Petascale Simulation for Accelerator-Based Science & Technology

Robert D. Ryne

Lawrence Berkeley National Laboratory

2006 Fall Creek Falls Meeting

Oct22-24, 2006

Fall Creek Falls, TN

OUTLINE

I. Accelerators and the US DOE

II. Challenges/opportunites in petascale accelerator S&T

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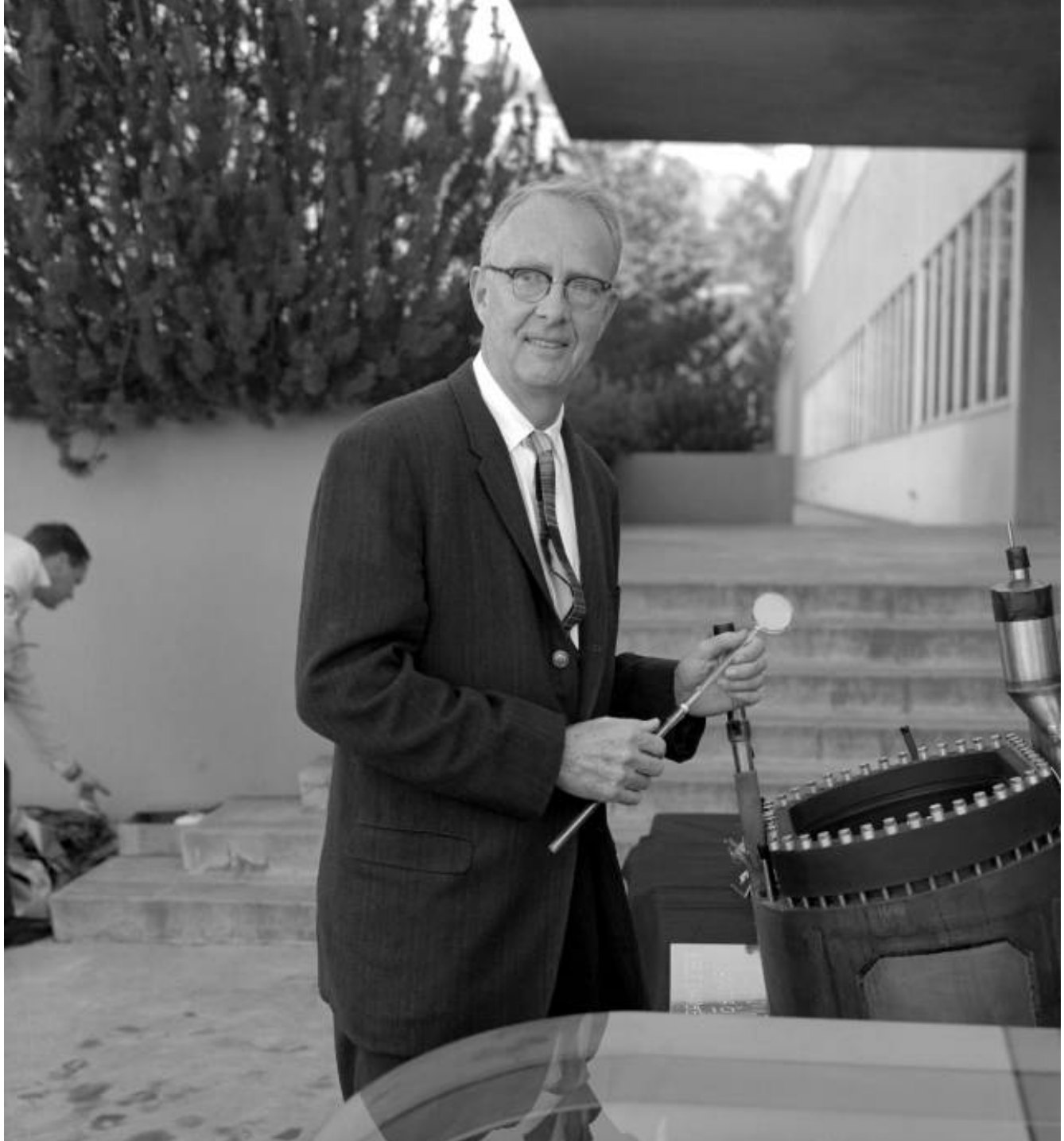
I. Accelerators and the US DOE

