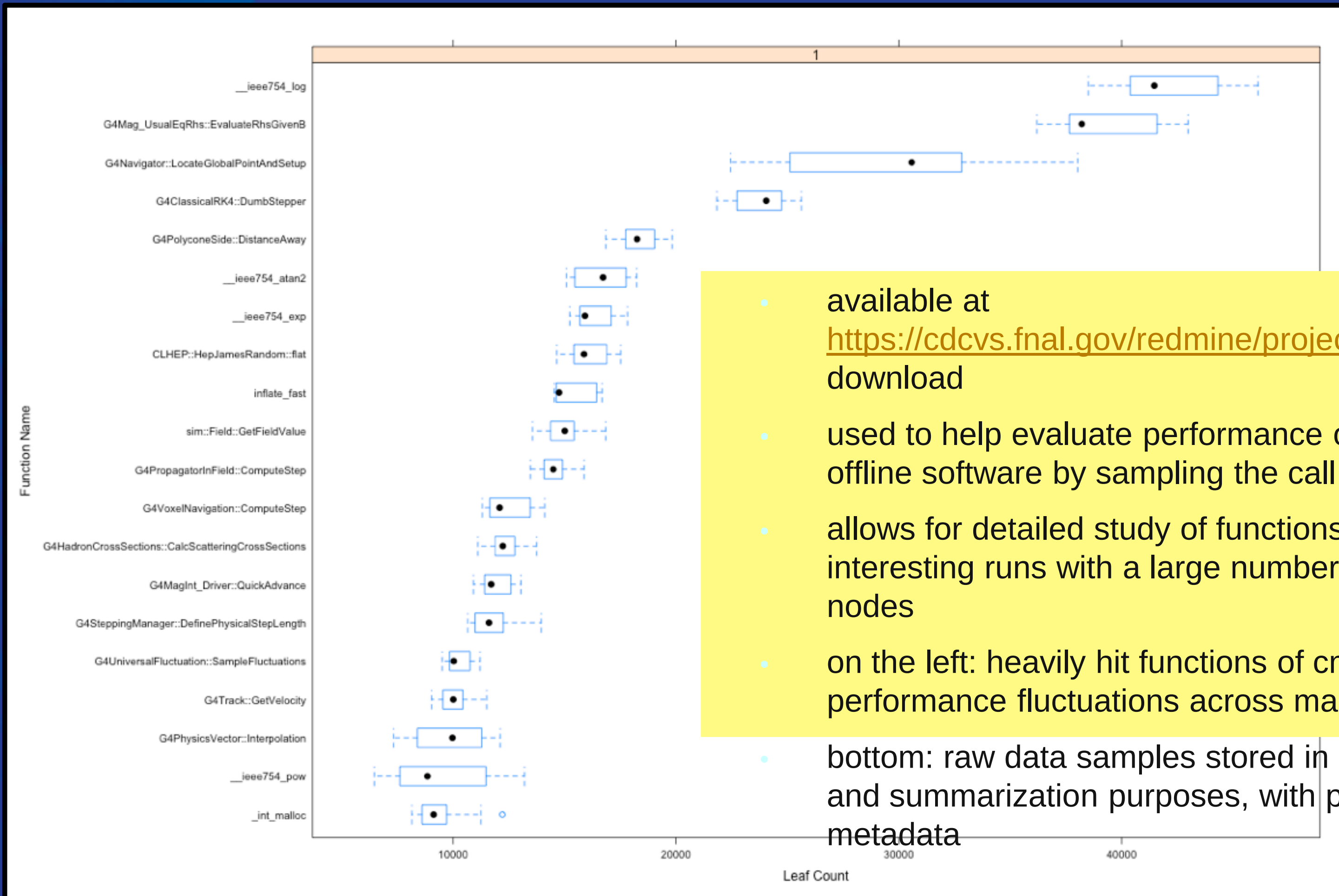
- Above picture just an example: there is a lot of work necessary (mostly incorporating data, x-checking, etc) for getting reliable neutrino generators
- This is a very important activity for the FNAL neutrino community, a possible growth area for our simulation activities

Event Processing Framework

- Packaged as a toolkit with a set of software libraries
- Easy distribution, setup, and management
- Existing applications: Mu2e, LAr offline



Sampling Profiler



- available at https://cdcvs.fnal.gov/redmine/projects/list_files/fast for download
- used to help evaluate performance of Geant4 within CMS offline software by sampling the call stack periodically
- allows for detailed study of functions and call paths for interesting runs with a large number of samples across nodes
- on the left: heavily hit functions of cms simulation, showing performance fluctuations across many nodes and runs
- bottom: raw data samples stored in database for download and summarization purposes, with provenance and other metadata

Program: cmsRun, Purpose: g4profiling

als	Exp	EPS Name	EPS	BFS Name	BFS	Trials	Events	Median Event Time	Wall Clock Time FNS (Δ from median) min	25%	median	75%	max	Leaf Count FNS (Δ from median) min	25%	median	75%	max
	1	1	1	1	1	33	3300	117	-1454	-109.0	11704	111.0	225	-932405	-8163.5	932405	92779.0	113889

Trial	Start Date	Events	Wall Clock Time	Leaf Count	CPU Vendor	Kernel	More Information
0_1	2010-08-03 13:23	100	11699	924554	AuthenticAMD	2.6.18-194.3.1.el5	View Library Calls Go
0_2	2010-08-03 16:38	100	11826	919162	AuthenticAMD	2.6.18-194.3.1.el5	View Library Calls Go

Issues

- We are already “doing more with less” in the simulation areas
  - as per D. Poneman’s recommendation
- All programs at the lab require support (building applications, consulting)
  - CMS, Mu2e, LAr applications supported at various levels, but more requests in the pipeline
- We have responsibilities within the G4 collaboration
- Effort reduction will result in no new initiative support , and most likely reduced contribution to G4 collaboration activities
  - Also, recent G4 re-org, possibly new collaboration strategy and new CERN group strategy affects our planning