II. Challenges/opportunites in petascale accelerator S&T

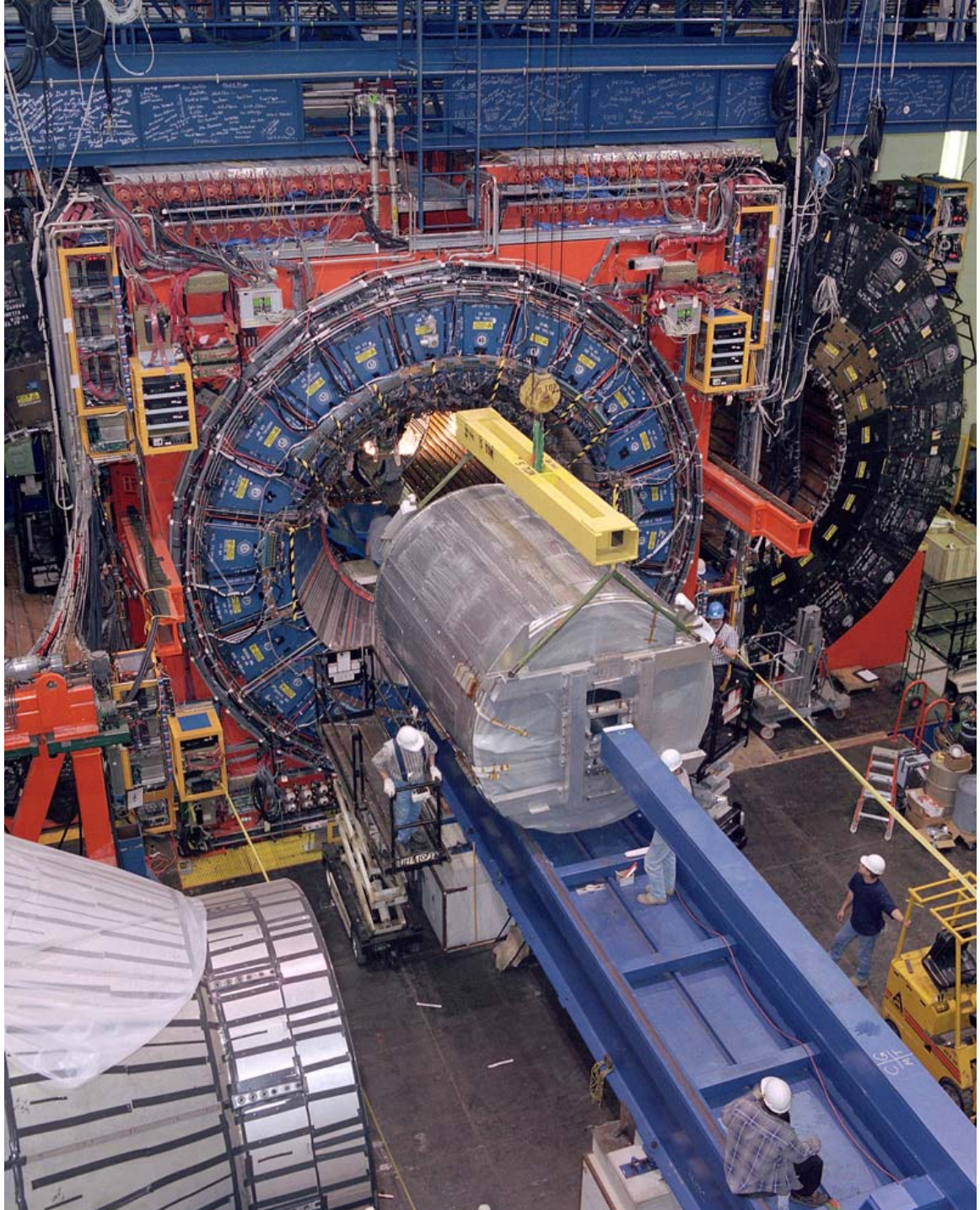
In ~75 years we have gone from…

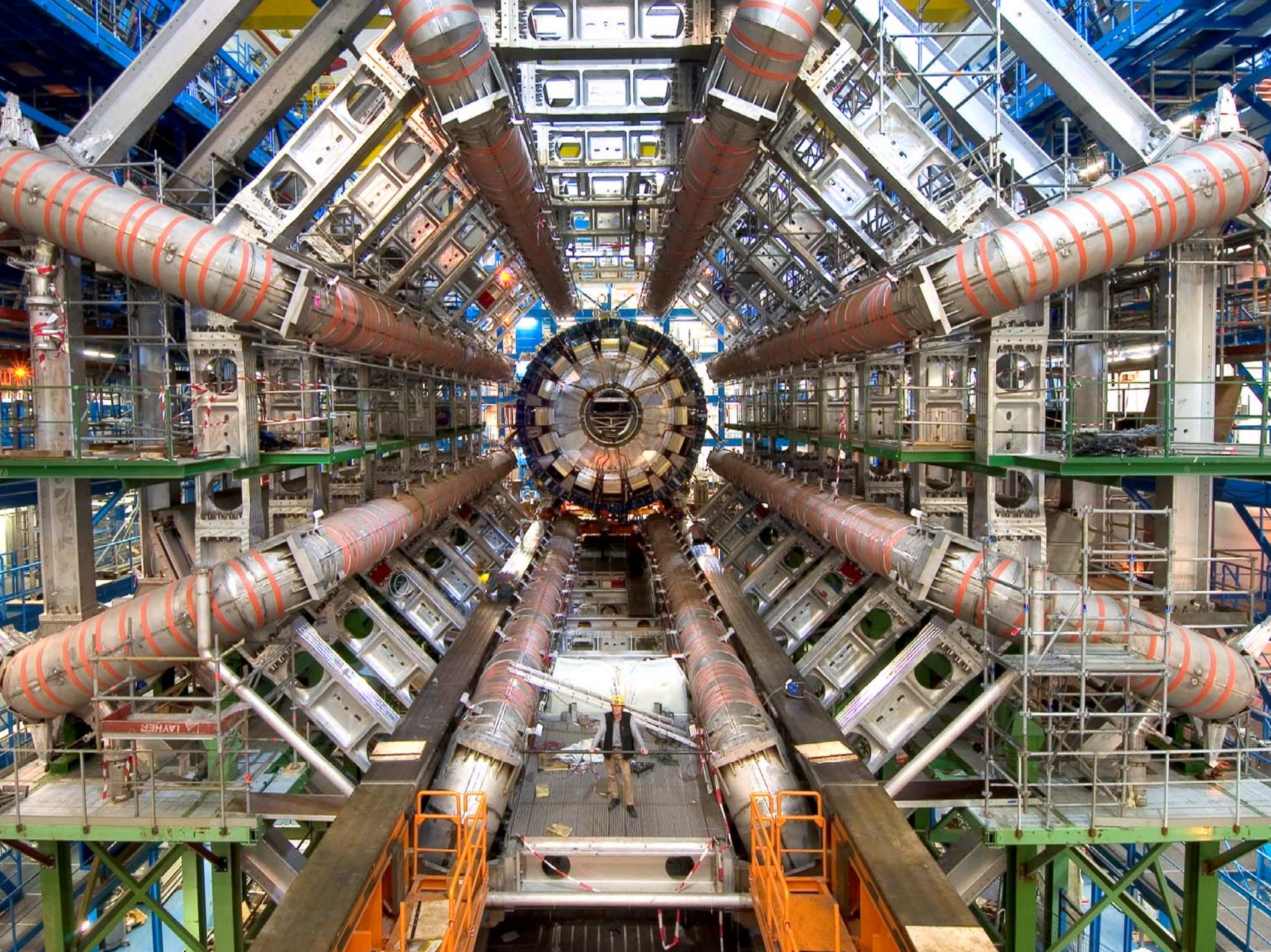
to…

And we have done from…



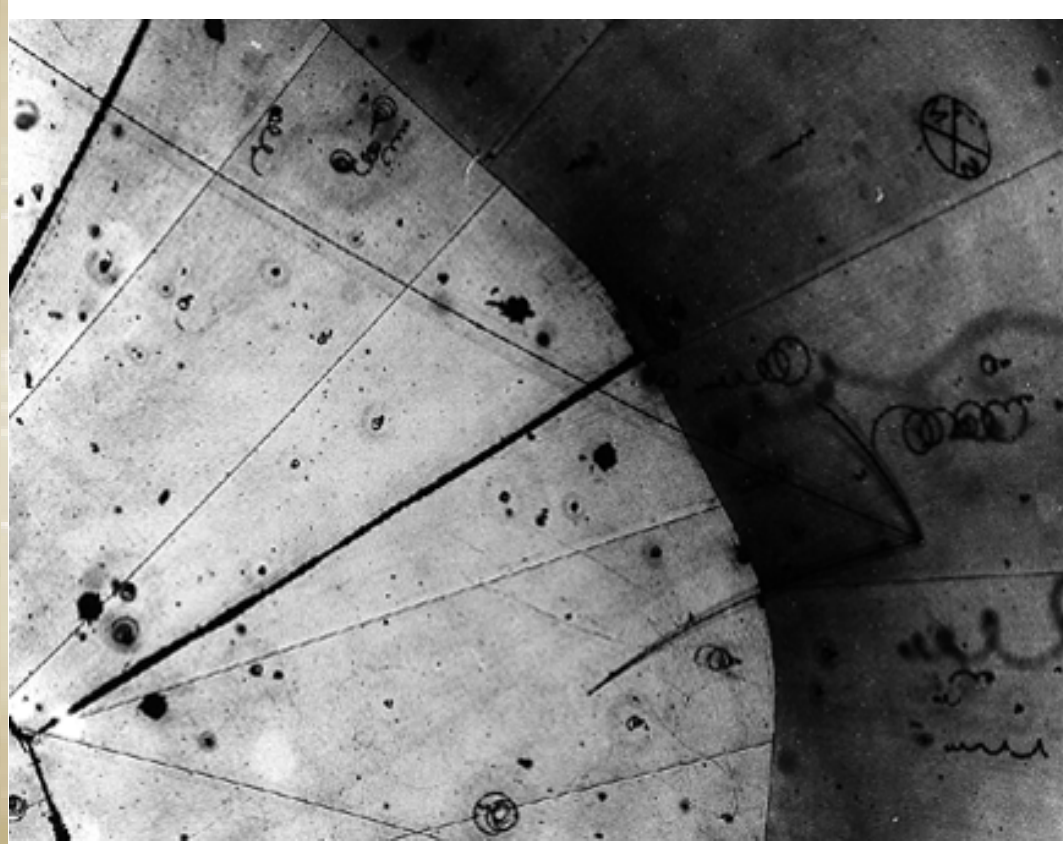
to…



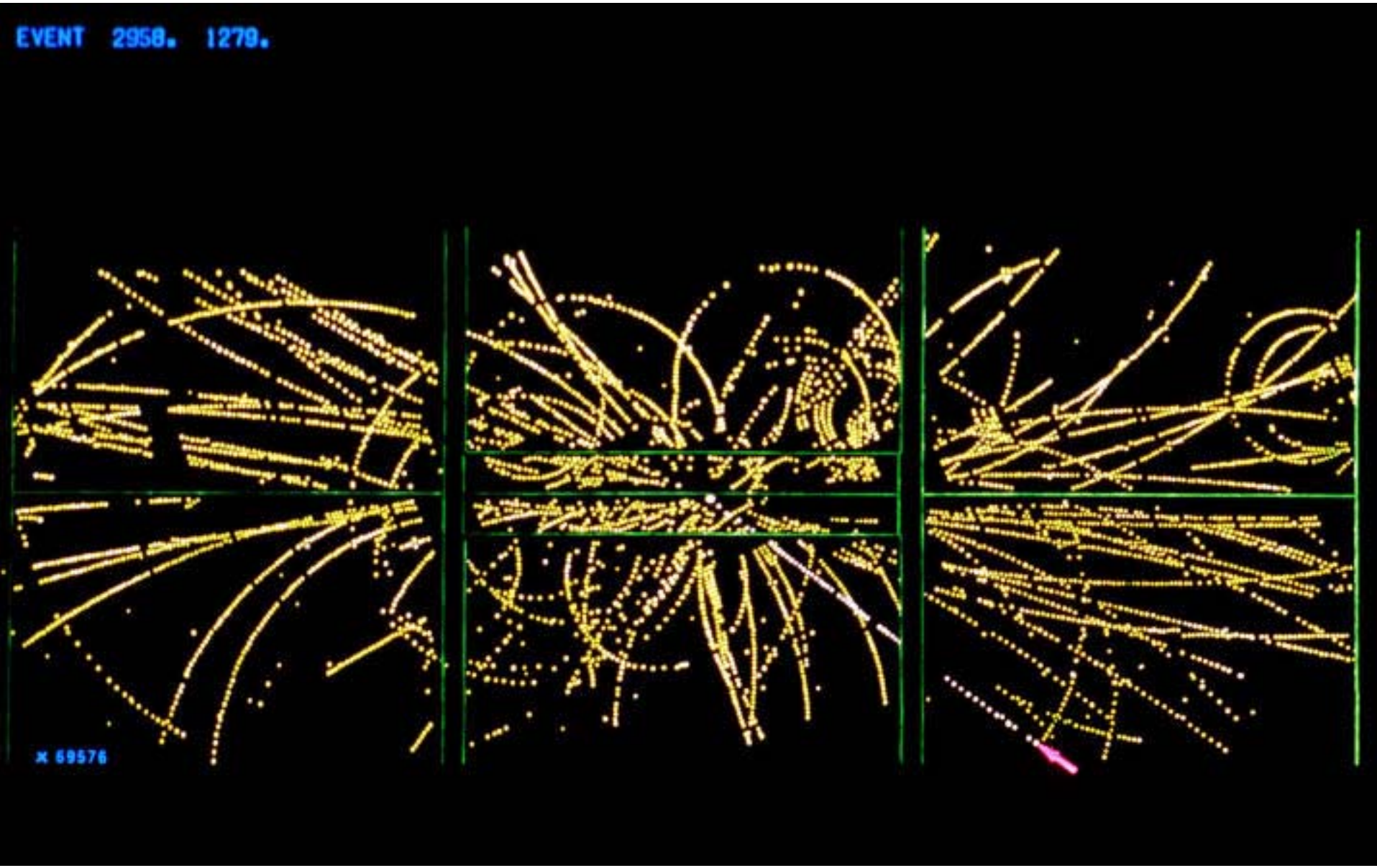


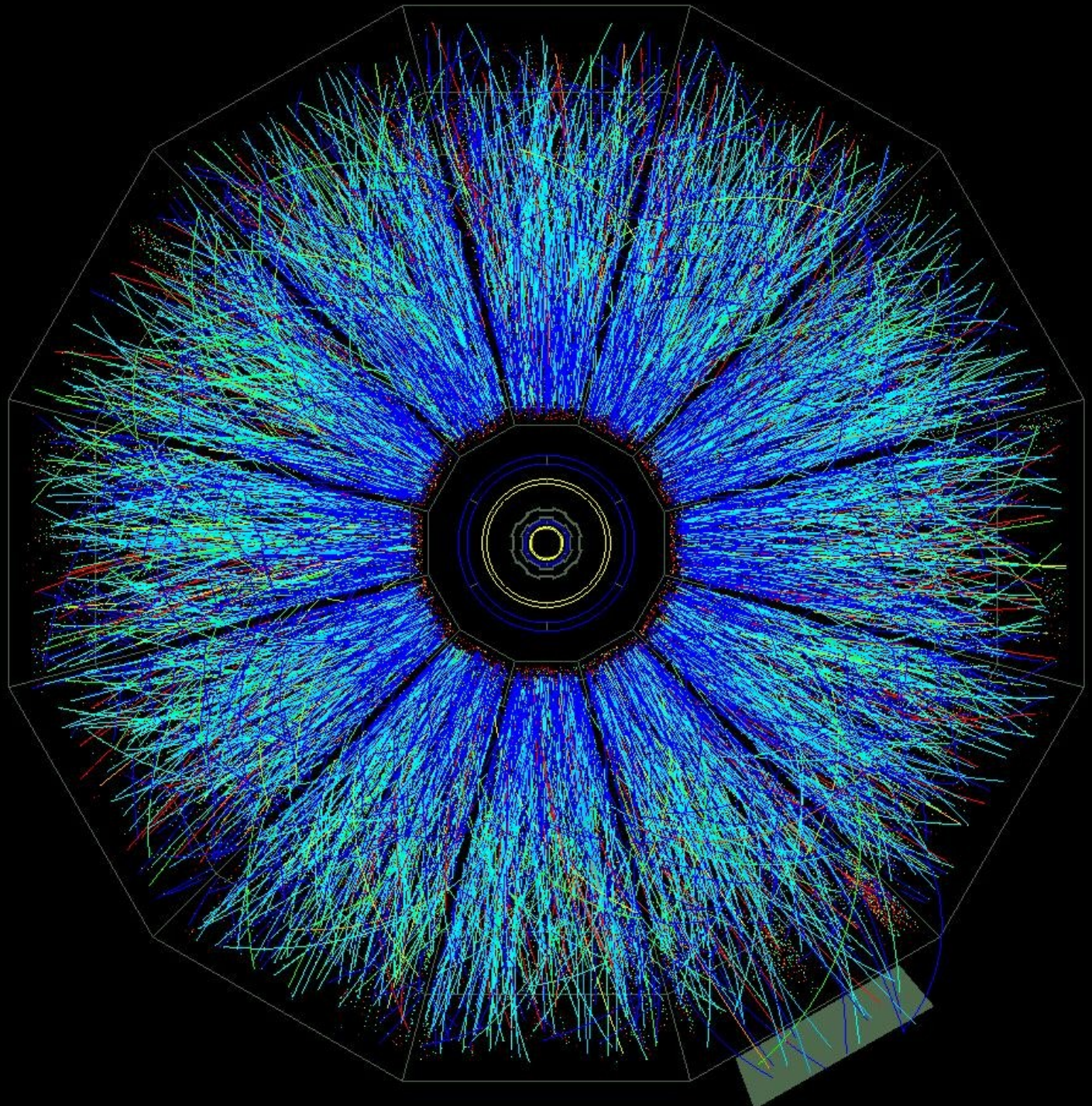
And we have gone from…

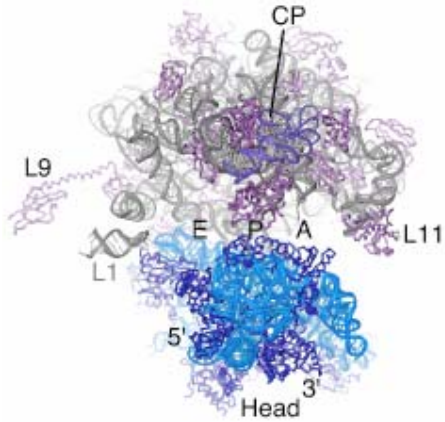
L
c
a
d
i
h
e
g
f
b
0
100
μ

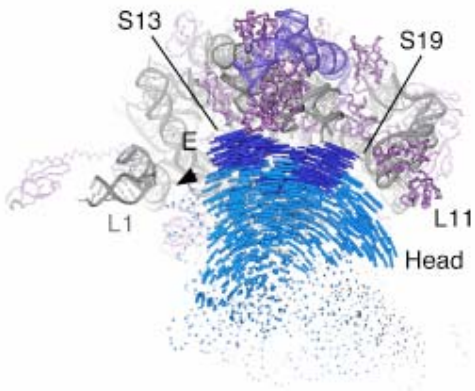


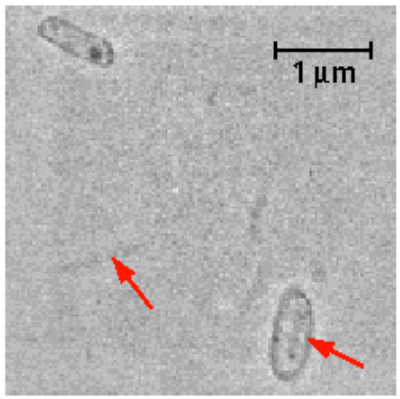
to…

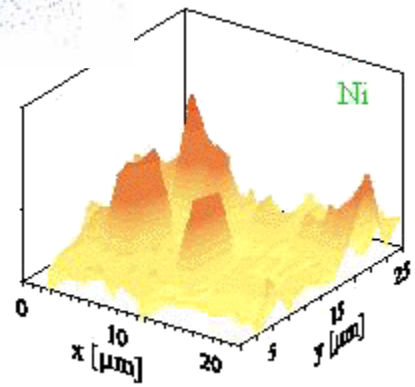

EVENT 2958. 1279.
X 69576

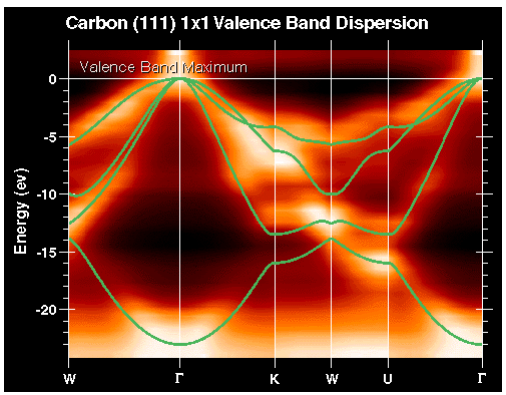

STAR

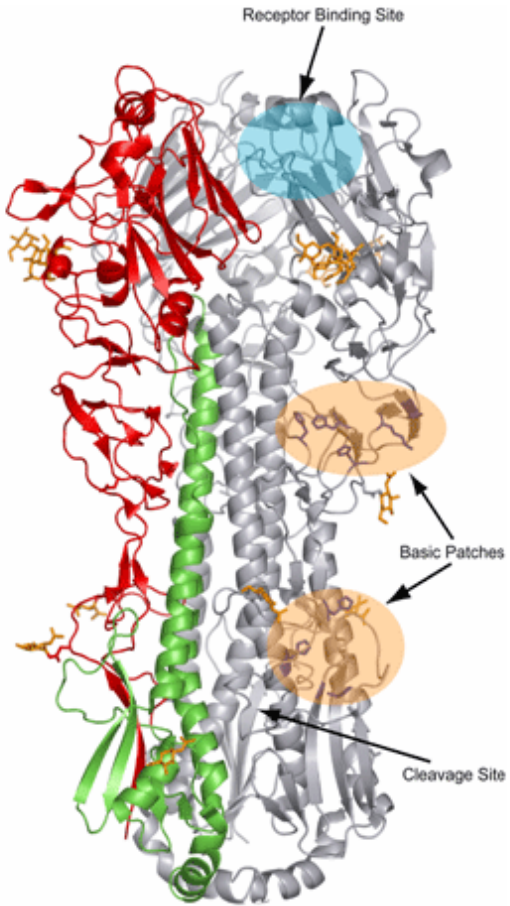

CP
L9
E
P
A
L11
L1
5'
3'
Head

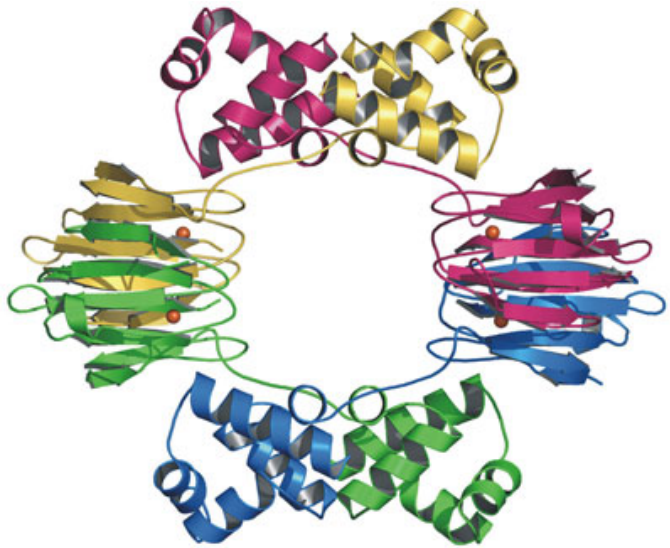

S13
S19
E
L1
L11
Head


1 µm


Ni
0
10
20
x [µm]
5
15
25
y [µm]

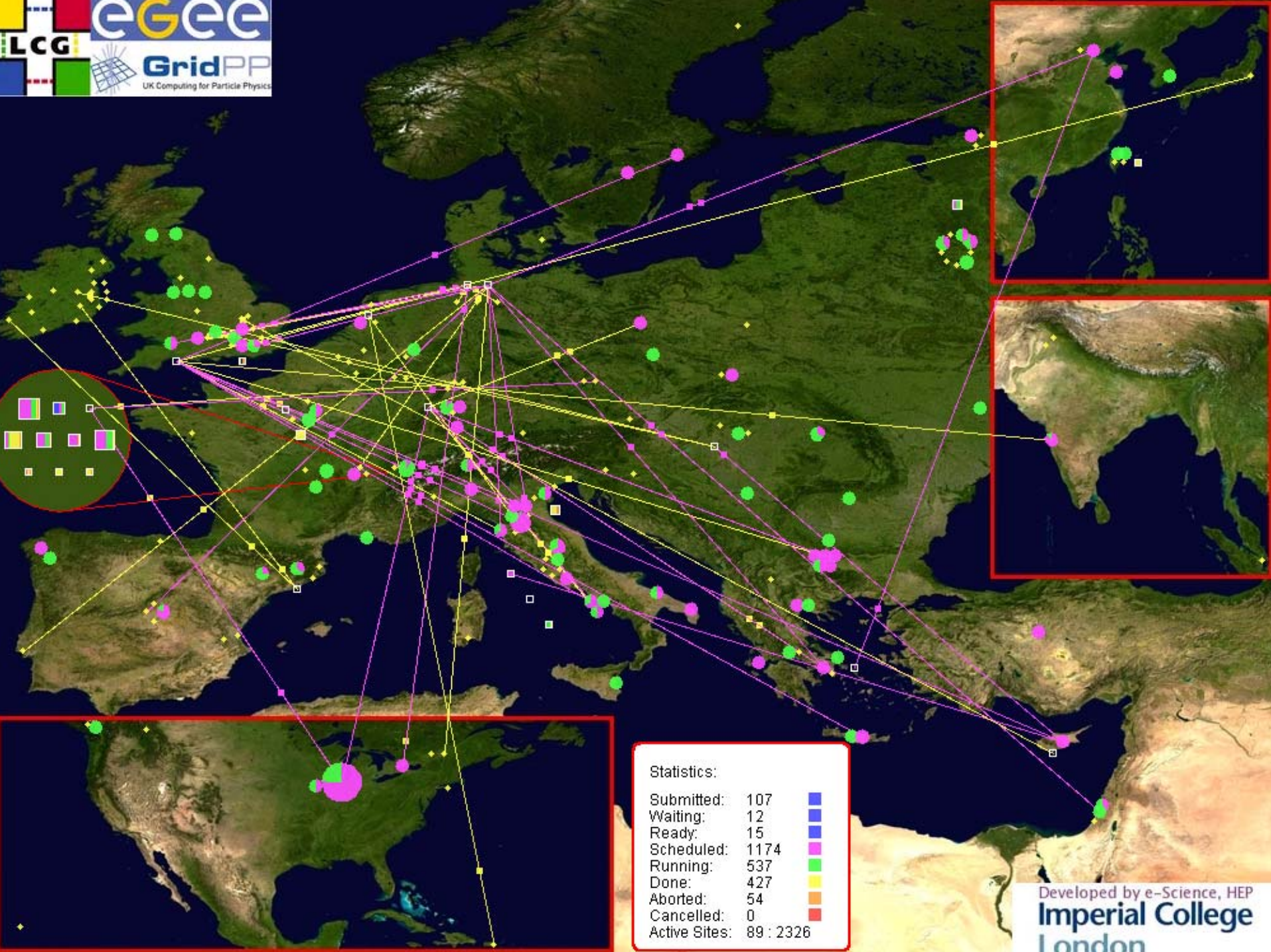

Carbon (111) 1x1 Valence Band Dispersion
Valence Band Maximum
Energy (ev)
0
-5
-10
-15
-20
W
Γ
K
W
U
Γ


Receptor Binding Site
Basic Patches
Cleavage Site



And we have gone from…

to…


LCG
eGee
GridPP
UK Computing for Particle Physics
Statistics:
Submitted: 107
Waiting: 12
Ready: 15
Scheduled: 1174
Running: 537
Done: 427
Aborted: 54
Cancelled: 0
Active Sites: 89 : 2326
Developed by e-Science, HEP
Imperial College London

Beyond fundamental physics, accelerators and accelerator technology are critical to:

- ✓US Science & Technology
- ✓US economy
- ✓National security
- ✓Energy/environmental security
- ✓Health/medicine
- ✓Quality of people’s lives

PORTAC

The Industry's Only Portable, All Weather, High Energy Linac.

| Ideal for field work | Superior to Isotopes | Flexibility | Simple Construction |
| Inexpensive | Easy Setup | Uses Reliable Components | Safe and Easy |

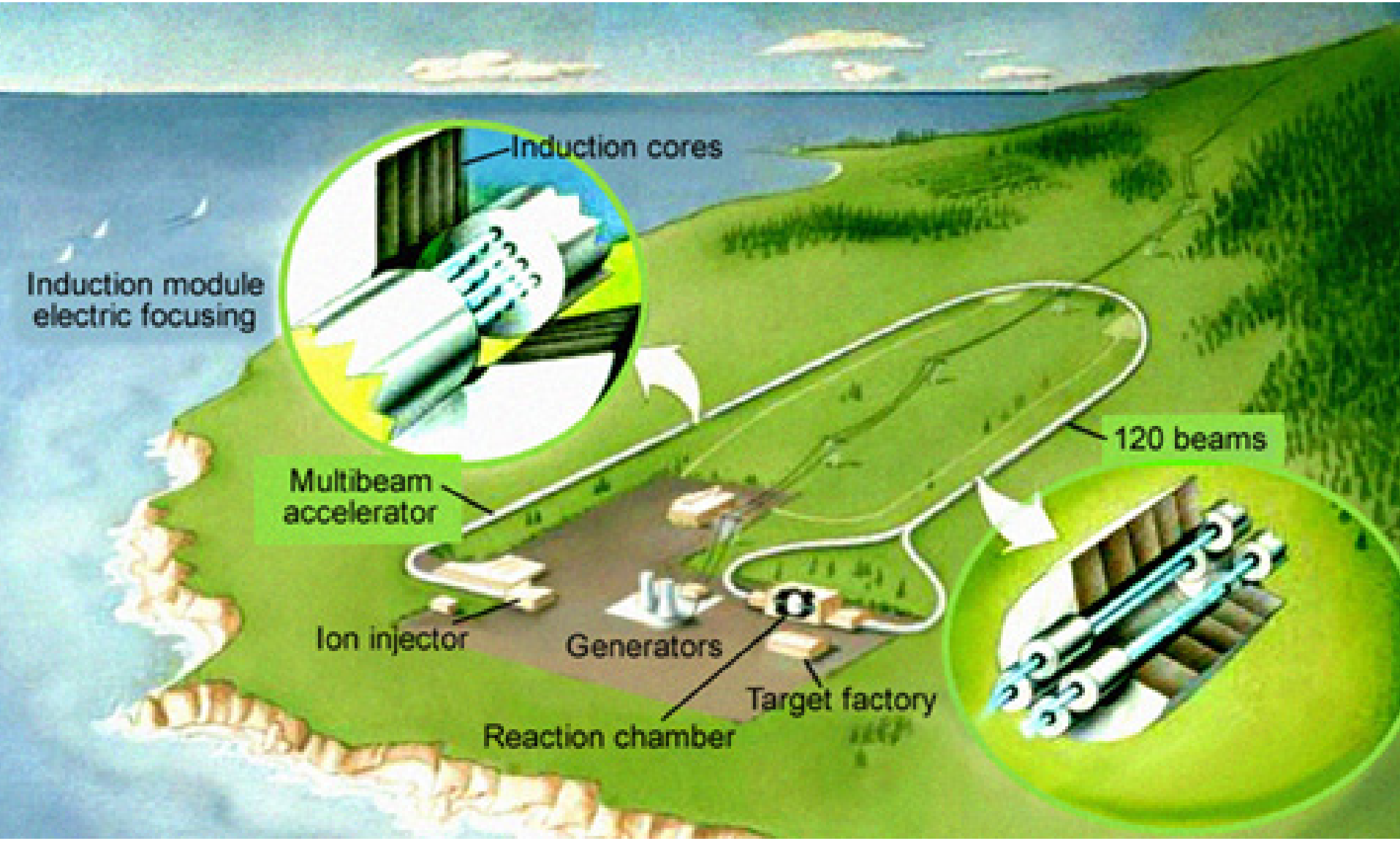
The PORTAC is *ideal* for demanding field and site operations on ...

- Pipelines
- Powerplants
- Shipyards
- Construction Sites
- Bridges

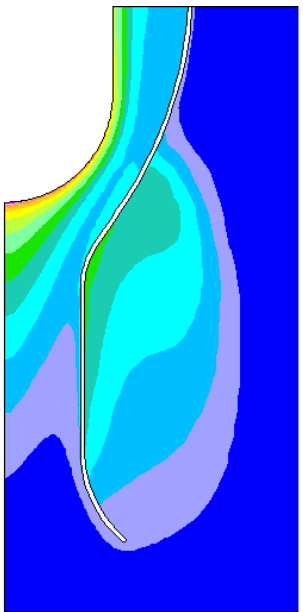
Ideal For Field Work.

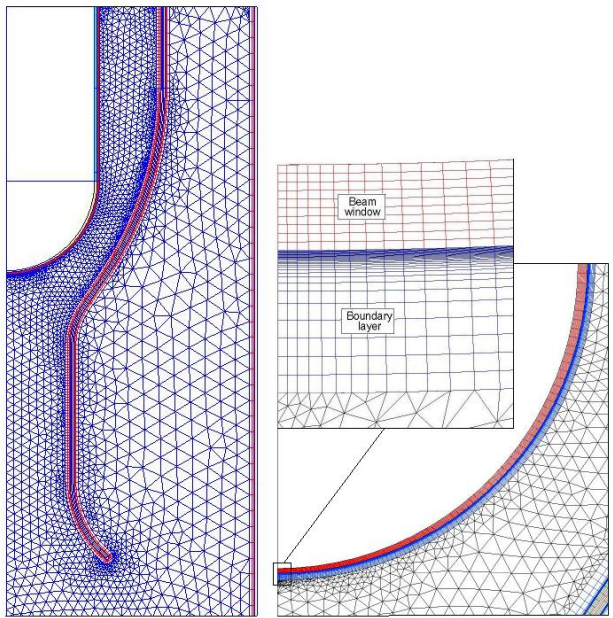
The PORTAC series of industrial accelerators was developed as a powerful, portable X-Ray source. The PORTAC is portable, rugged, all weather, high energy linac available. It is capable of operating in any environment with a minimum of setup. It can be transported by air or by truck over rough terrain. Once on site, it can be assembled and ready for use in less than 15 minutes.

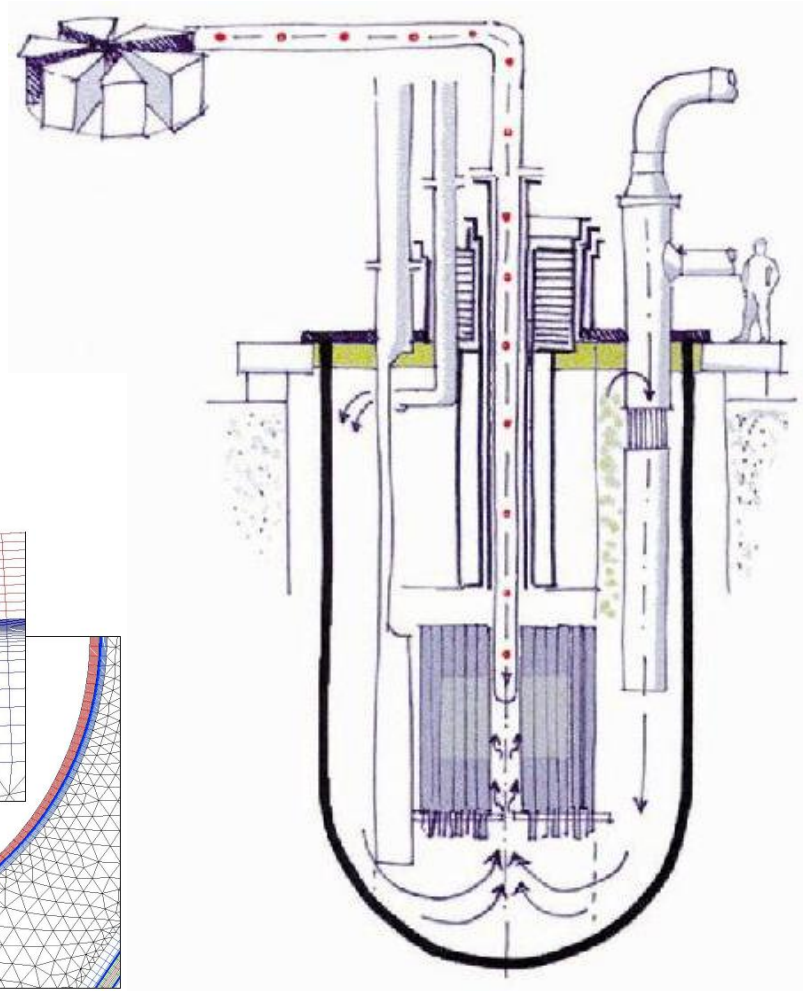
The PORTAC has been tested through shock and vibration routines at temperatures from


Induction cores
Induction module
electric focusing
120 beams
Multibeam
accelerator
Ion injector
Generators
Target factory
Reaction chamber

- **Transmutation of waste**
- **Accelerator-driven energy production (Energy Amplifier)**
- **Proton radiography**

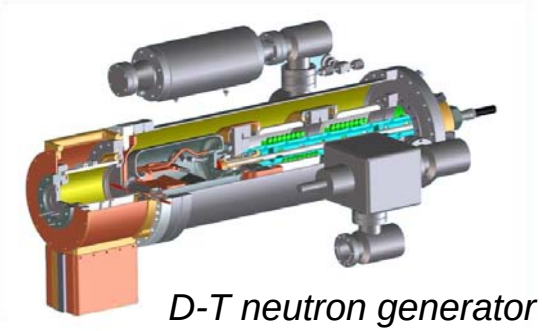






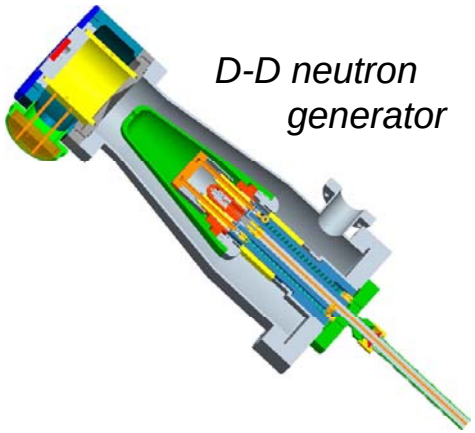
Accelerator Technologies for Homeland Security

- **Accelerator technology can be used to mitigate vulnerabilities in our homeland security**
  - **Sea-going cargo containers**
    - **10 million cargo containers enter the US annually thru 22 ports**
    - **only a few percent presently undergo screening**
  - **Airport cargo, border crossings…**

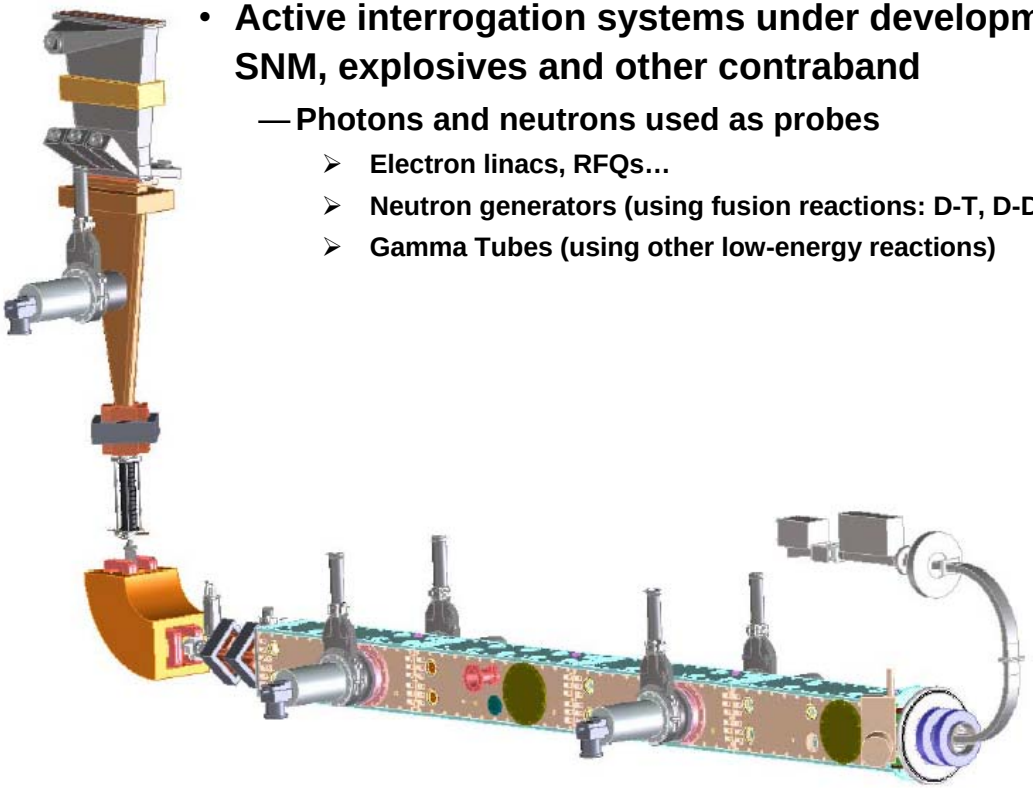


D-T neutron generator

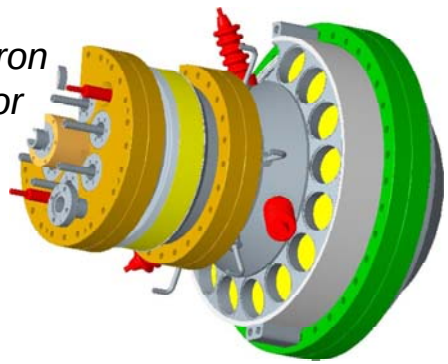
- **Active interrogation systems under development to detect SNM, explosives and other contraband**
  - **Photons and neutrons used as probes**
    - **Electron linacs, RFQs…**
    - **Neutron generators (using fusion reactions: D-T, D-D, T-T)**
    - **Gamma Tubes (using other low-energy reactions)**



D-D neutron generator



RFQ-based neutron source



T-T neutron generator

Importance of accelerators is evident from "Facilities for the Future of Science"

13 of the 28 facilities are accelerators!

Facilities for the Future of Science:
A Twenty-Year Outlook

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Priority: Tie for 3	Joint Dark Energy Mission (JDEM)	16
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	Protein Production and Tags	17
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Priority: Tie for 7	Characterization and Imaging of Molecular Machines	19
	Continuous Electron Beam Accelerator Facility (CEBAF) 12 GeV Upgrade	20
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	Spallation Neutron Source (SNS) 2-4MW Upgrade	25
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Priority: Tie for 18	Double Beta Decay Underground Detector	27
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Priority: Tie for 21	National Synchrotron Light Source (NSLS) Upgrade	30
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US DOE Office of Science (DOE/SC) is the steward of nearly all of the nation's major accelerator facilities

- HEP: High energy physics machines
- NP: Nuclear physics machines
- BES: Light sources, neutron sources

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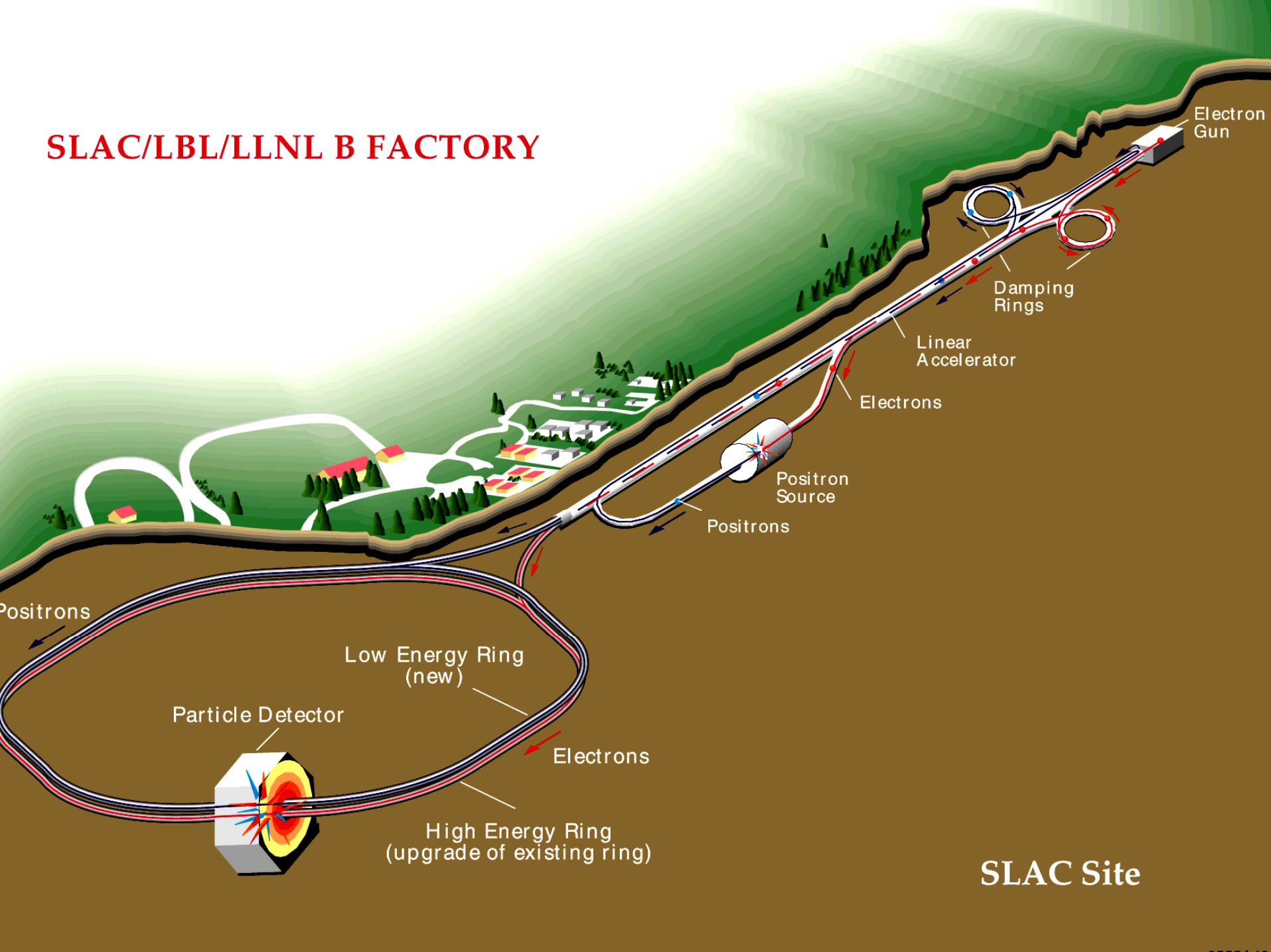
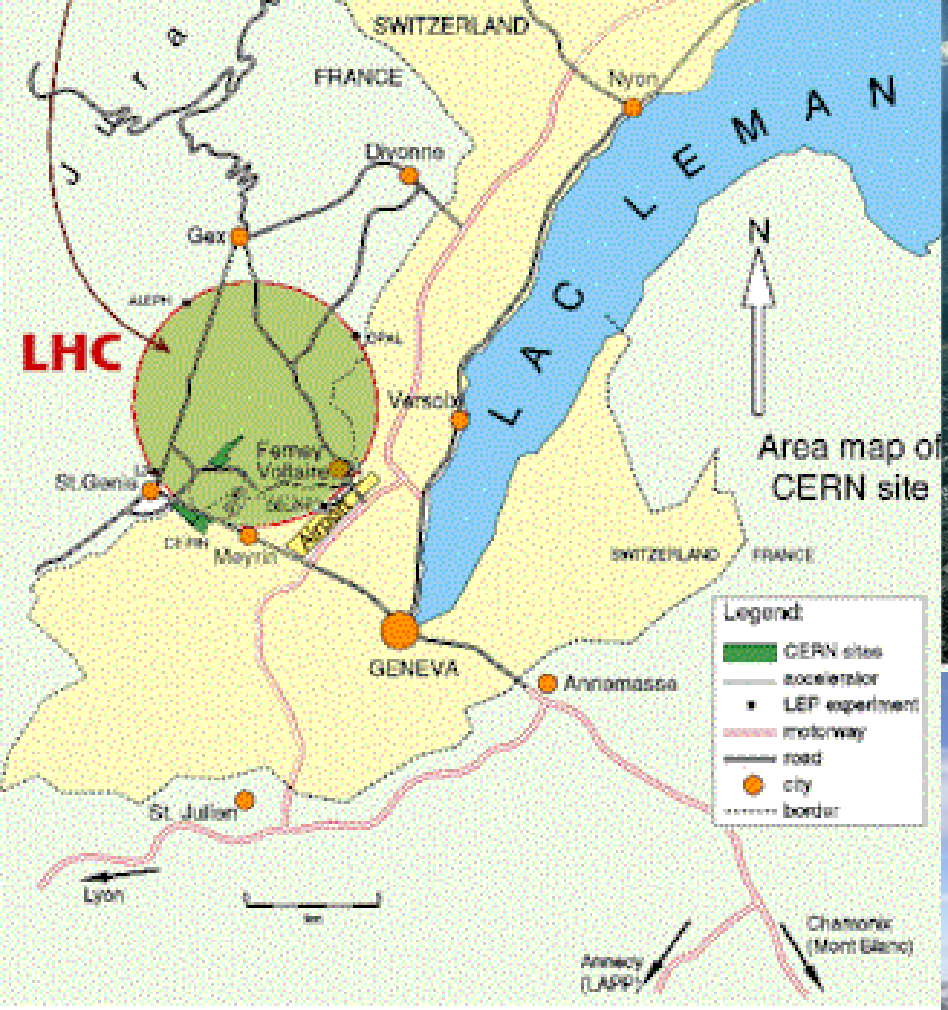
SLAC
Stanford Linear Accelerator Center