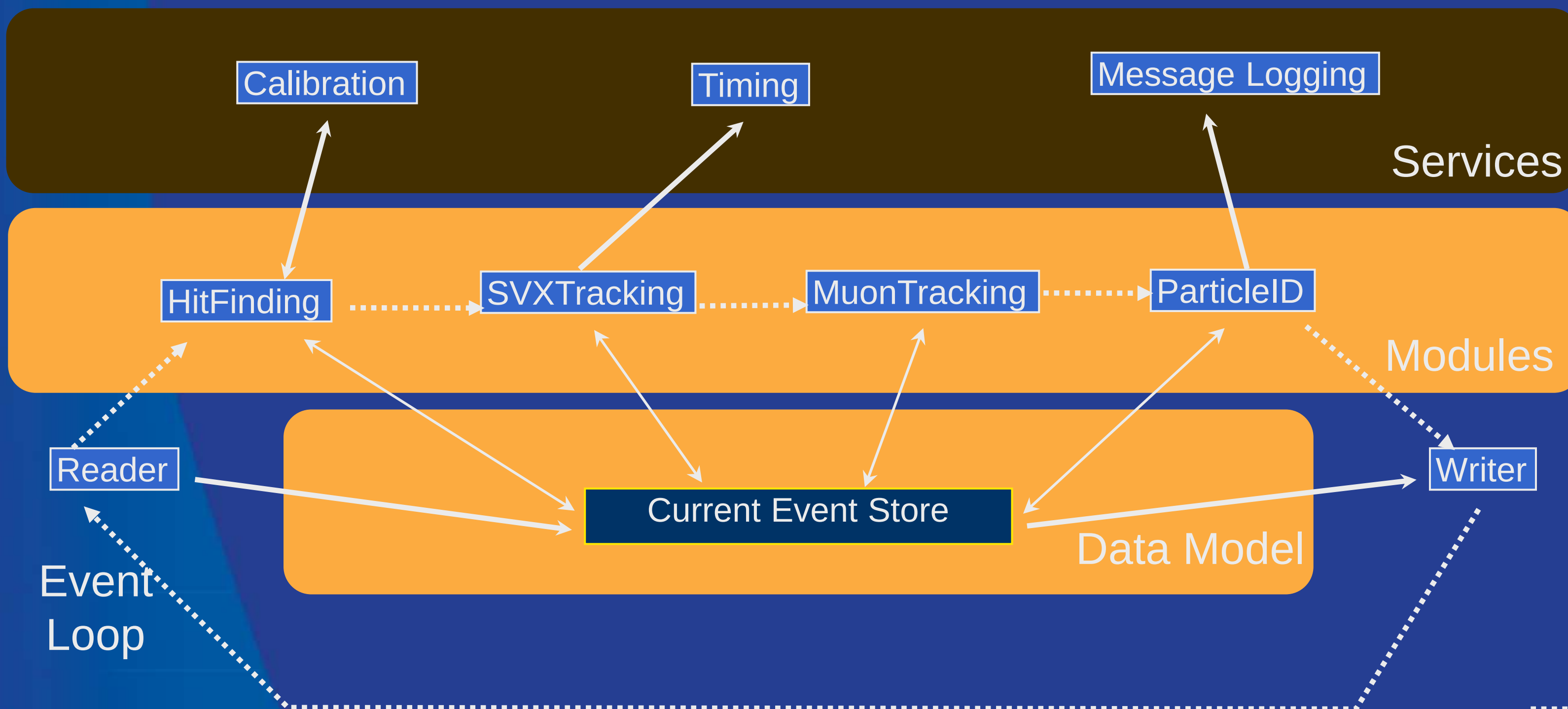
Extras

Computational Accelerator Physics mission

- Develop computational tools
  - Realistic physical system modeling (accelerator dynamics, accelerator components)
  - Algorithm and application optimization
    - Emphasis on High Performance Computing (HPC)
- Provide expertise on deployment and utilization of computational tools
  - Both internally (FNAL) and externally developed
  - On local, distributed, and non-local facilities
- Develop or contribute to the development of applications of such tools

HEP experiment analysis

Event Processing Framework: Software that coordinates the processing of collision events by pluggable reconstruction, filtering, and analysis modules. Events and modules are independent. Modules add data to and retrieve data from one event at a time.



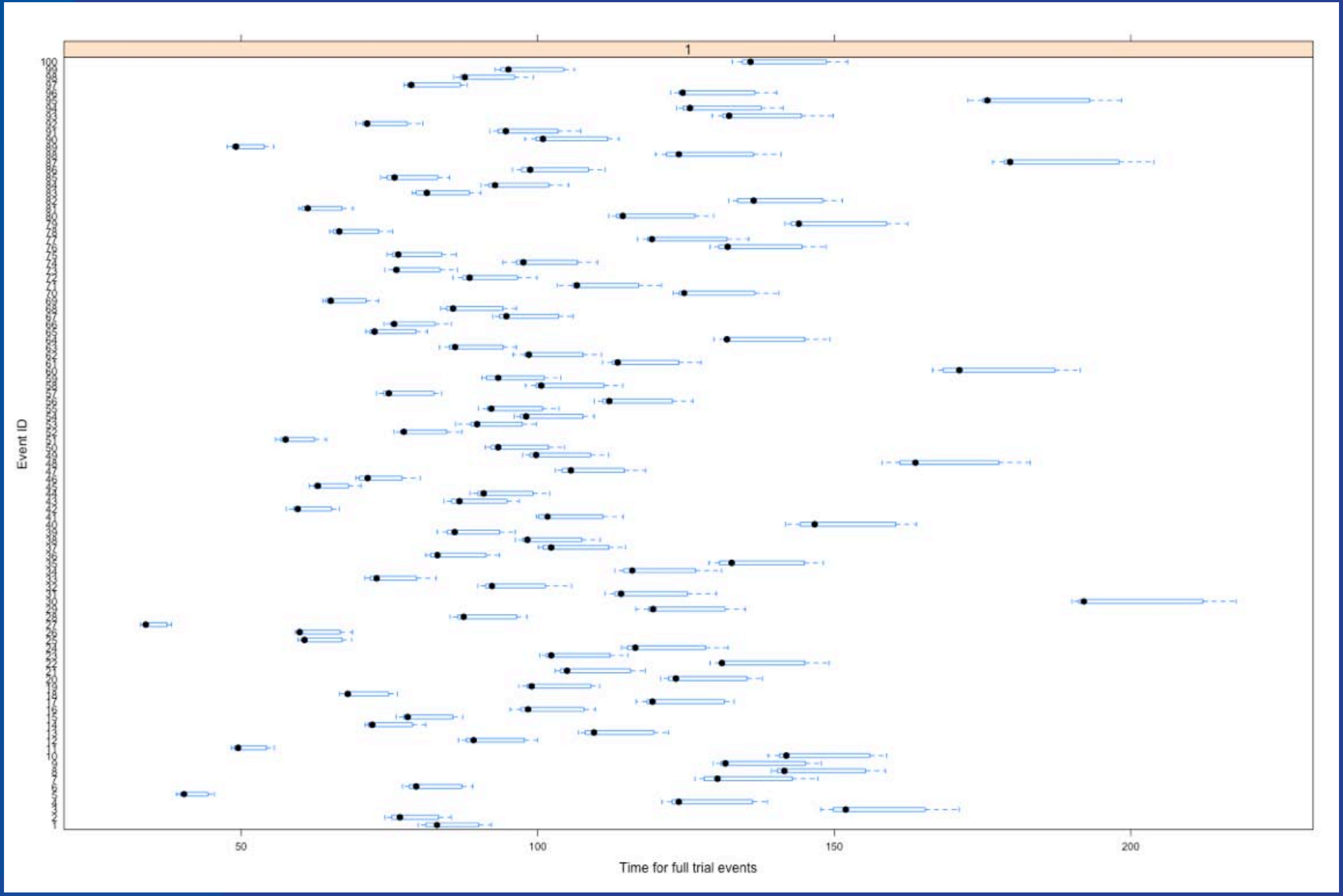
- Event: unit of data, an interaction or period of collected data
- Two other key features are provenance tracking and configuration