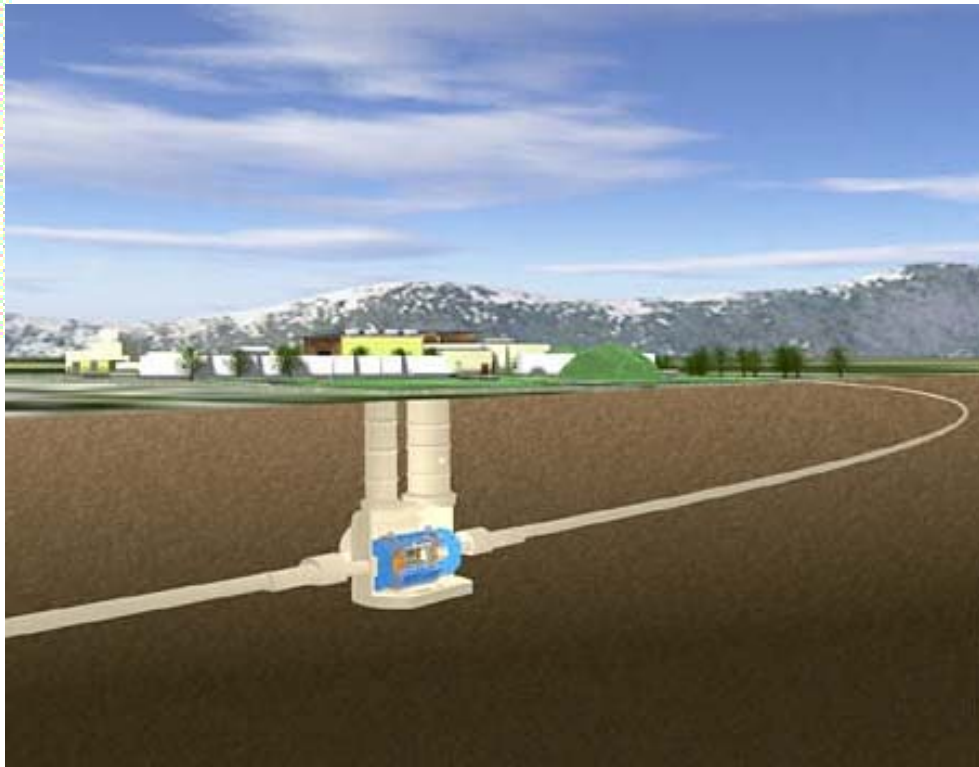
SLAC/LBL/LLNL B FACTORY



BABAR™

BABAR TM & L de Brunhoff


SWITZERLAND
FRANCE
Nyon
Divonne
Gex
LHC
ALEPH
OPAL
Versoix
Ferney Voltaire
St.Genis
CERN
Meyrin
AIRPORT
LAC LEMAN
N
Area map of CERN site
SWITZERLAND
FRANCE
GENEVA
Annemasse
St. Julien
Lyon
Legend:
CERN sites
accelerator
LEP experiment
motorway
road
city
border
Chamonix (Mont Blanc)
Annecy (LAPP)



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- HEP: High energy physics machines
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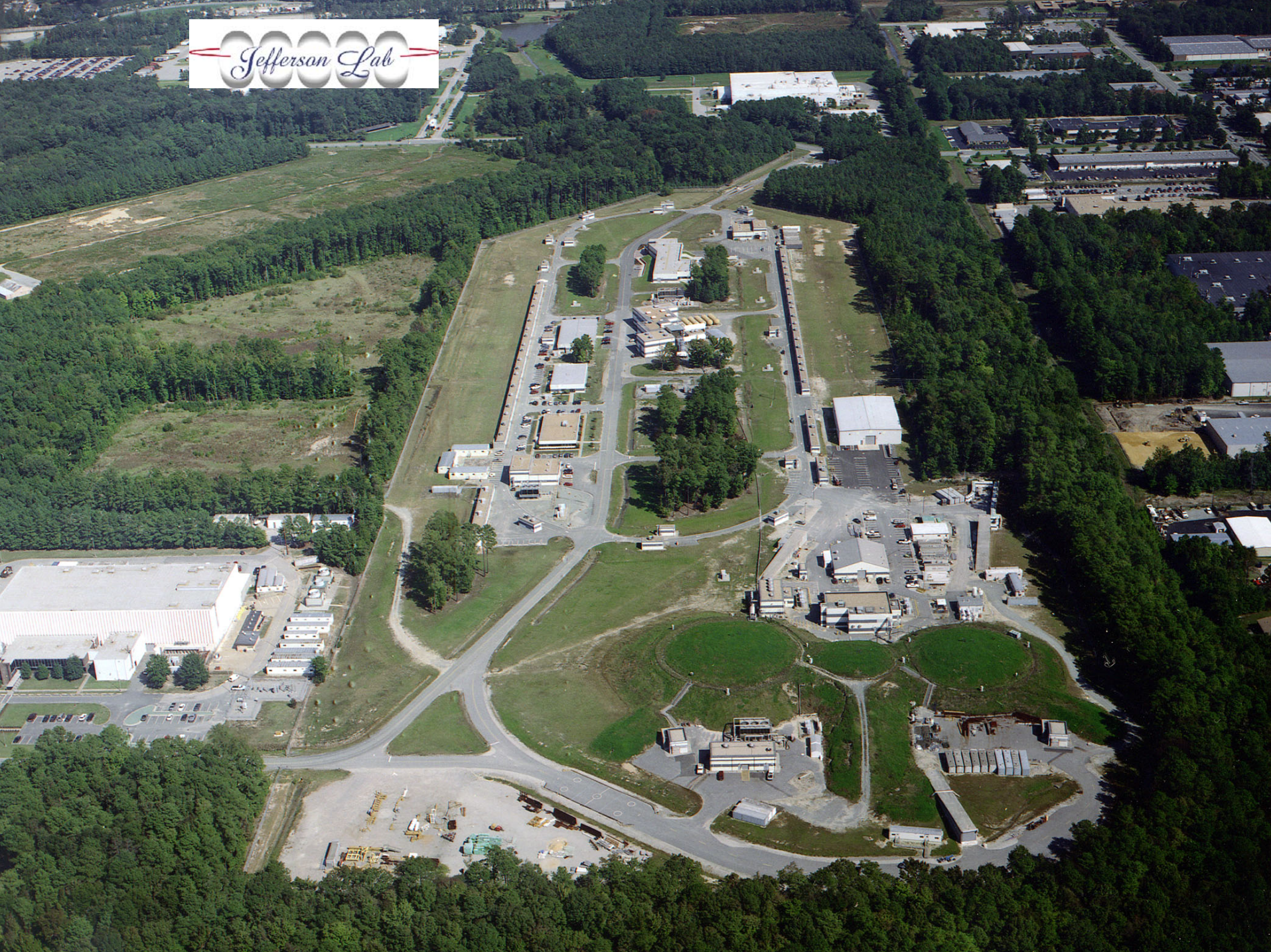
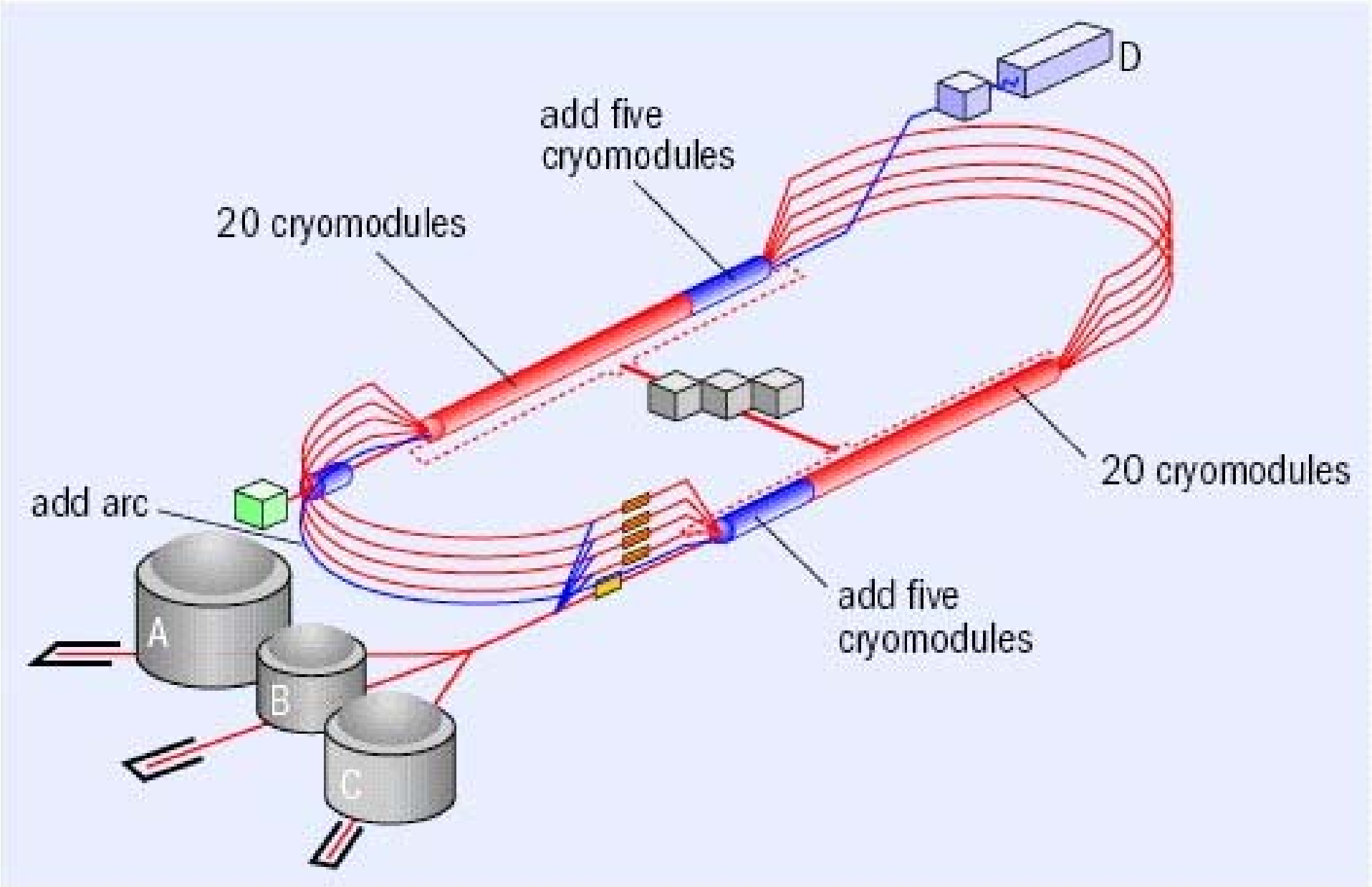
12:00 o'clock
Sextant 10/11
Sextant 12/1
PHOBOS
10:00 o'clock
BRAHMS
2:00 o'clock
RHIC
Sextant 2/3
PHENIX
4:00 o'clock
Sextant 6/7
STAR
Sextant 4/5
(First sextant to be tested)
BOOSTER
G-2
LINAC
AGS
TANDEMS

NORTHROP GRUMMAN


Jefferson Lab


D
add five
cryomodules
20 cryomodules
20 cryomodules
add arc
add five
cryomodules
A
B
C

hribf
Home

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- HEP: High energy physics machines
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nsls
IR
UV
X

APS

SSRL

Berkeley Lab
75
Years of World-Class
Science
1931-2006

SNS
A U.S. Department of Energy multilaboratory project
Spallation Neutron Source

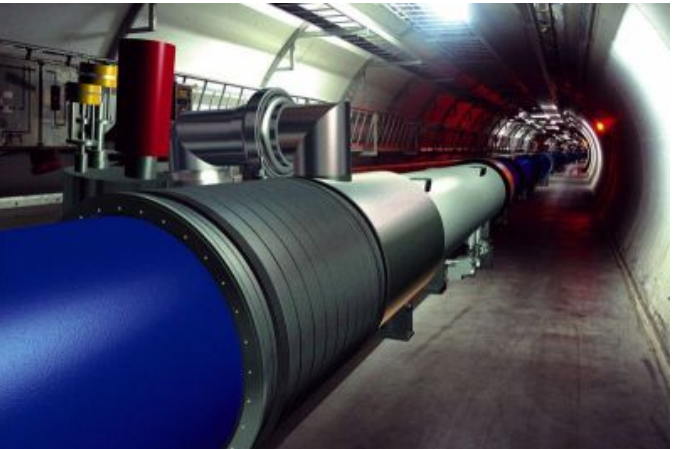
LANSCE

NSF accelerator facilities

- National Supercondcuting Cyclotron Lab @ MSU
- Indiana Univ. Cyclotron Facility
- CESR/CHESS @ Cornell
- Many small university programs

Besides CERN (already mentioned), DOE/SC has many other collaborations w/ international accelerator labs

- A few examples…



～宇宙と物質の
起源と構造を探る～

KEK

高エネルギー加速器研究機構

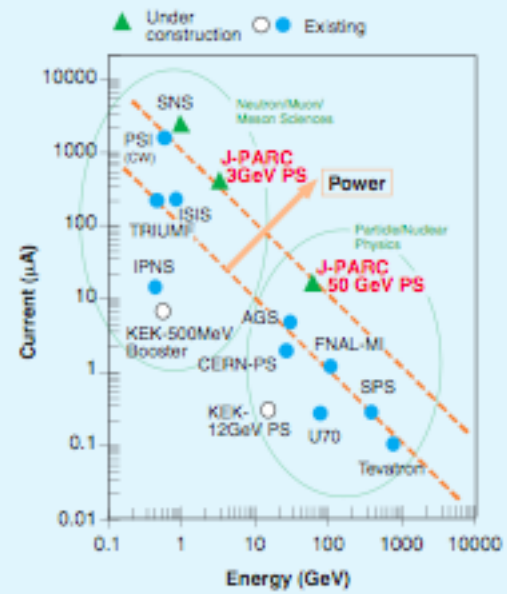
J-PARC
High Intensity Proton Accelerator Facility

J-PARC: Towards High Intensity Frontier!

J-PARC, Japan Proton Accelerator Research Complex, is a joint project of KEK and JAERI (Japan Atomic Energy Research Institute). The construction started at the Tokai campus of JAERI, about 70 km northeast of KEK, in 2001, and the first beam is expected around 2007. The facility aims to create a world's leading accelerator complex with its high beam power. Using intense proton beams at 3-GeV and 50-GeV proton synchrotrons, a variety of secondary beams will be produced, and a broad range of sciences, from nuclear and particle physics to materials and life sciences, will be pursued.

Nuclear and Particle Physics with a Variety of Secondary Beams!

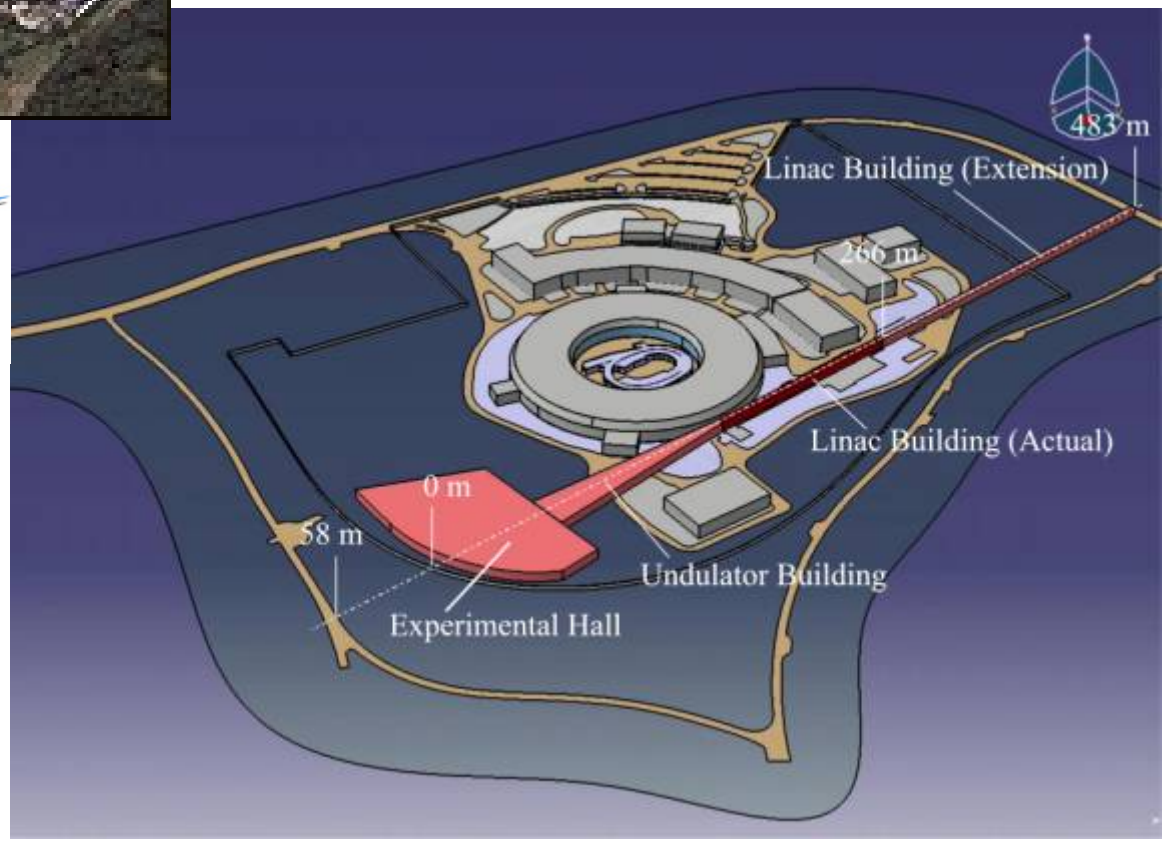
http://j-parc.jp/



J-PARC will be a world's leading Mega-Watt class accelerator facility.

Accelerator components are being fabricated and tested.

FERMI @elettra



GSI

The software developed under the SciDAC Accelerator Science & Technology (AST) project has been applied to projects at most of the previously mentioned facilities

SciDAC Accelerator Science & Technology (AST) Project

Goals: Develop & apply an advanced, comprehensive simulation environment to solve the most challenging problems, and to enable new discoveries, in 21st century accelerator science & technology

Participants:

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

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

SciDAC/AST codes have been applied present & future DOE projects + projects of our international collaborators

1. Tevatron
2. LHC
3. NLC
4. ILC
5. PEP-II
6. FNAL booster
7. FNAL Main Injector
8. L'OASIS LWFA experiments
9. SLAC PWFA experiments
10. Plasma afterburner design
11. RHIC
12. RIA
13. SNS
14. LCLS
15. Photoinjector design
16. Advanced streak camera design
17. CERN SPS
18. JPARC commissioning
19. FERMI design
20. Int'l code benchmarking @ CERN PS

SciDAC/AST project 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

Multiple models needed:

- **Maxwell,Vlasov, Poisson/Vlasov,Maxwell/vlasov, static PIC, EM PIC, Fokker/Planck, multi-species**

Multi-physics

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)

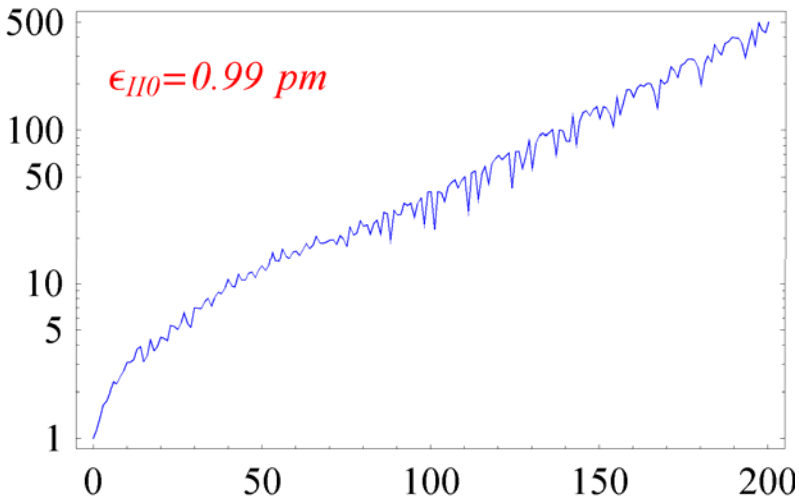
- First 100M simulation of a linac for an x-ray light source w/ self-consistent 3D space charge (IMPACT-Z; I. Pogorelov, J. Qiang)

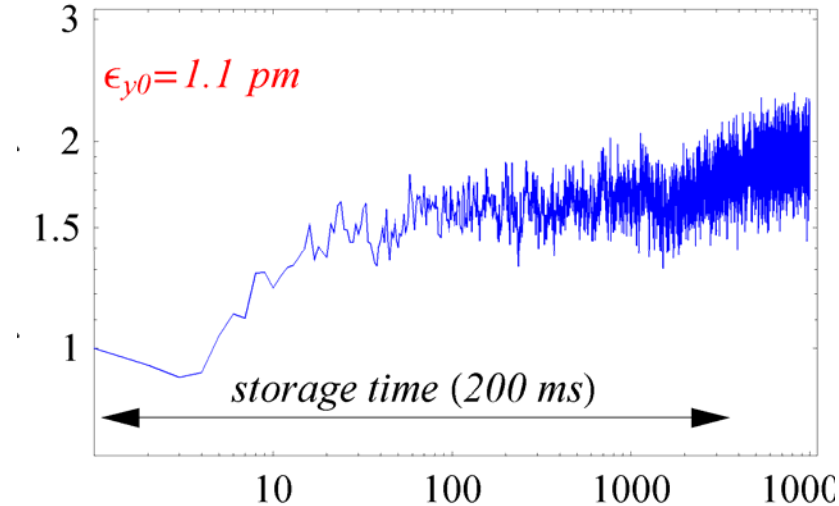
- First self-consistent electromagnetic simulation of an intense beam in an ILC 'crab' cavity (VORPAL; J.R. Cary, C. Nieter & VORPAL team)

- First 3D simulation of a 1TeV Afterburner stage (QuickPIC; C.K.Huang et al.)

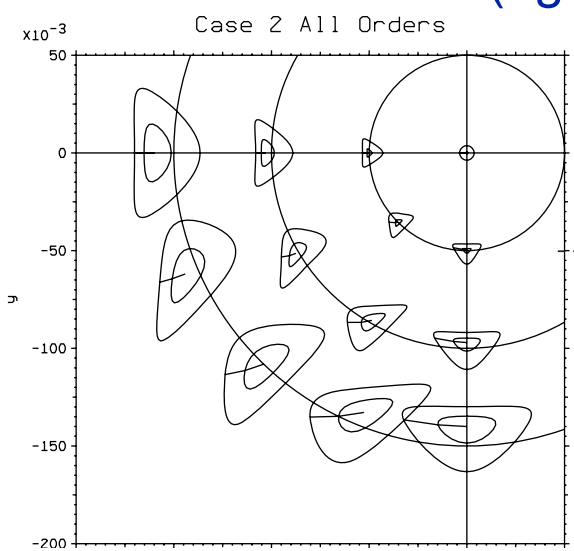
- First 3D simulation of a GeV LWFA stage (OSIRIS; F.S.Tsung, W.Lu, M. Tzoufras et al.)

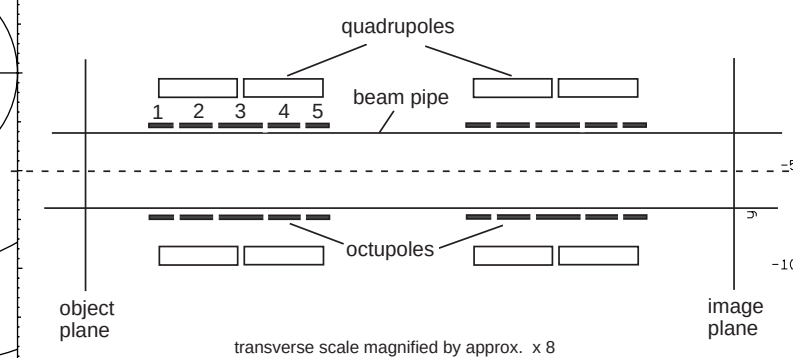
ML/I examples

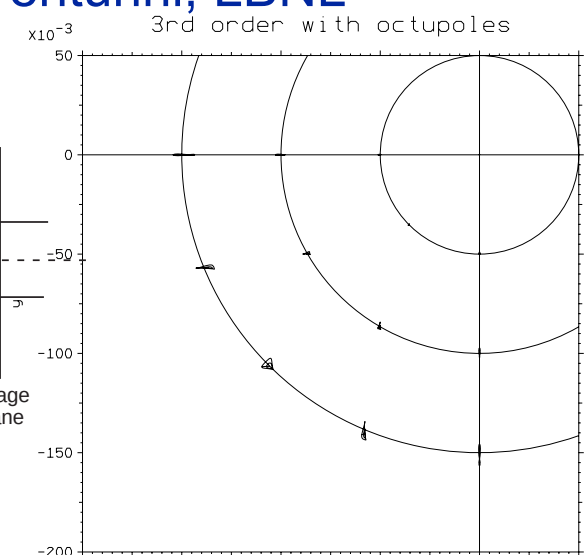




ILC damping ring simulations showing emittance growth w/ linear (left), nonlinear (right) space-charge models. M. Venturini, LBNL

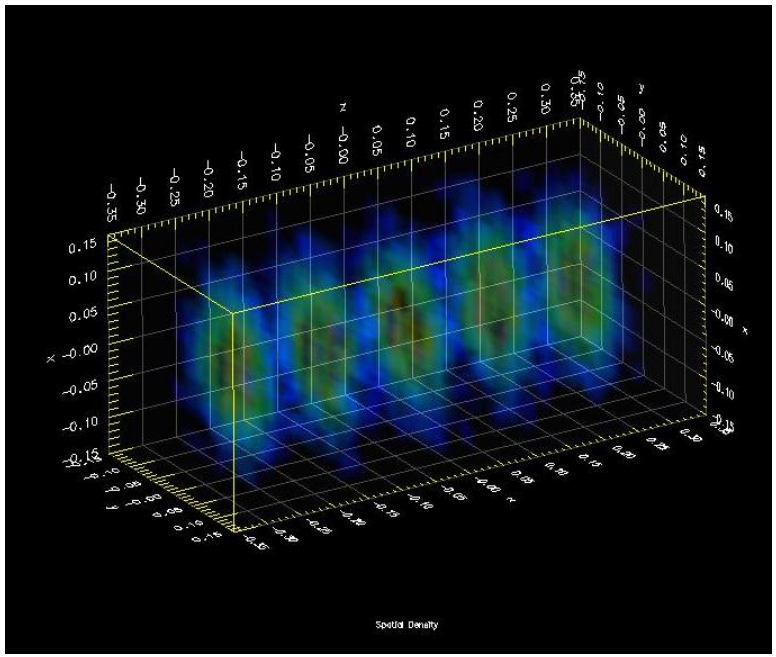






Web plots showing aberrations in uncorrected (left) and octupole-corrected (right) imaging system. P. Walstron and F. Neri, LANL)

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

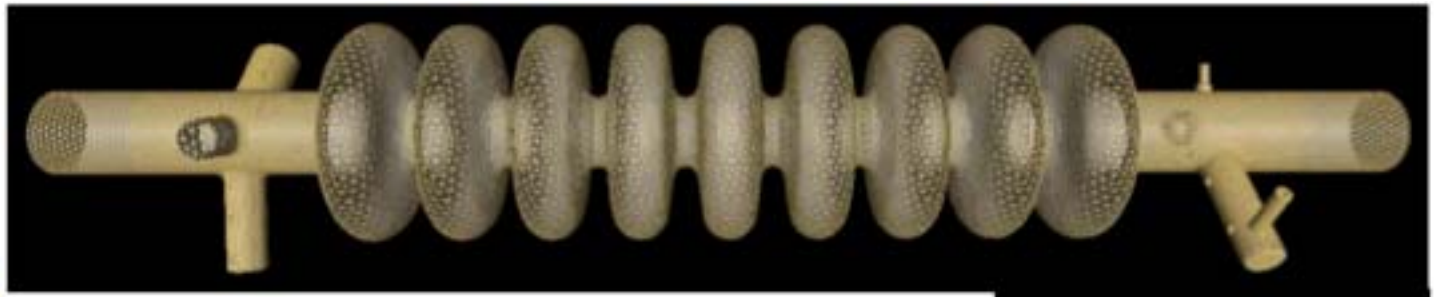


Merging of 5 microbunches in the FNAL booster (J. Amundson, P. Spentzouris)

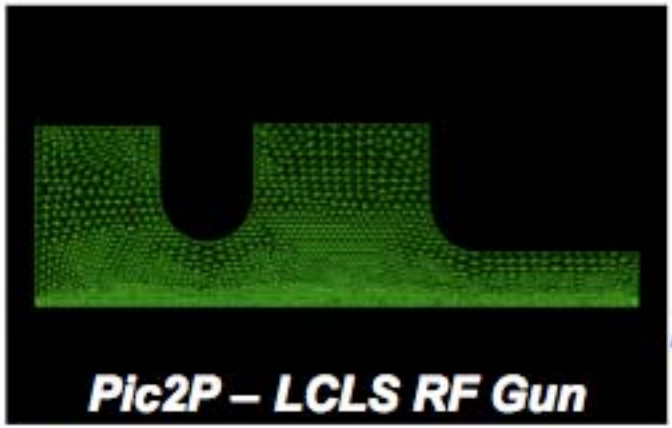
- Self-consistent 3D space-charge model
- 2nd order maps (arbitrary order possible)
- Use 33x33x257 grid and ~ 5,000,000 particles
- Multi-turn injection
- Machine ramping with position feedback
- 6-D phase space beam matching

FNAL Booster simulations follow 5 200 MHz Linac micro-bunches in a 37.8 MHz PhS slice.