Control-flow

Data-flow

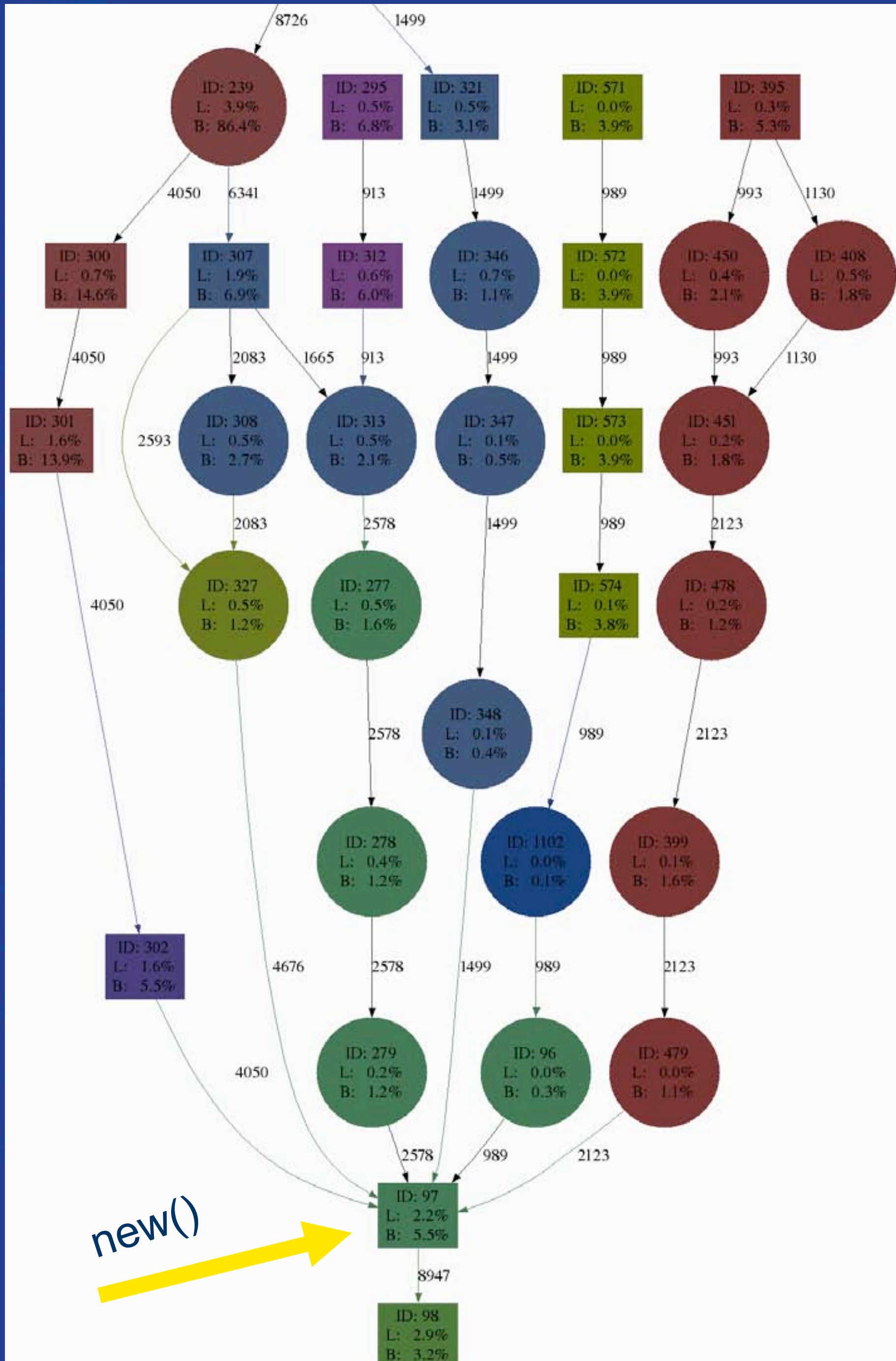
Fermilab

Event processing time fluctuations

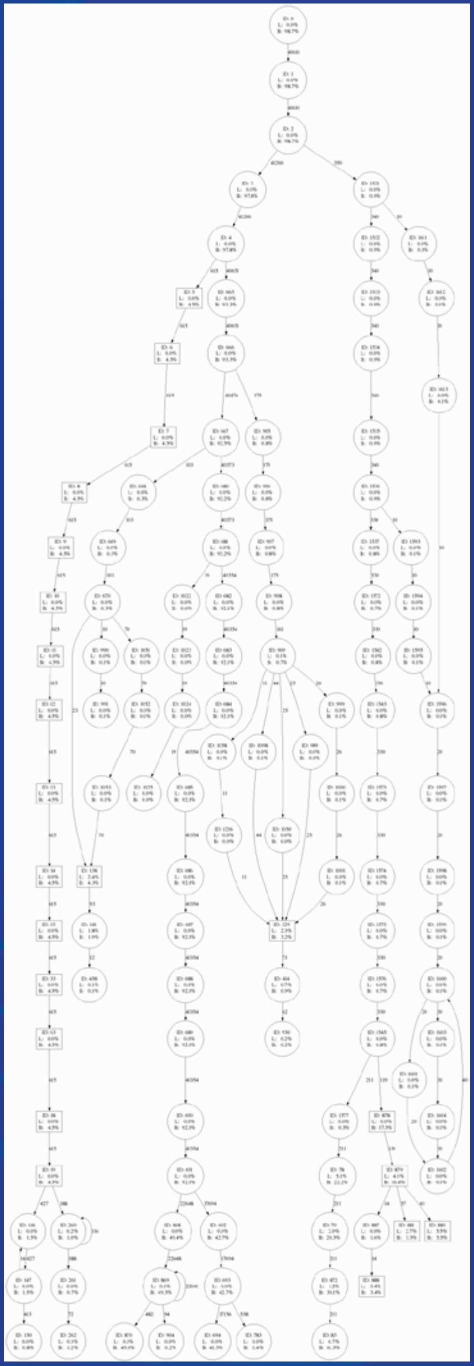


Fermilab

Locating Features

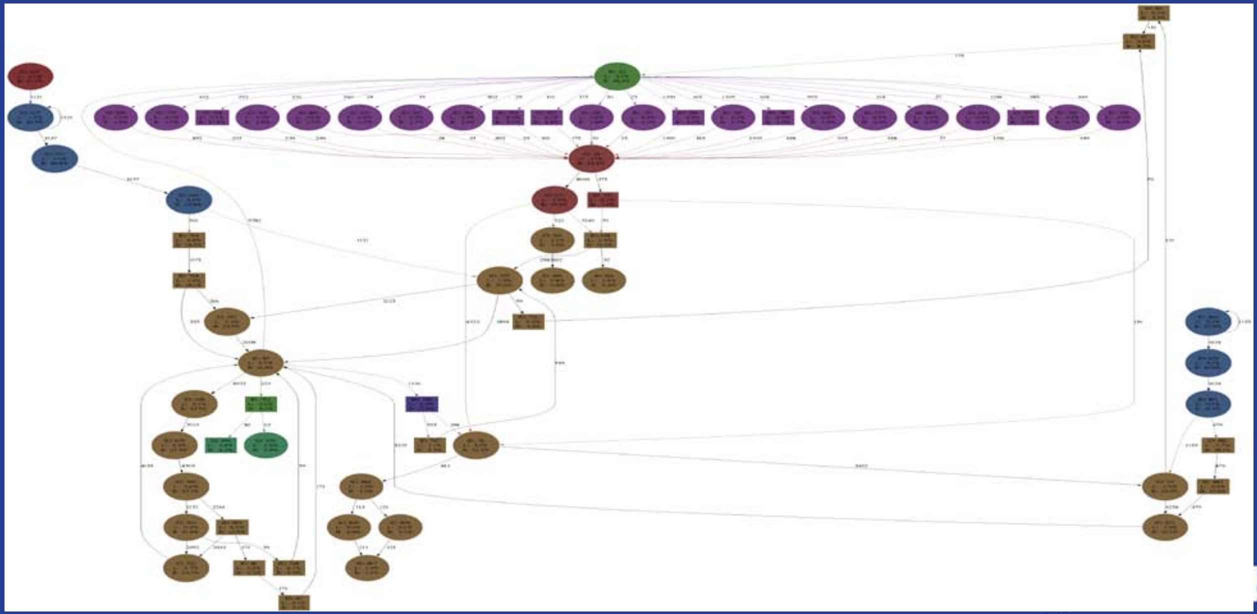


- Look at sample counts for function + children instead of just leaf counts.
- “operator new” chosen as example:
  - Remove all paths containing less than 1% of the samples
  - Graph built directly from remaining path data
  - Can trace up high enough to locate leading cause
  - Can look downward to find where the target spends its time
- Main points about the graph
  - It has the right amount of information on it
  - It answers the question we had about major causes
  - Always generated from path data

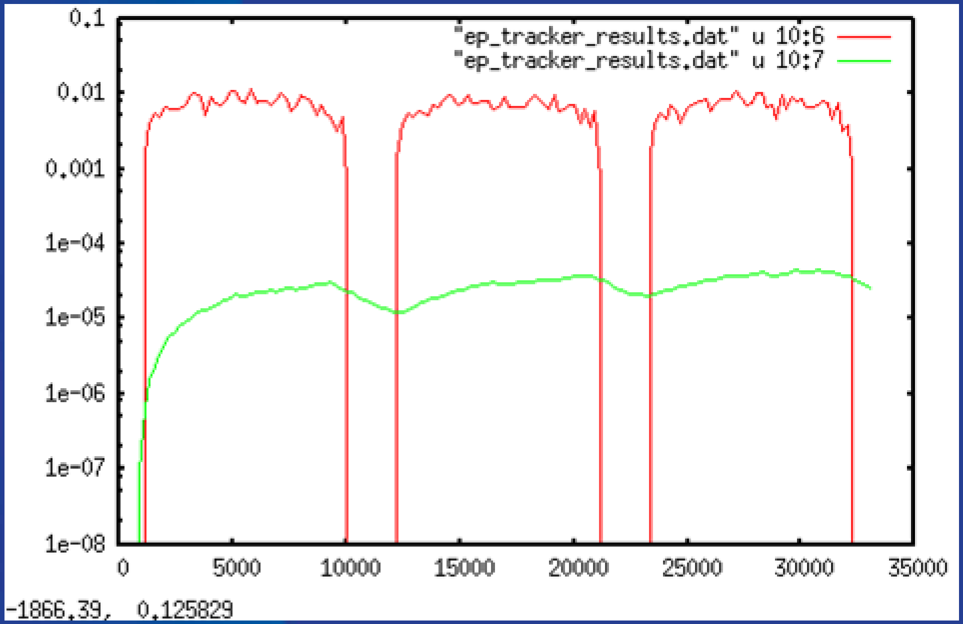


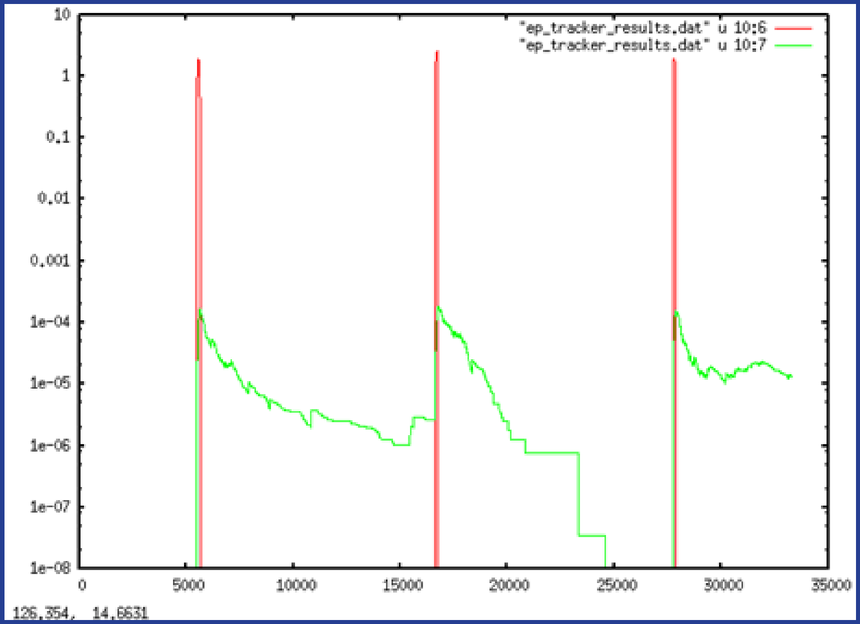
Additional Benefits

- Can see structure of program
- A good guide to what gets called from where when you know nothing about the application
- Can group by library



Code development: enhance ORBIT e-cloud module for multi-bunch applications





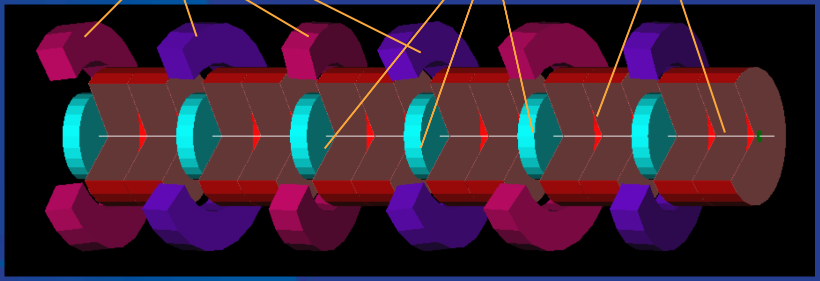
- Work on addressing issues with multi-bunch e-cloud applications in ORBIT to utilize tool in Project-X applications

Application specific tools: Methodical Ionization Cooling Channel Design (MICCD)

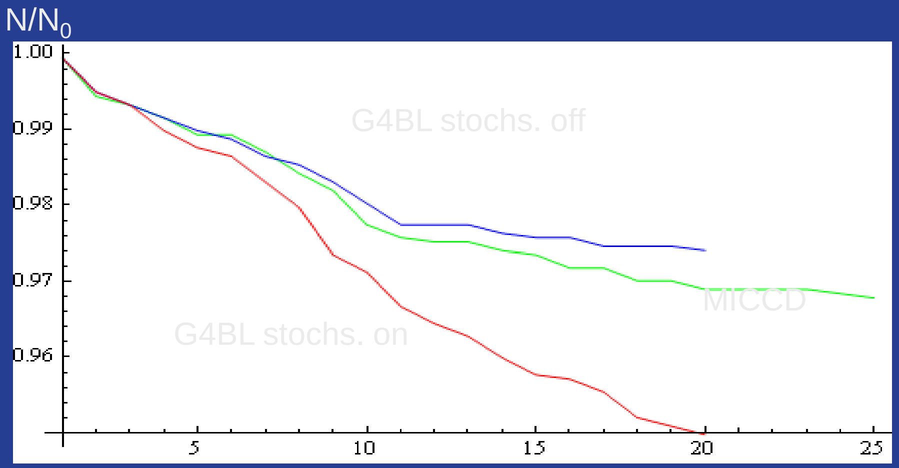
A MAD-like code (in *Mathematica*) which includes:

- long-range fields of tilted and displaced off-axis magnetic elements,
- fully coupled 6D optics functions calculation in presence of strong damping,
- analysis of higher order effects on beam dynamics
- particle tracking (w/o stochastic effects yet)

MICCD was successfully used for Helical FOFO snake design for the 1st stage of ionization cooling,
helped to find bugs in G4beamline (tracking code used in ionization cooling studies)



HFOFO snake layout (1 period = 6.12 m)



Transmission vs period #

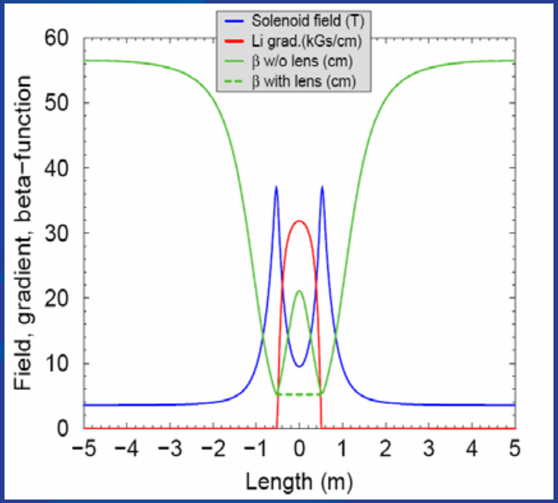
After fixing bugs in G4BL it gives very close results

App. specific tools: LLSC (Lithium_Lenses_Solenoid_Cooling)

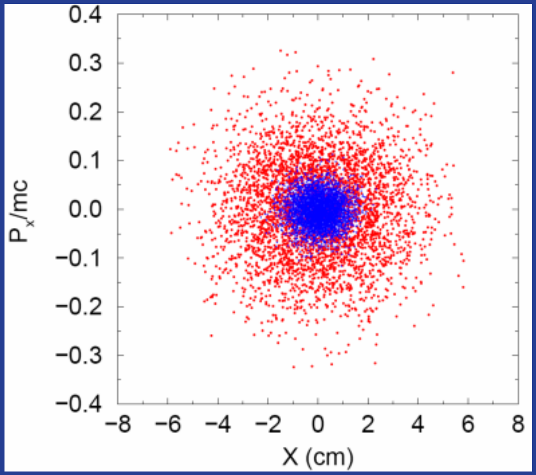
The program is designed for tracking and ionization cooling simulation in a channel with Li lenses, solenoids, and RF cavities, including:

- Calculation and tabbing of magnetic field of arbitrary solenoid coils, as well as the field of Li lenses of variable diameter.
- Calculation of standard channel parameters like beta-functions, tunes, etc.
- Tracking of a particle with arbitrary initial conditions to plot its trajectory in usual or phase space.
- Cooling simulation and the beam parameters calculation and plotting.

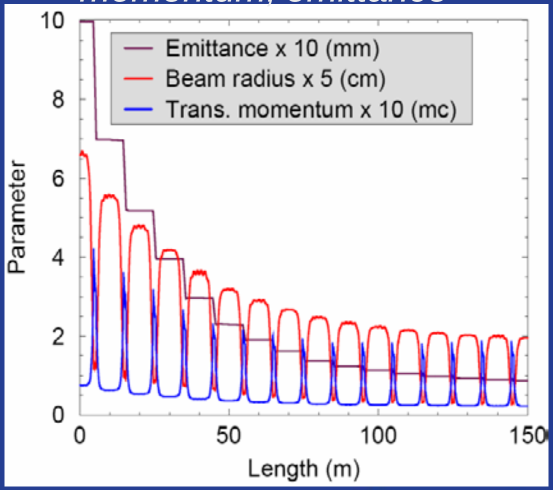
Example 1: Axial solenoid field, Li lens gradient, and beta-function of a cell



Example 2: Transverce phase space before (red) and after (blue) the cooling



Example 3: Beam evolution in 15-cell cooling channel: r.m.s. radius, transverse momentum, emittance

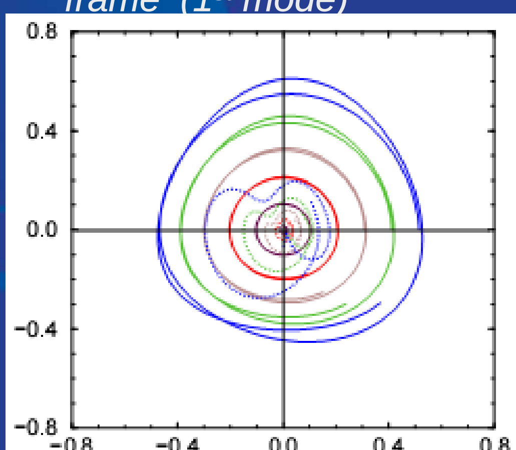


Application specific tools: HELIX

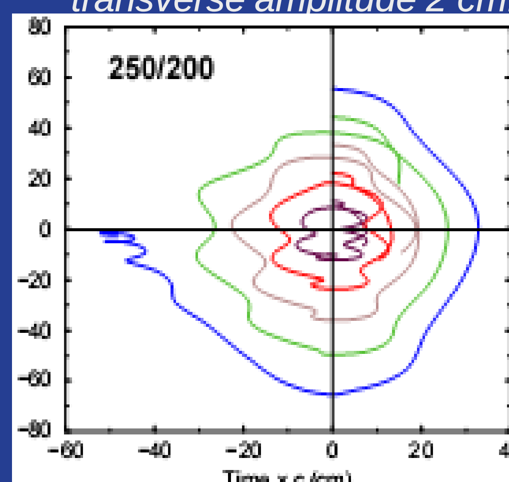
The program is designed for tracking and ionization cooling simulation in a gas filled Helical Cooling Channel with wedge absorbers and RF cavities, including:

- Calculation and tabbing of magnetic field containing arbitrary set of multipoles.
- Calculation and tabbing of magnetic field of a helical solenoid.
- With obtained helical field, determination of the natural frame and calculation of the channel beta-functions and tunes.
- Generation and injection of matched beam.
- Tracking of a particle with arbitrary initial conditions and plotting of trajectories in usual or phase space.
- Cooling simulation and the beam parameters calculation in the natural frame.