ILC BPM



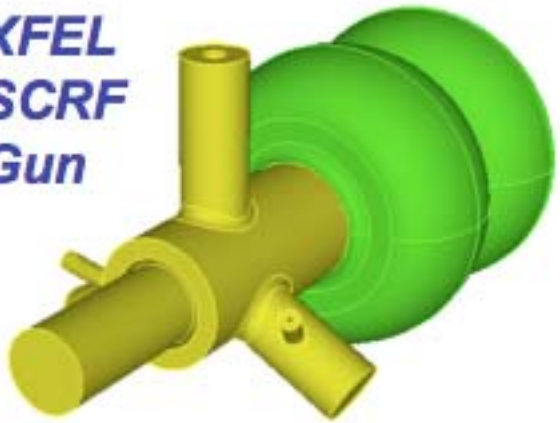
ILC Crab Cavity



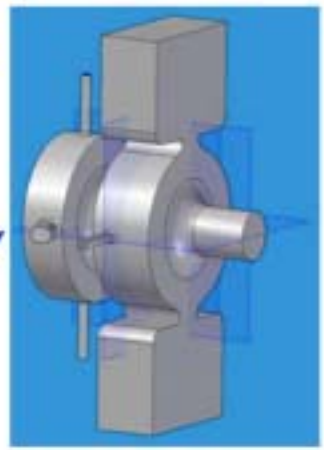
Pic2P – LCLS RF Gun

PEP-II BPM

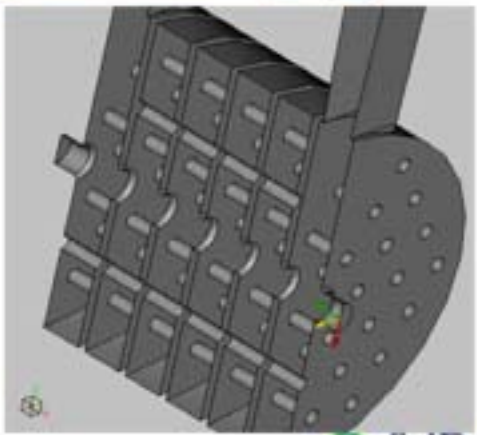
XFEL SCRF Gun

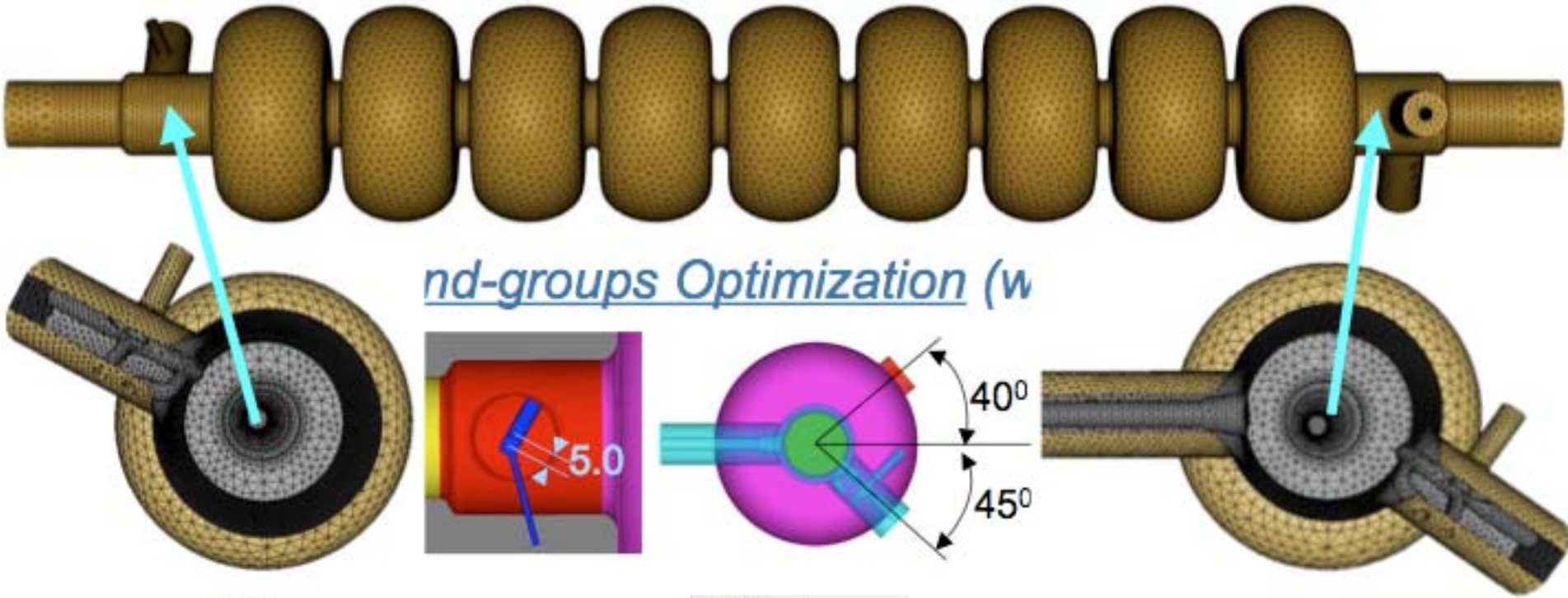


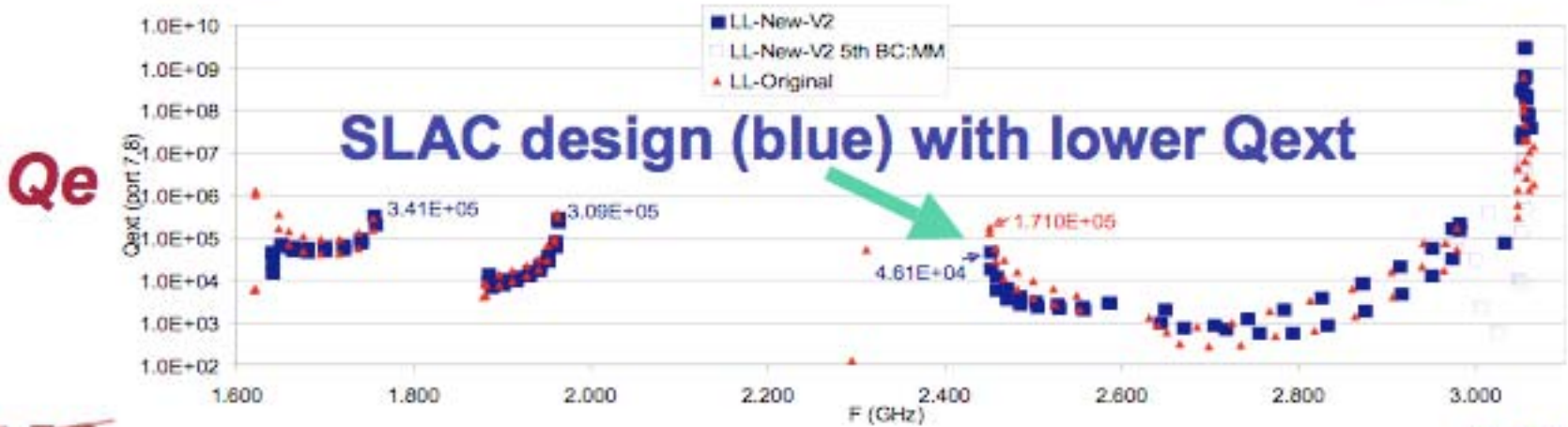
LCLS RF Gun Cavity



MIT PBG

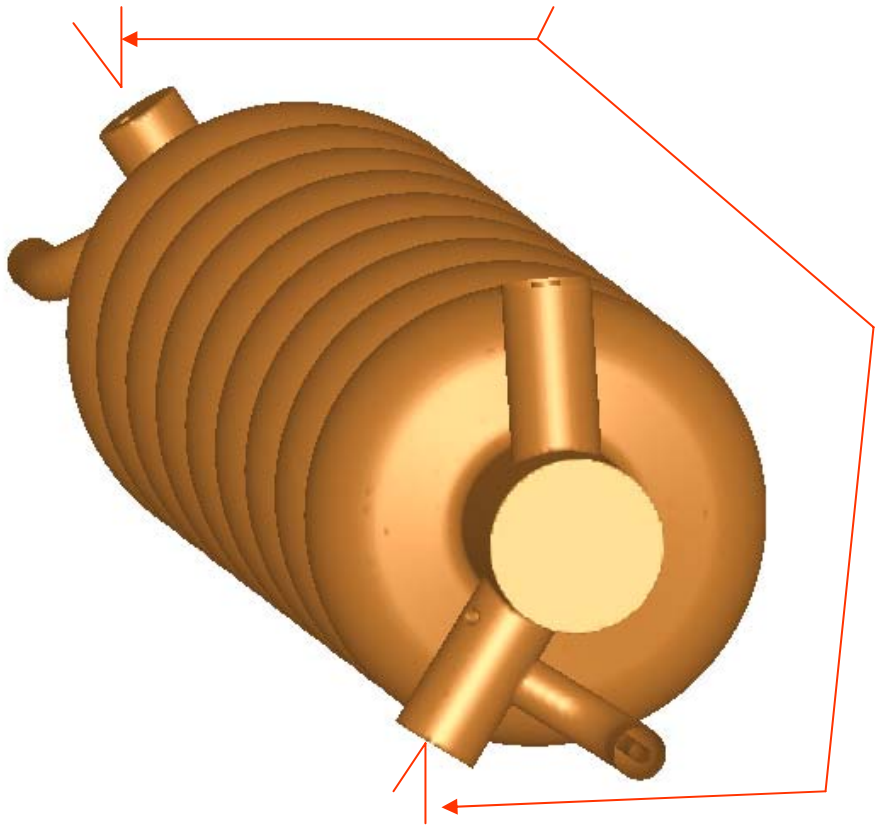


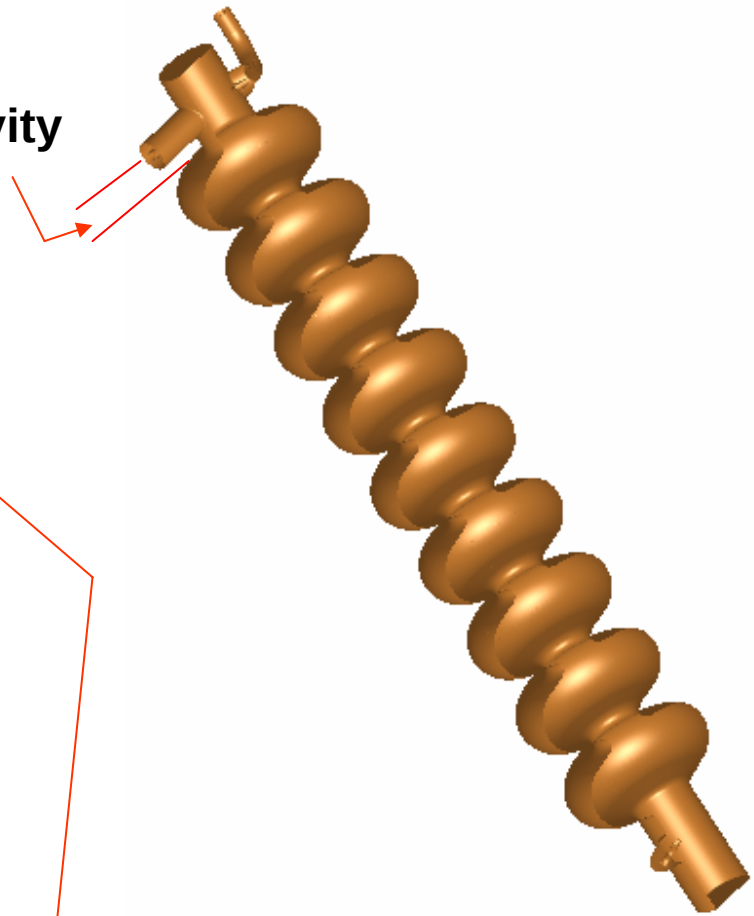

nd-groups Optimization (w
5.0
40⁰
45⁰

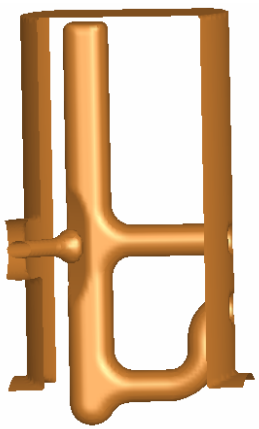

Qe
LL-New-V2
LL-New-V2 5th BC:MM
LL-Original
SLAC design (blue) with lower Qext
Qext (port 7,8)
1.0E+10
1.0E+09
1.0E+08
1.0E+07
1.0E+06
1.0E+05
1.0E+04
1.0E+03
1.0E+02
3.41E+05
3.09E+05
1.710E+05
4.61E+04
1.600
1.800
2.000
2.200
2.400
2.600
2.800
3.000
F (GHz)

ILC cavity modeling w/ VORPAL (Tech-X Corp)

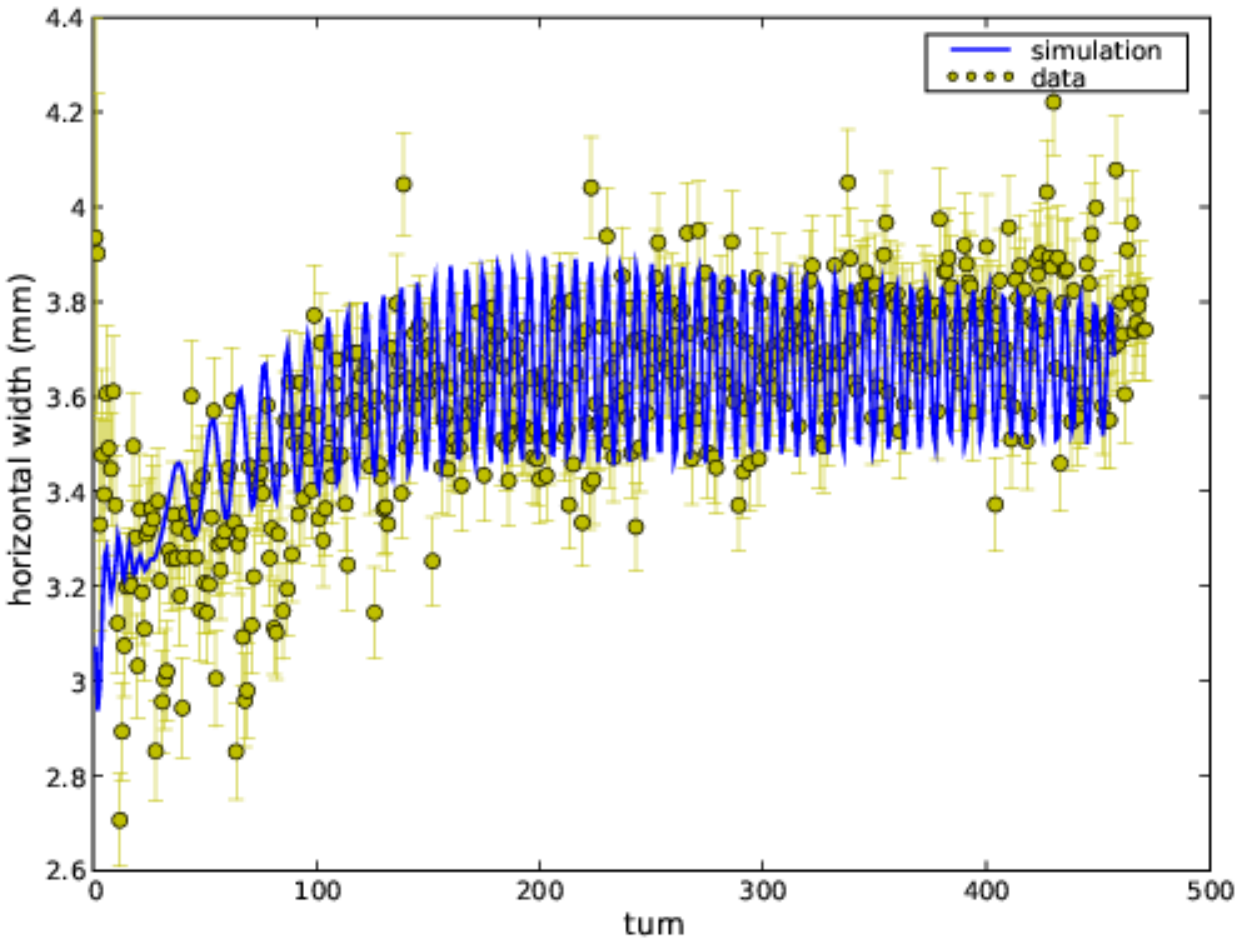
- **HOM Couplers are:**
  - **— Properly distanced from the cavity**
  - **— Properly oriented around axis**





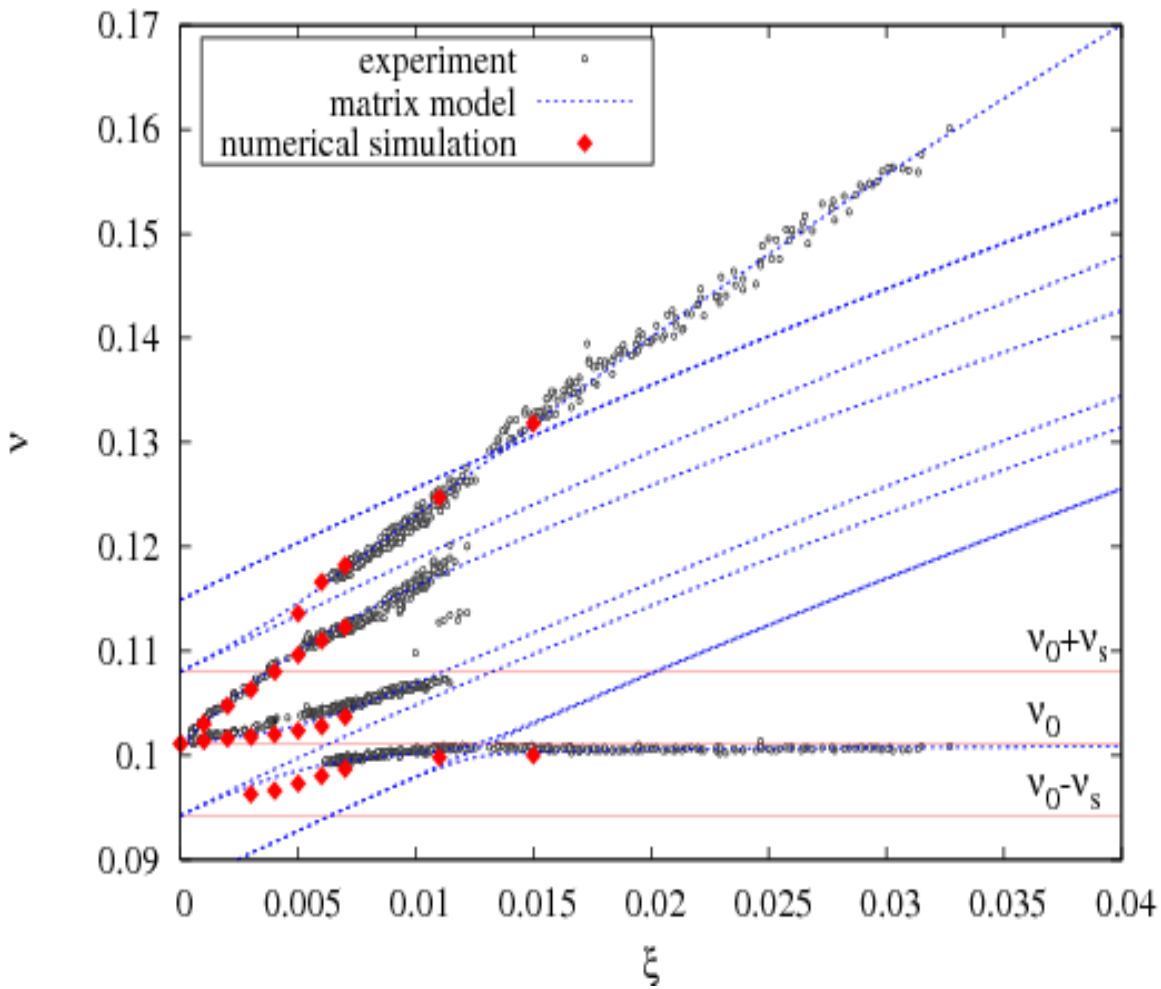


Booster simulations studied halo creation and emittance dilution

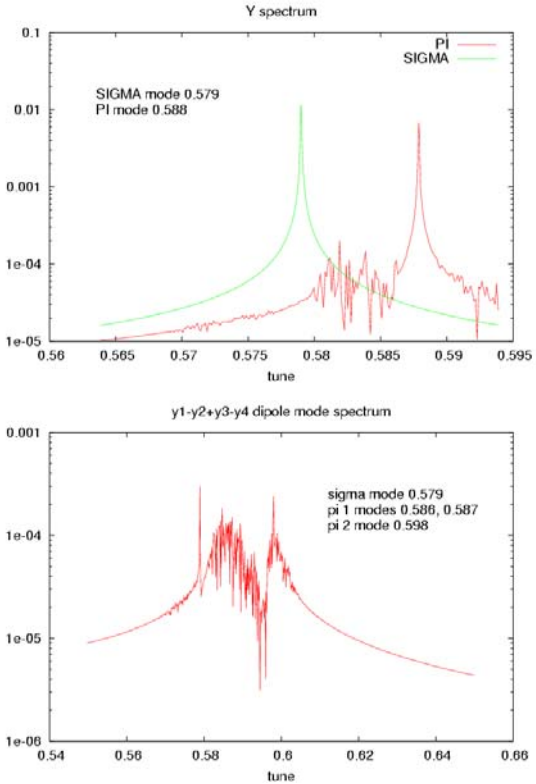


3D Booster simulation including injection, rf ramping, etc.
Comparison with experimental data (J. Amundson, P. Spentzouris, FNAL)