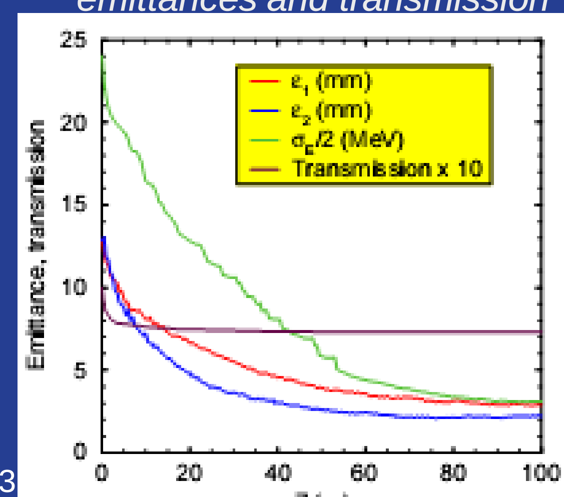
Example 1: Transverse phase trajectories in natural frame (1st mode)



Example 2: Longitudinal phase trajectories at transverse amplitude 2 cm.



Example 3: Beam evolution in 100 m cooling channel: r.m.s. emittances and transmission



LARP beam-beam simulations

Beam-beam code (BBSIM) for 6D weak-strong simulations of hadron colliders.   Authors: T. Sen and H.J. Kim

Devices in model

- Wire for compensation of long-range interactions
- Electron lens for head-on compensation
- Crab cavity
- Multiple harmonic cavities
- AC dipole

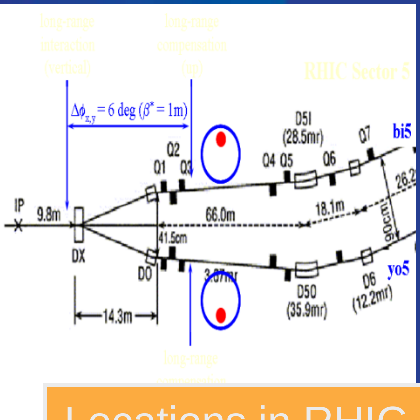
Diagnostics include

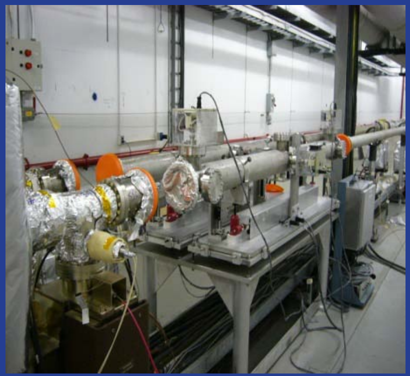
- Tune footprints, dynamic aperture
- Frequency maps
- Amplitude diffusion
- Beam transfer function
- Emittance growth
- Lifetimes, loss rates

Applied to LHC, RHIC, SPS & Tevatron

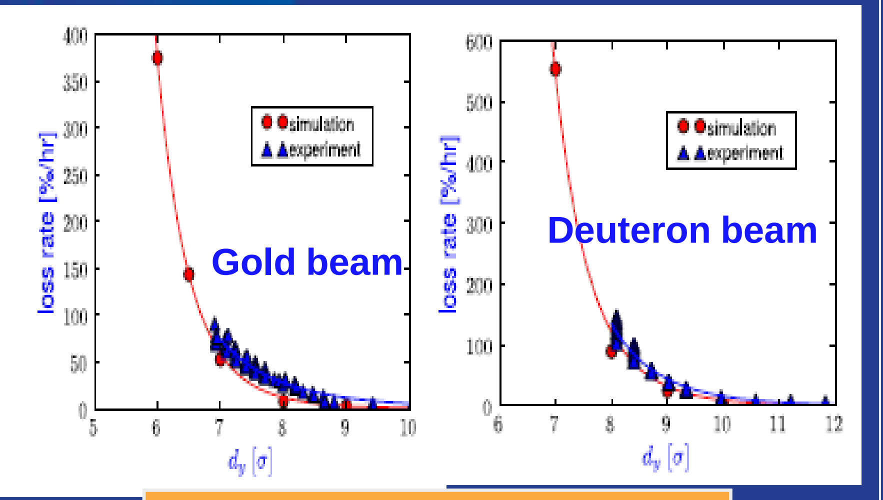
BBSIM Applications

Wire Compensation



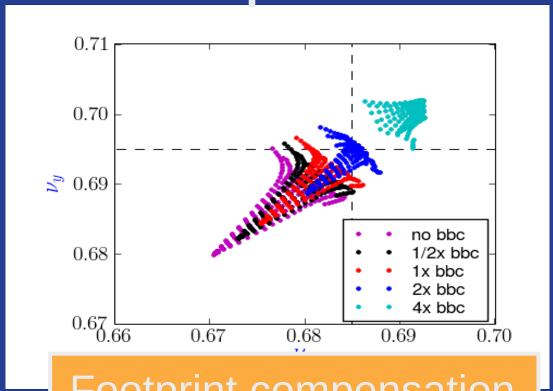


Locations in RHIC

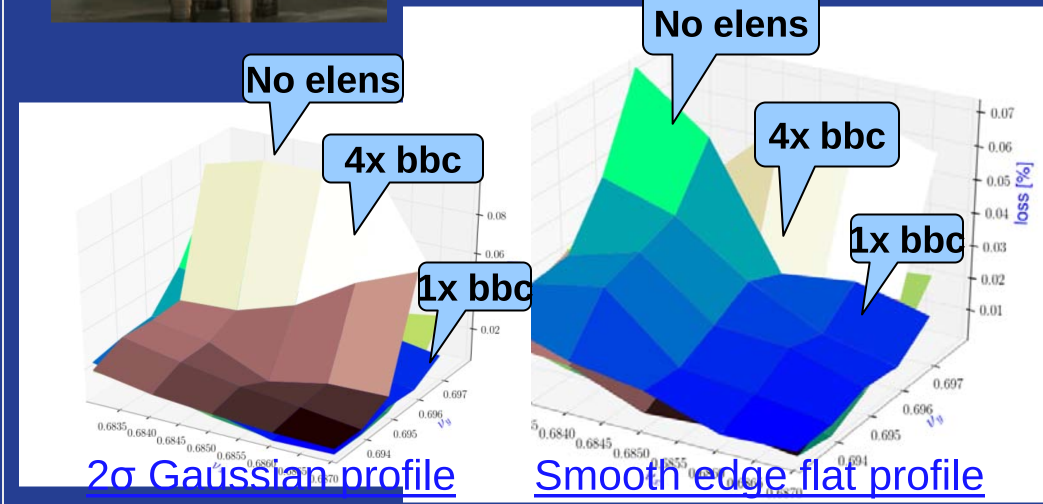


DC wire in RHIC: beam loss vs beam-wire separation

Electron lens compensation



Footprint compensation



2σ Gaussian profile

Smooth edge flat profile

Tune scan of loss rates w/wo electron lens compensation. 1xbbc=nominal electron lens Intensity.

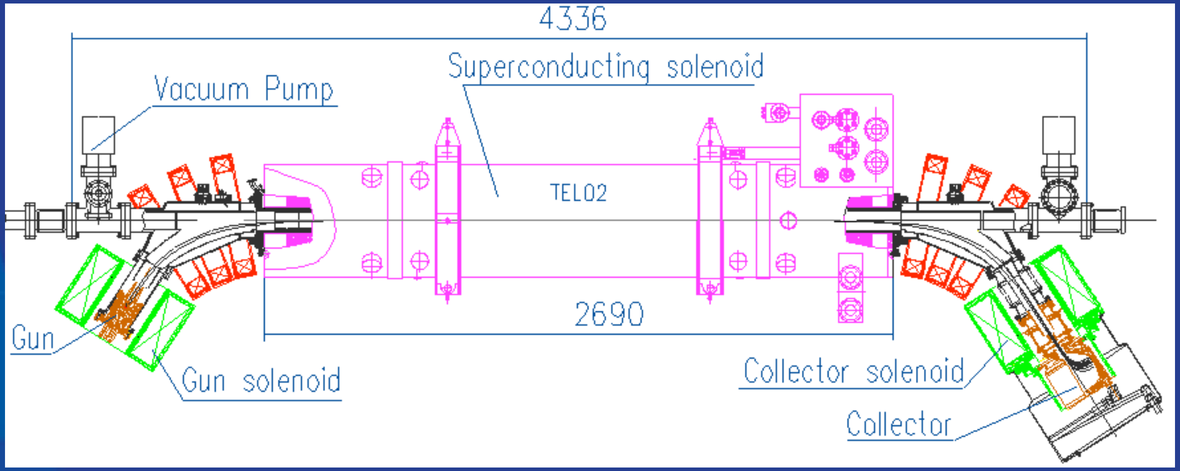
Accelerator Science application: collimation of high-intensity protons with hollow electron beams

Modeling/simulations of effects on core, collimation efficiency

Kick maps in overlap region:
- analytical form / ideal case ☑
- 2D from measured profiles (Poisson solver) ☑
- 3D particle-in-cell Warp code:
    - effect of TEL2 bends
    - profile evolution
    - misalignments
    - time structure

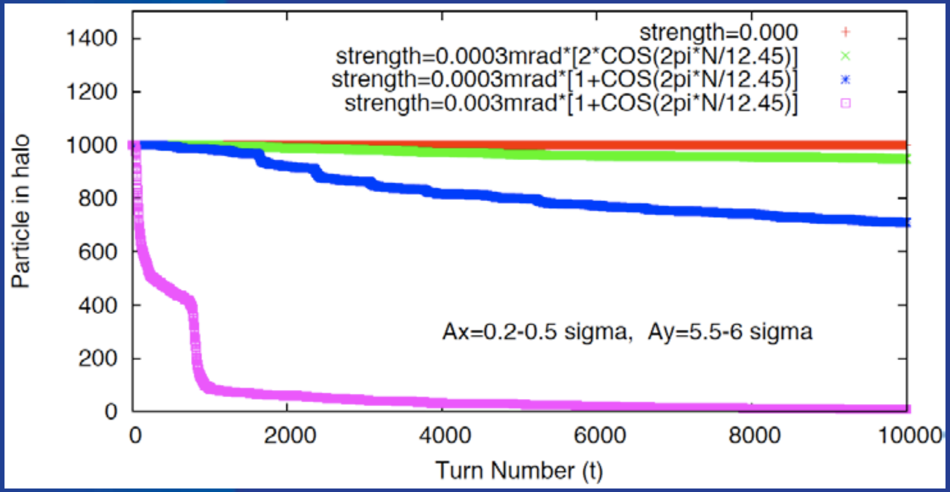
→

Tracking software
with lattice and apertures:
- STRUCT ☑
- Lifetrac ☑
- OptiM
- MAD / SixTrack



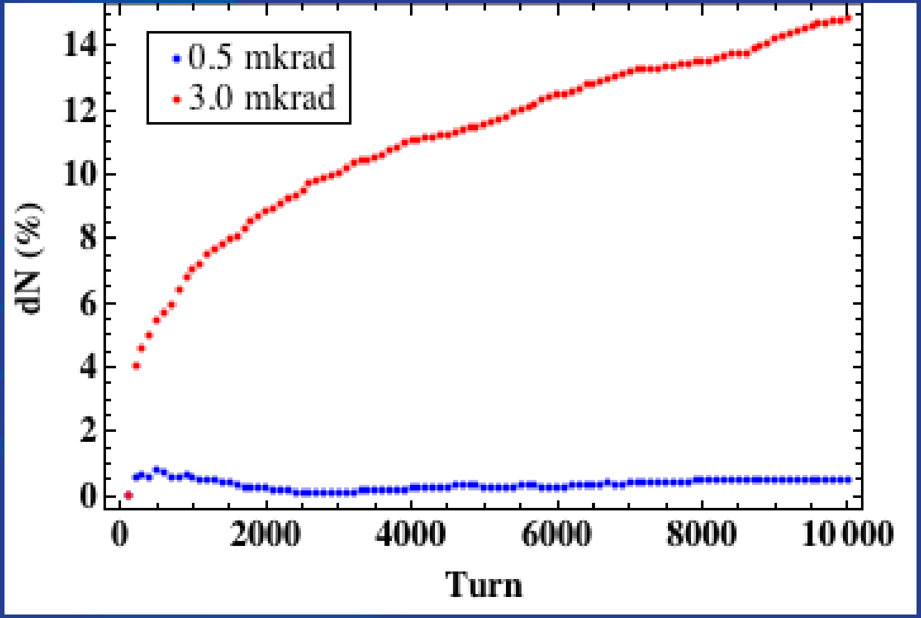
A. Drozhdin, G. Stancari, A. Valishev

Simulations of halo cleaning with ideal hollow beam vs. kick strength and pulsing pattern. Effects should be observable in the Tevatron at 980 GeV



A. Drozhdin

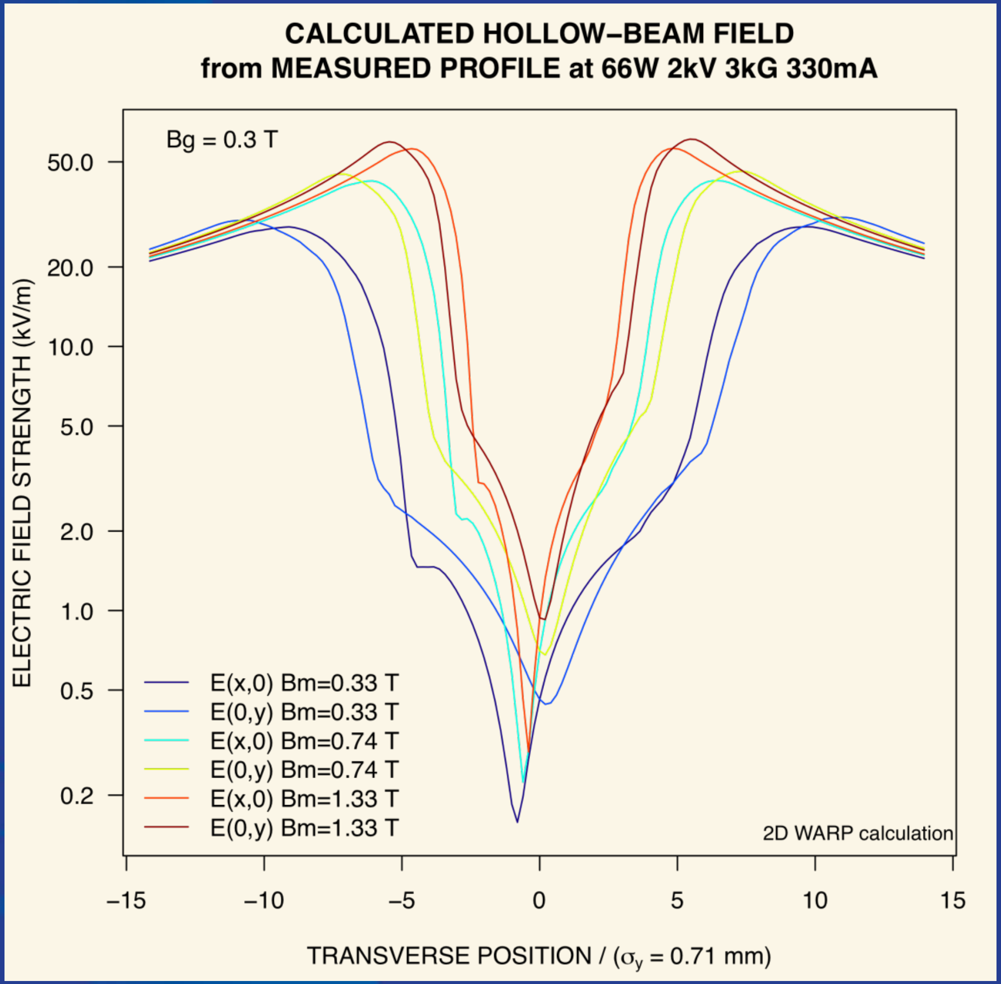
STRUCT
Apertures / helices / rf cavities / sextupoles
Pulsed lens