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



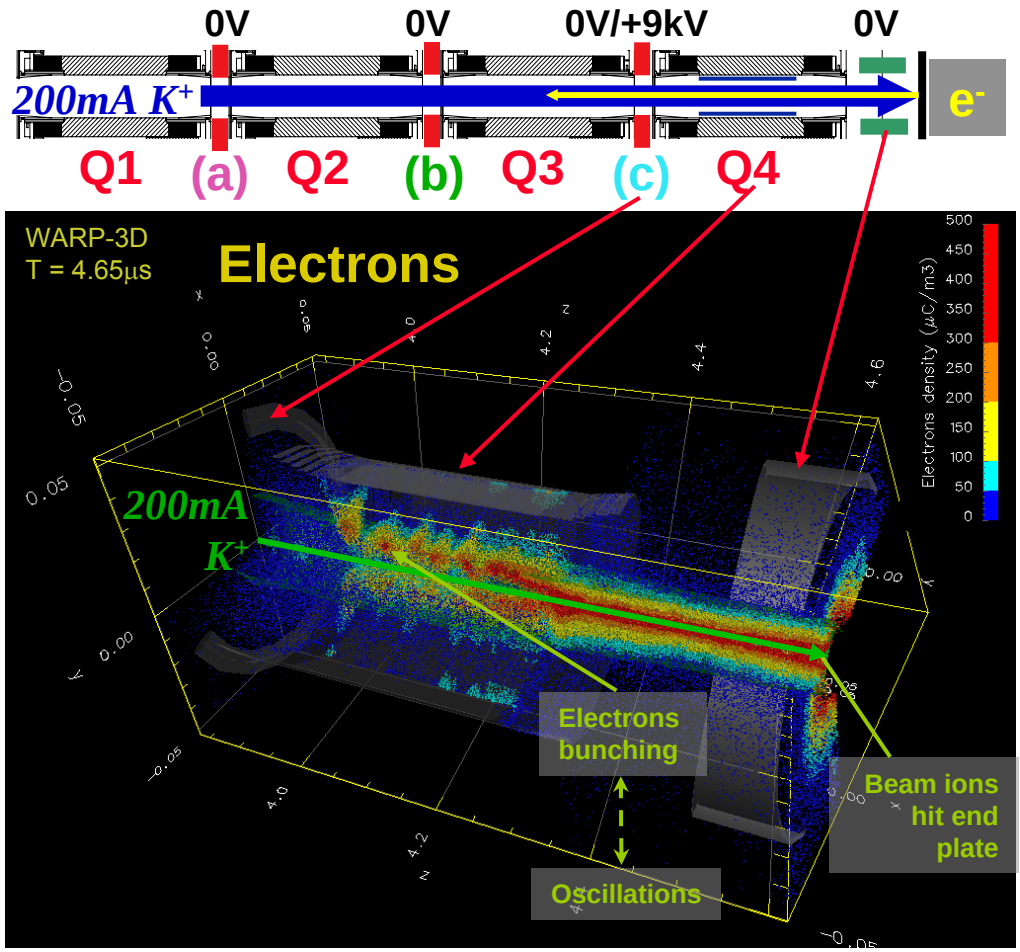
Beam-beam code validation comparing with VEPP-II data



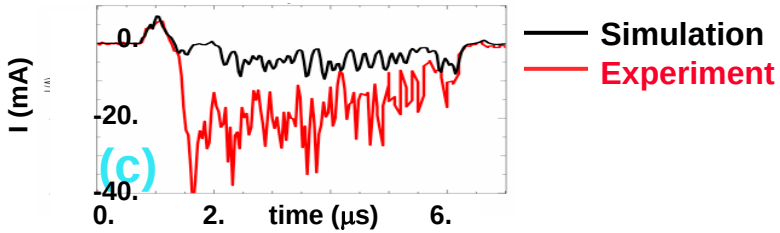
2-bunch coherent (top)
4-bunch coherent (below)

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

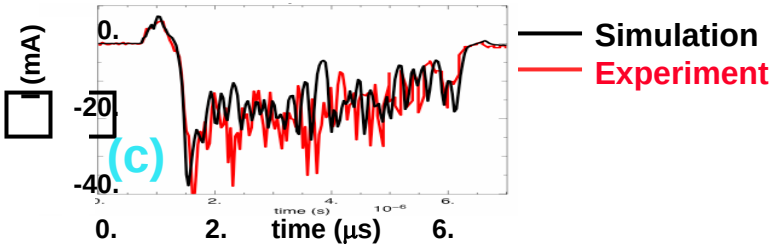
6 MHz signal in clearing electrode: simulation & expt



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



2. **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

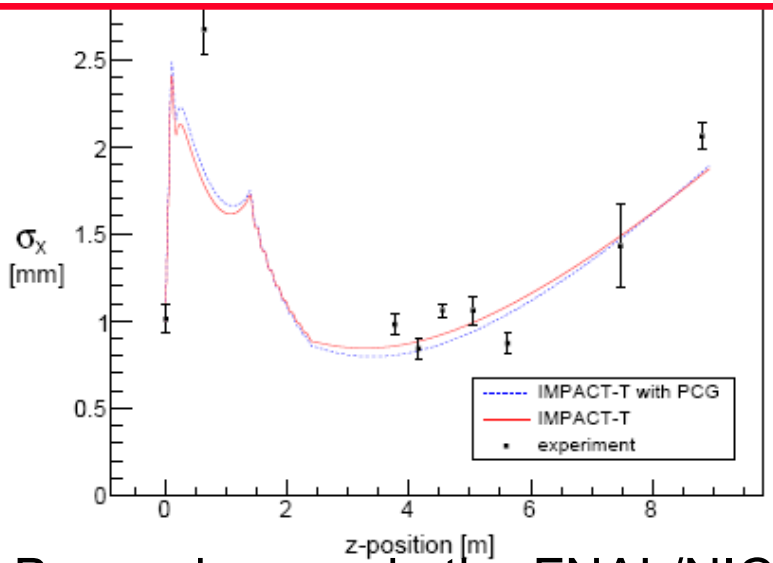
M. Furman, J.-L. Vay (LBNL); A. Friedman, R. Cowan (LLNL); P. Stoltz (Tech-X); P. Colella (LBNL)

Illustrates the strong cross-cutting nature of accelerator modeling across DOE/SC: An OFES code (WARP), combined w/ a OHEP code (POSINST) into a unique parallel capability that will serve both communities.

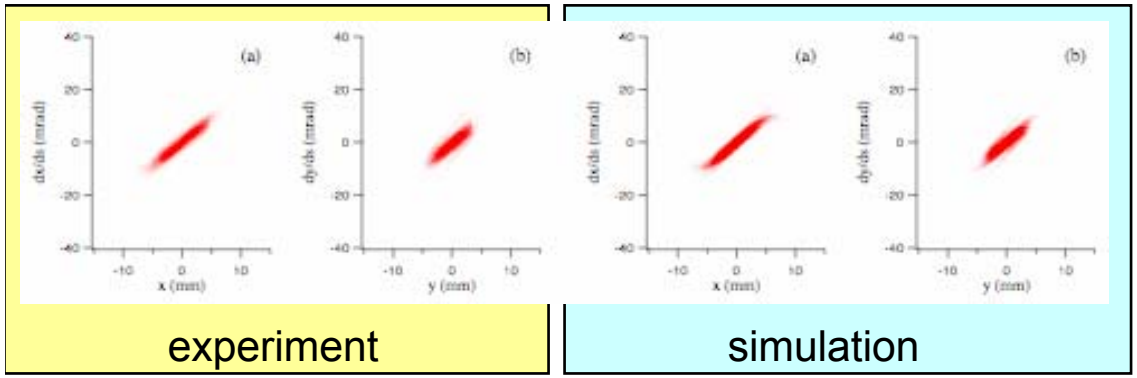
- Future apps include e-cloud studies for ILC, LHC, FNAL MI, possibly RHIC

Broad impact

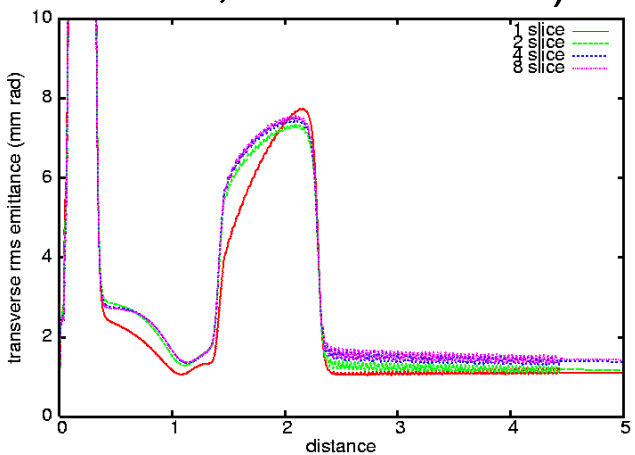
Example IMPACT applications: HEP, NP, BES



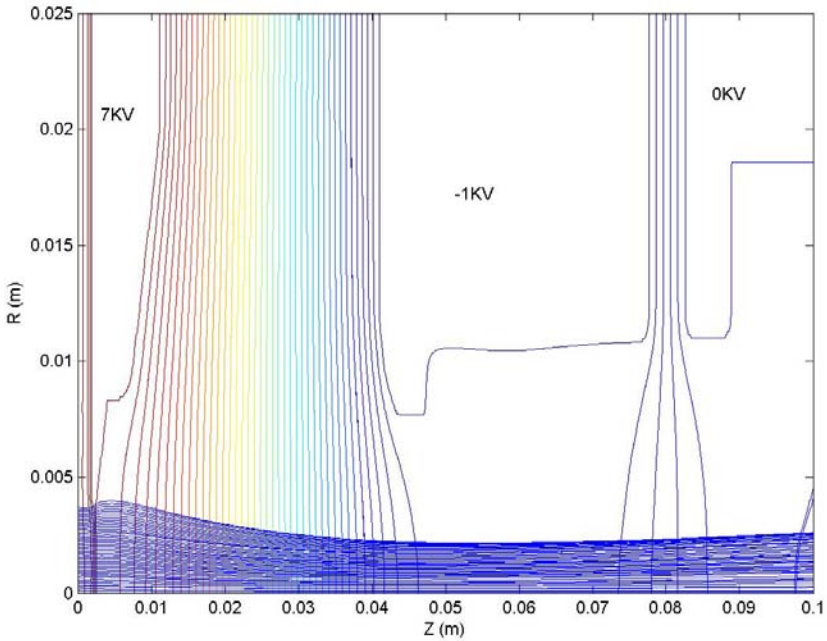
Beam size vs z in the FNAL/NICADD photoinjector: simulation & experiment (C. Bohn/NIU, F. Piot/FNAL)



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

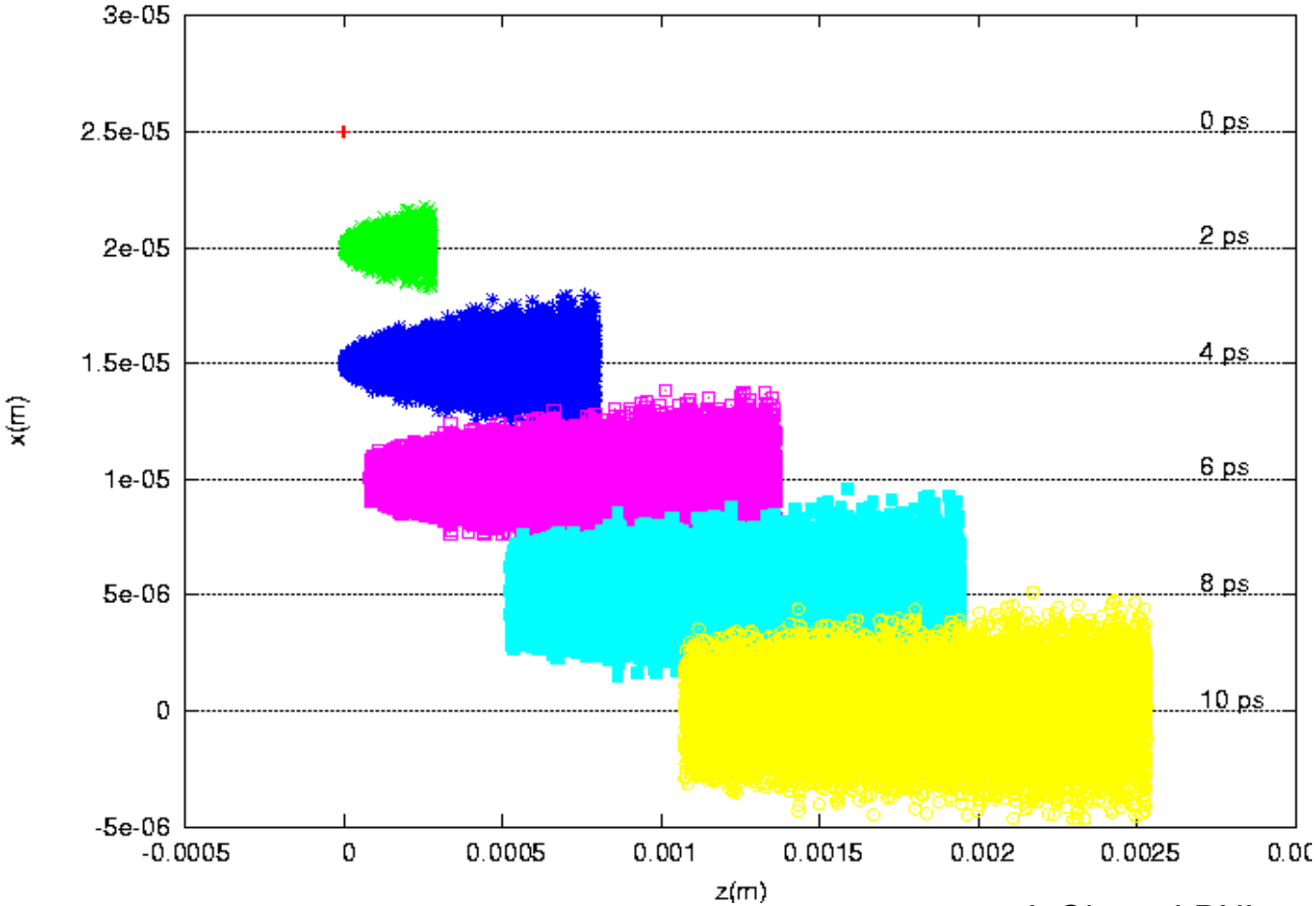


LCLS photoinjector emittance evolution (J. Qiang/LBNL, C. Limbourg/SLAC)