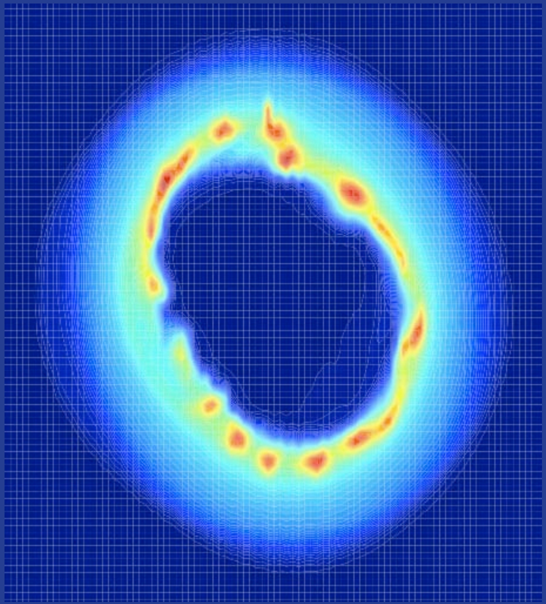


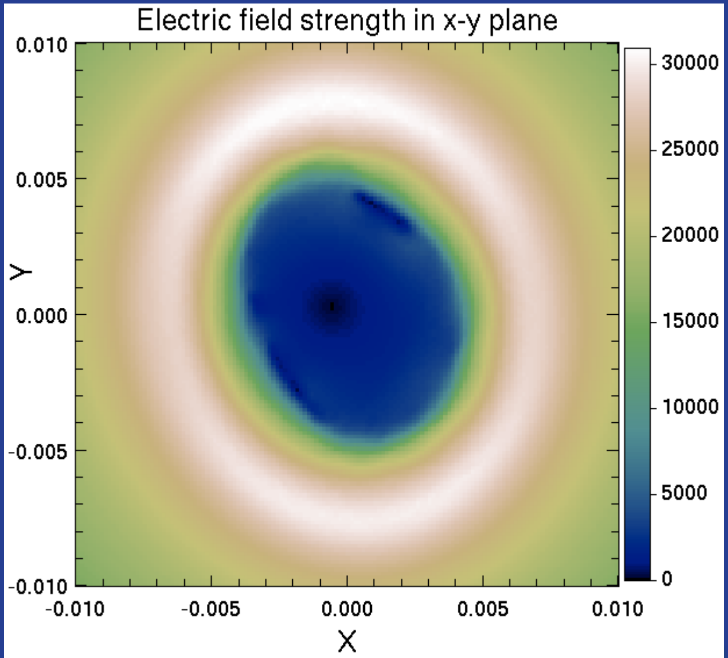
A. Valishev

Lifetrac
3D beam-beam / nonlinearities / chromaticity
simplified apertures
DC lens

Calculation of 2D fields from measured profiles, using Warp's 2D Poisson solver



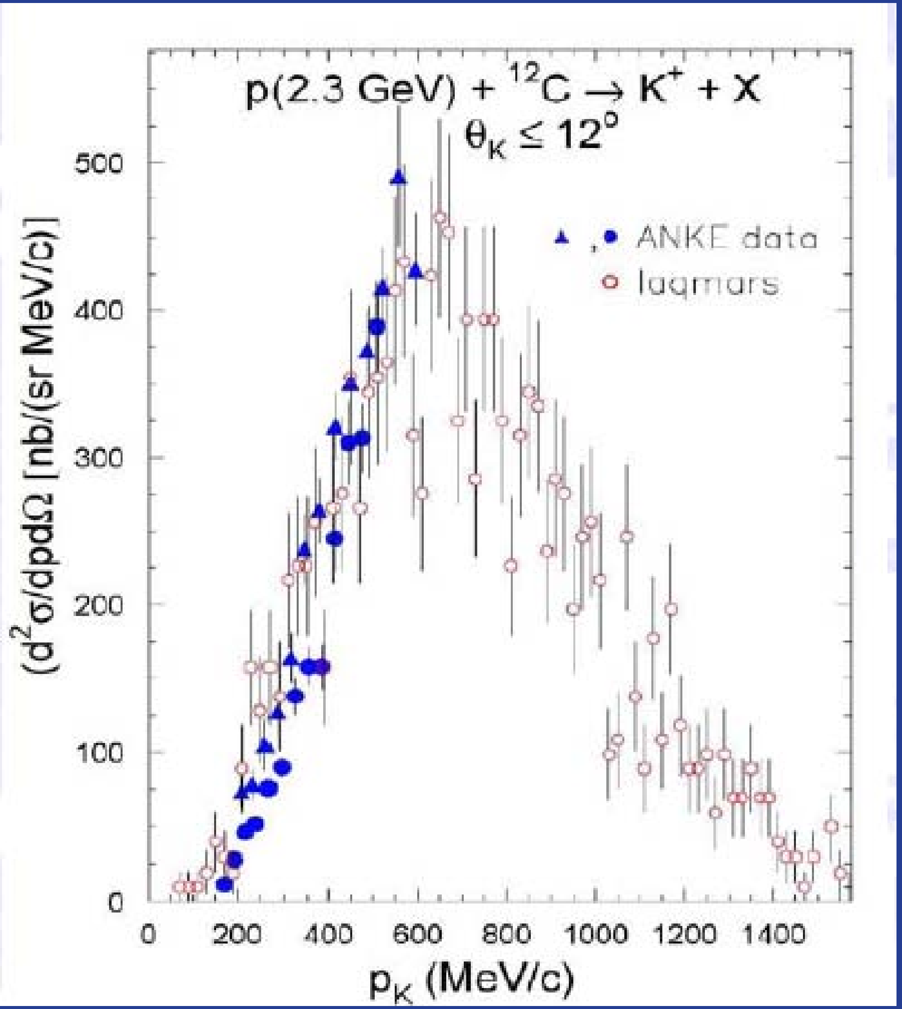




G. Stancari

MARS15

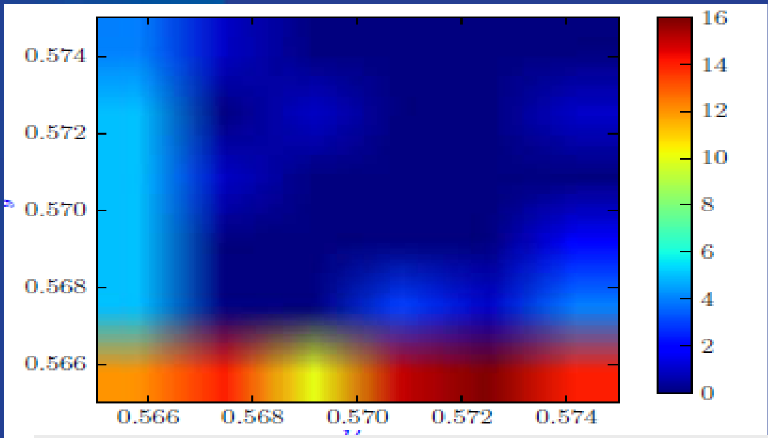
- The MARS15 code system is a set of Monte Carlo programs for the simulation of hadronic and electromagnetic cascades used for shielding, accelerator design, and detector studies. It covers a wide energy range: 1 keV-100 TeV for muons, charged hadrons, heavy ions and electromagnetic showers and 0.00215 eV-100 TeV for neutrons.



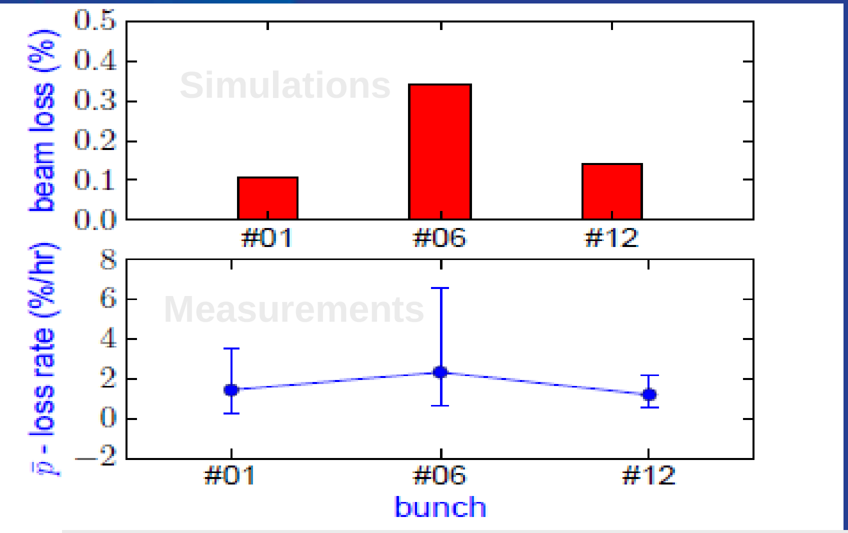
Simulation of the challenging region between 1-4 GeV/c p beam momentum.

Applications (2)

Tevatron: pbar loss rates at collision



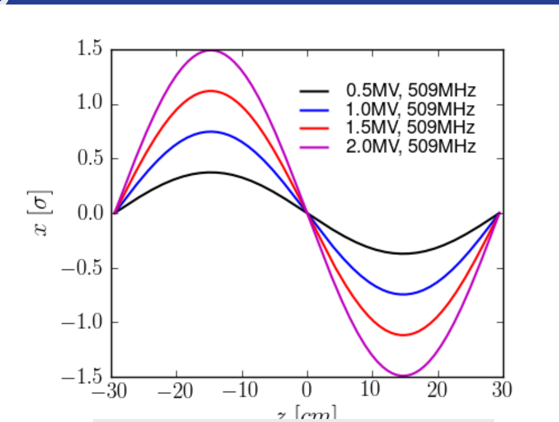
Tune scan of loss rates; bunch 6



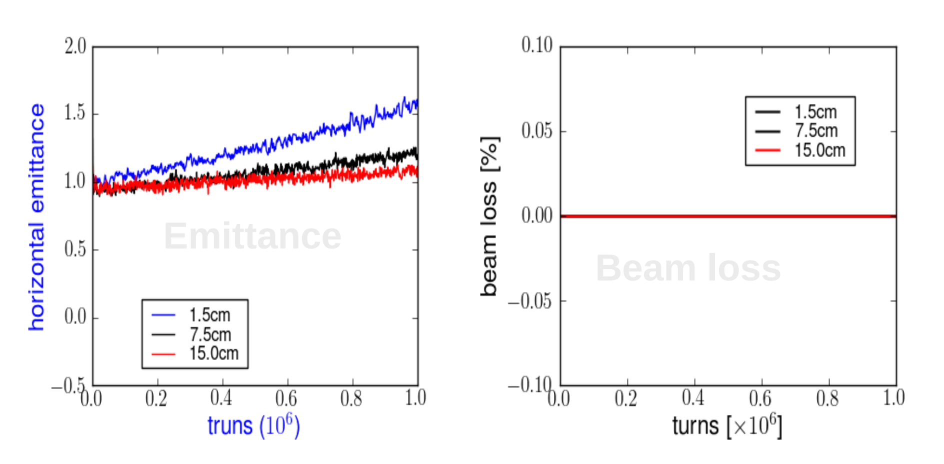
Comparison of losses for 3 bunches

Crab cavity test in SPS

KEK crab cavity



Closed orbit vs z



Emittance growth and beam loss for different bunch lengths with crab cavity at a zero dispersion location.

Summary of results

- Wire compensation: Detailed comparison with measurements in RHIC showed good agreement. Onset of sharp losses with beam-wire separation agreed to 0.5σ. In the LHC, simulations showed that chosen wire parameters are close to optimal
- Electron lens compensation: Wide electron lens expected to reduce losses from head-on interactions in RHIC.
- Beam lifetimes in Tevatron: Optimum working point and bunch by bunch losses are in reasonable agreement with observations.
- Crab cavity test: Single crab cavity in SPS will have little impact on beam quality if tunes and dispersion at crab cavity are well chosen. Study for LHC in progress.

Tevatron setup dance

The Tevatron is unstable at high intensities

Adding chromaticity can improve stability

Chromaticity causes losses and radiation

Beam-beam force is stabilizing

During setup, beam-beam force is reduced

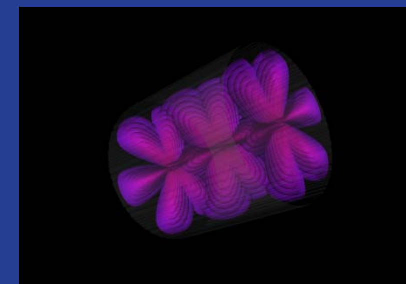
But is it enough to give beam stability?

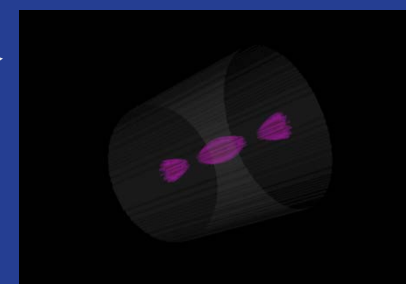
Accelerator modeling tools development

- Strategy: apply state-of-the-art computing to enable state-of-the-art accelerator modeling
  - Move beyond the era of one code per one effect
  - Develop modeling capabilities to be integrated in realistic applications
    - Advance to muti-physics, multi-scale models
  - Develop and apply expertise in parallel computing from clusters with O(100) processors to capability machines with O(100,000) processors
    - Synergistic with Lattice QCD effort
  - Leverage experience with providing support for user-oriented software

Fermilab

Accelerator design: multi-scale, multi-physics problem

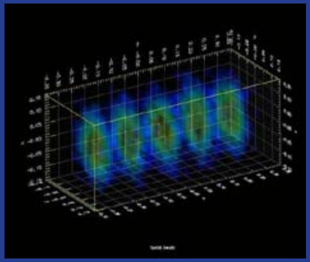


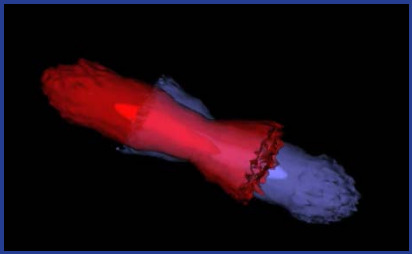


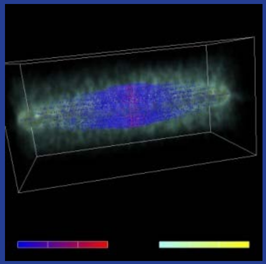
- Wide range of scales:
  - accelerator complex (10^3m) → EM wavelength (10^2-10 m) → component (10-1 m) → particle bunch (10^{-3} m) → PIC (10^{-12})
  - Simulations need to connect scales and allow inclusion of multiple physics effects at each level
  - Requires efficient utilization of HPC

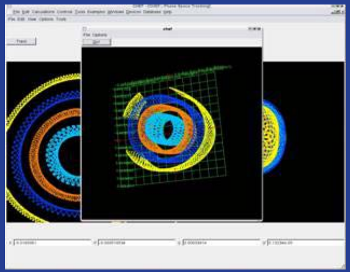
Computationally challenging physics, common to most applications

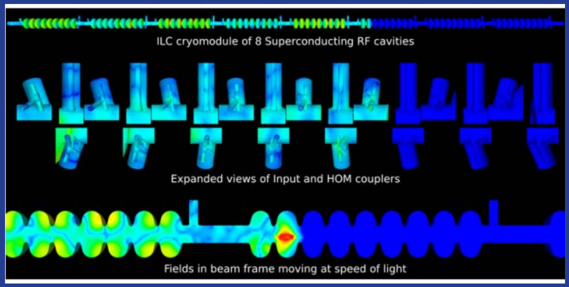
- Machine design: particles affected by machine components, other beam particles or beams **[Beam Dynamics]**
  - Space charge
  - Beam-beam
  - Electron cloud
  - Electron cooling
  - Intrabeam scattering
  - Accurate description (optics, position, feedback, etc)
- Component design **[Electromagentics]**
  - Impedance
  - Wakefields
  - multipacting
  - Thermal, mechanical
- New accelerator technologies **[Advanced Accelerators]**
  - Laser and plasma wakefields
  - Ionization cooling
- Multi-parameter optimization

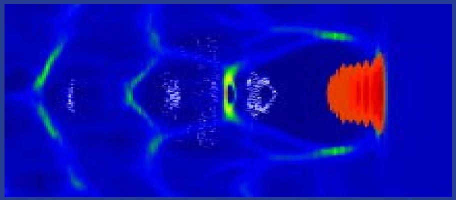












Synergia applications: FNAL Booster

- Extensive modeling of the Booster with Synergia
  - 400 MHz structure debunching and 37.7 MHz capture
  - Including machine ramping
- Emittance growth and halo formation studies
  - Including comparison with experiment
  - Used to help optimize operating parameters
    - Work with AD proton source department personnel
  - NIMA570:1-9,2007