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

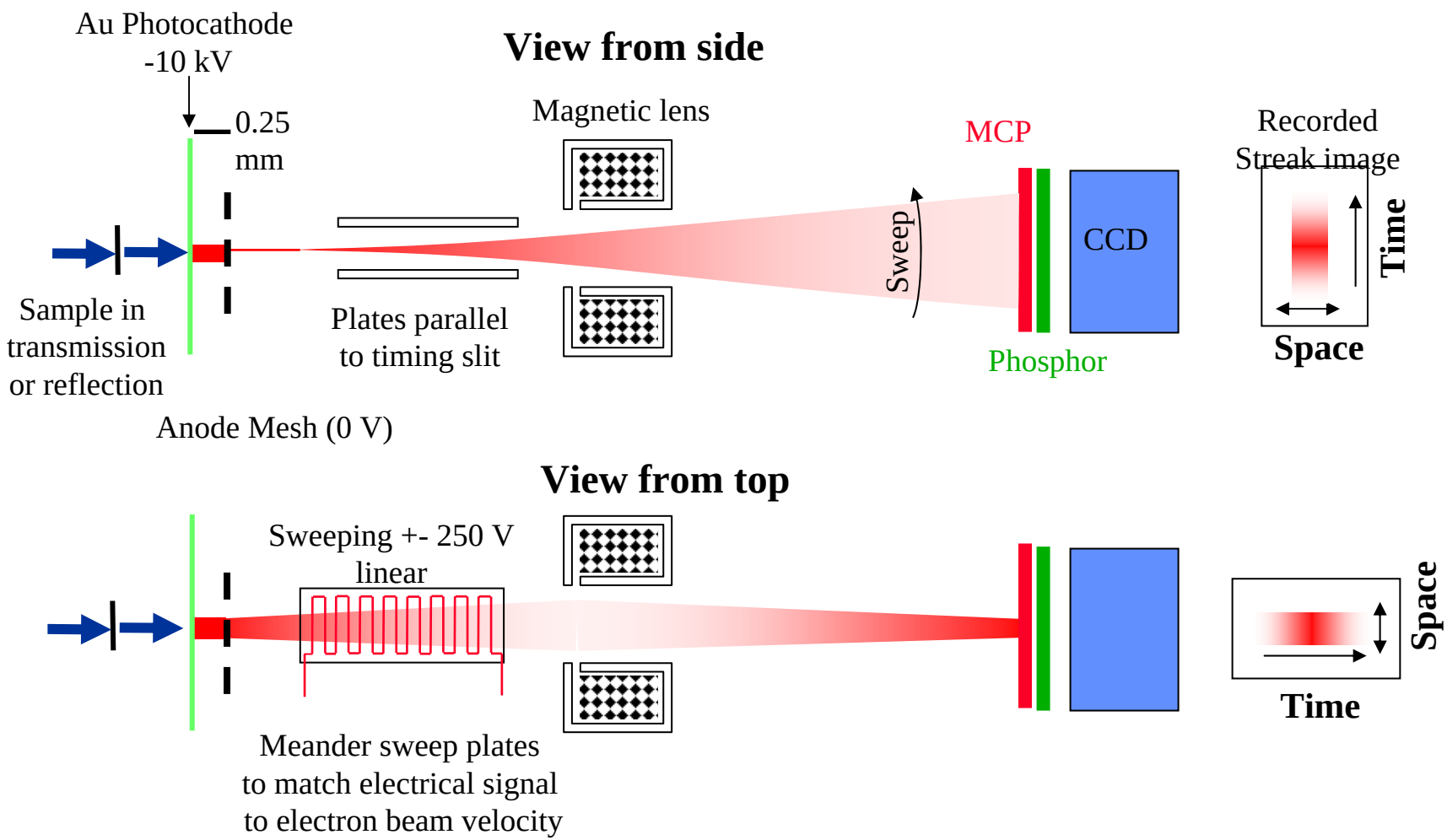
Photoinjector modeling using IMPACT-T



J. Qiang, LBNL

IMPACT-T simulation of electron emission from a nano-needle tip

Modeling Streak Camera Using IMPACT-T



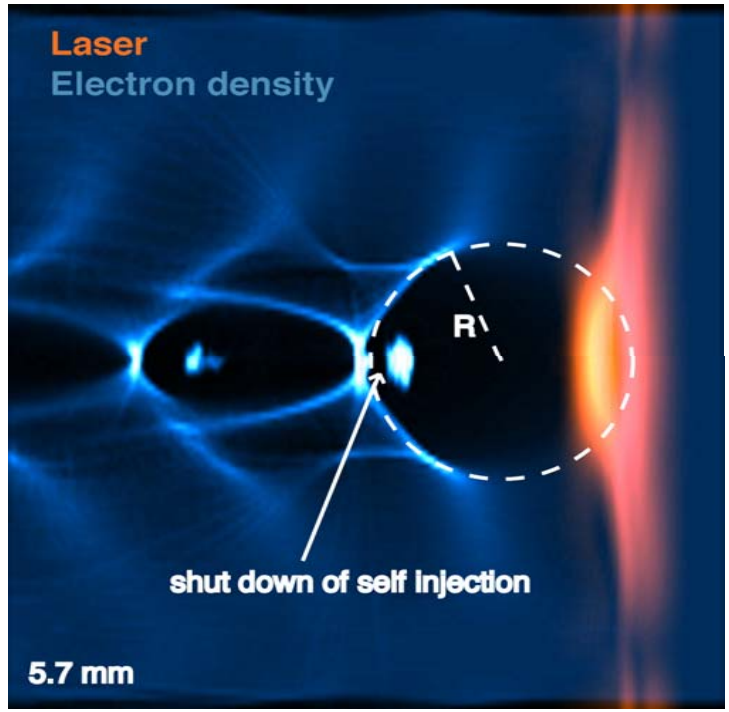
Progress in laser/plasma based concepts has accelerated significantly in recent years

- **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)

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)

OUTLINE

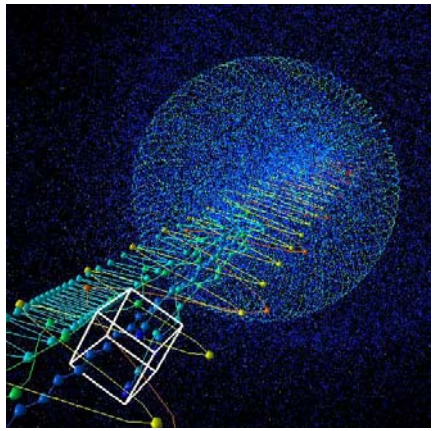
I. Accelerators and the US DOE

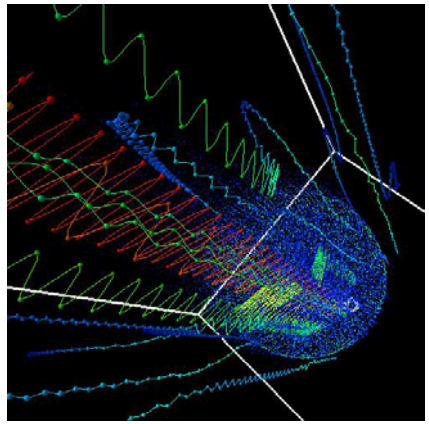
II. Challenges/opportunites in petascale accelerator S&T

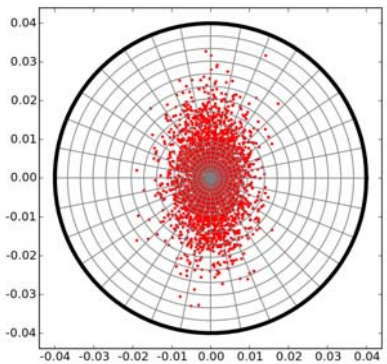
Collaborations w/ Applied Math & Comp. Sci

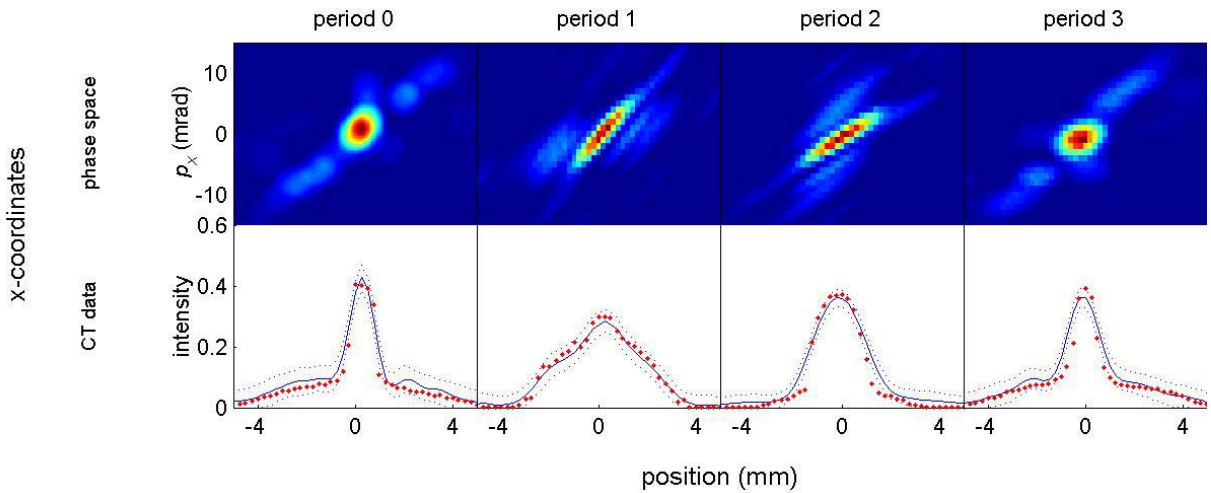
SciDAC ISICs (TOPS, APDEC, TSTT, PERC) & SAPP

- Linear solvers, eigensolvers
- Poisson solvers
- Meshing
- Parallel PIC methods
- Performance optimization
  - SC06 presentation
- Statistical methods
  - Calibration, forecasting, prediction
- Visualization









UT-BATTELLE

Computational Beam Dynamics for SNS Commissioning and Operation

Jeff Holmes

ICAP 2006

Chamonix, France

October 2, 2006

SNS
SPALLATION NEUTRON SOURCE

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Spallation Neutron Source (SNS)

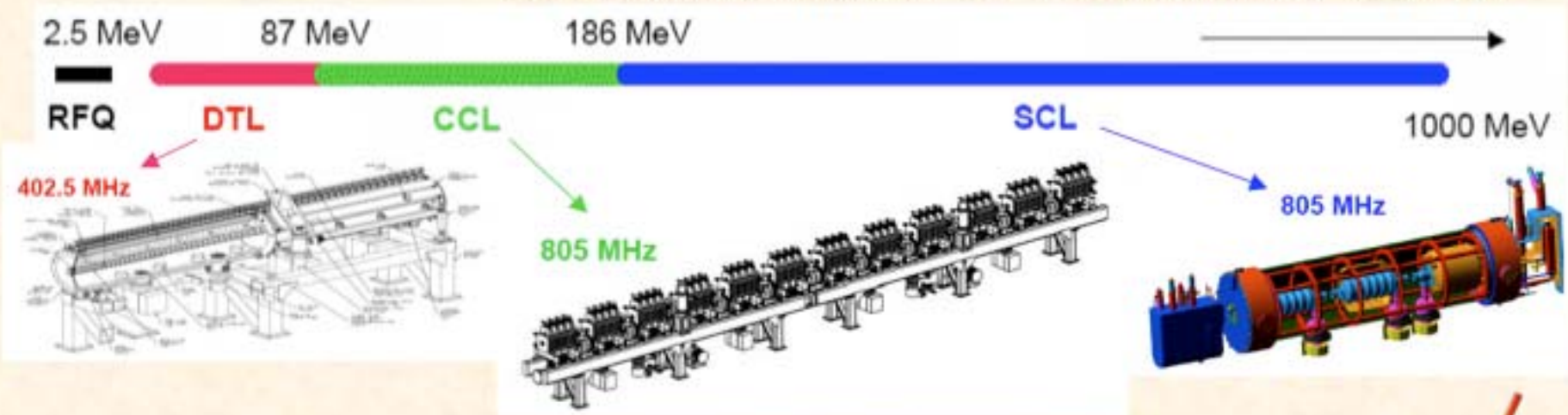
H^- ions are created and bunched.

Ions are accelerated to 1GeV.

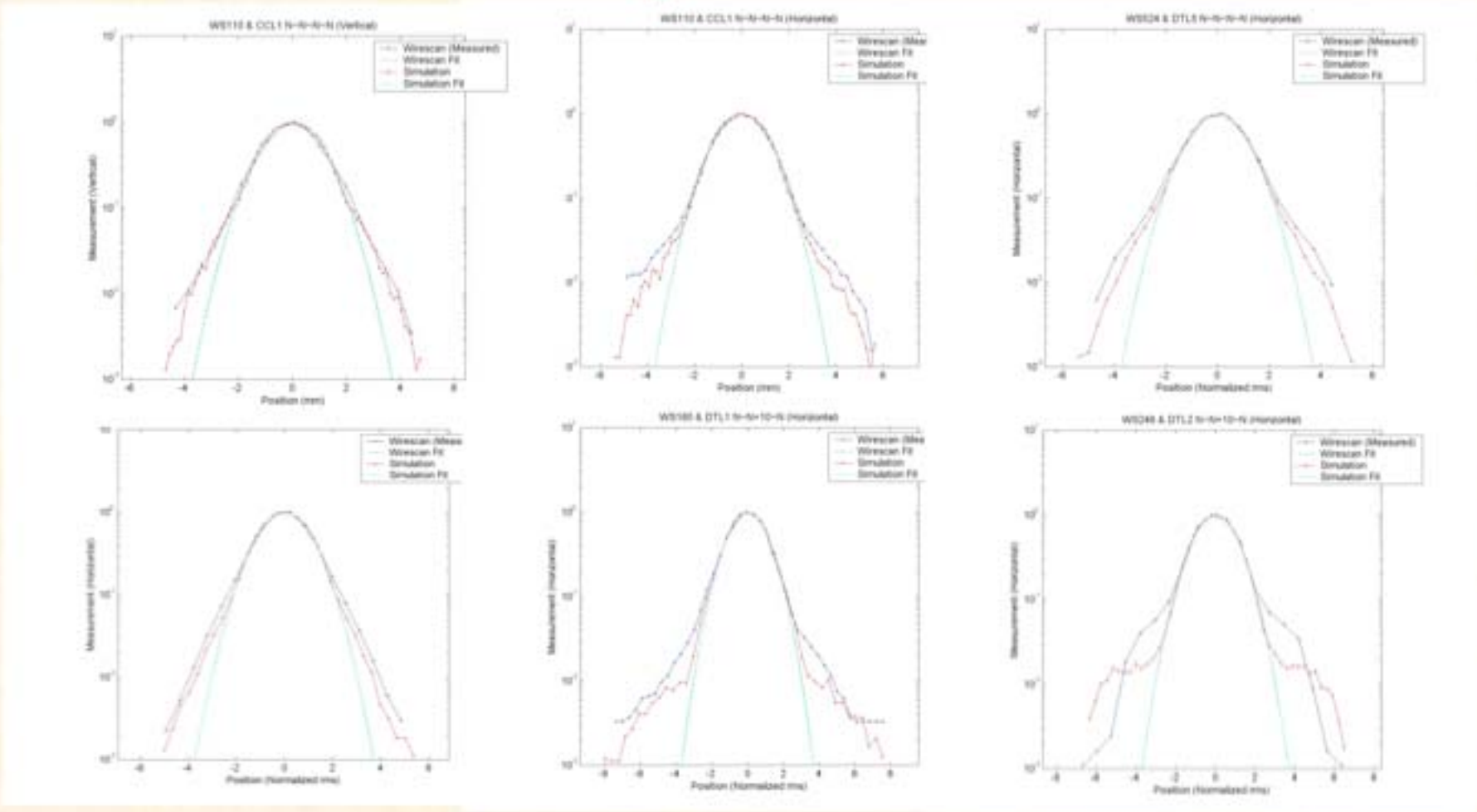
Delivers 1micro-second pulses.

Liquid mercury target produces neutrons.

60 Pulses/second, 1.5×10^{14} protons/pulse, 1.44 MW



Simulation vs. Experimental Data

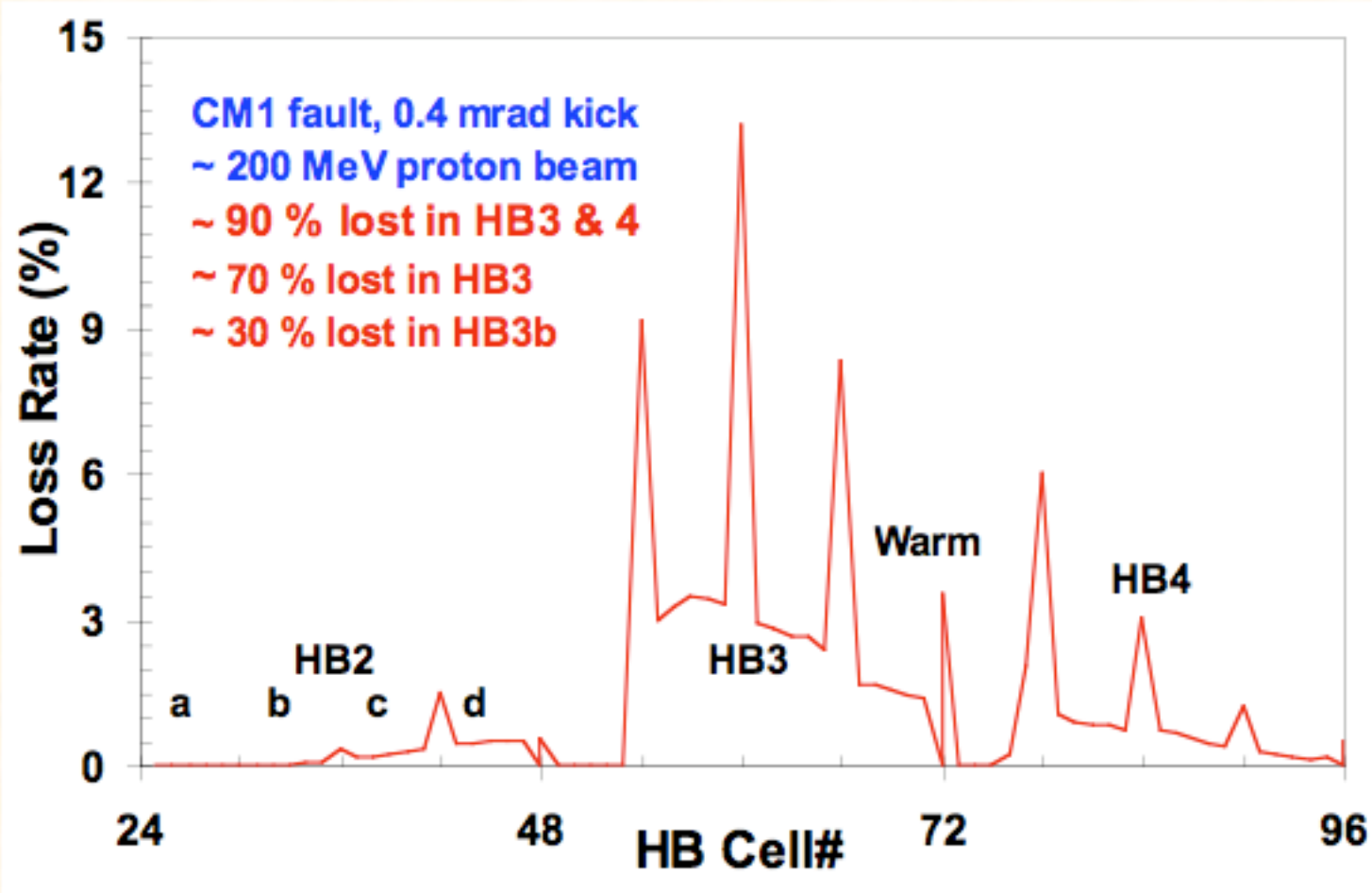


- **Partial success in simulating profiles.**

An "Actual" Fault of the 1st Modulator

~10 % acceleration field change of 12 cavities

~ 20° RF phase change of only the first MB cavity would give similar results

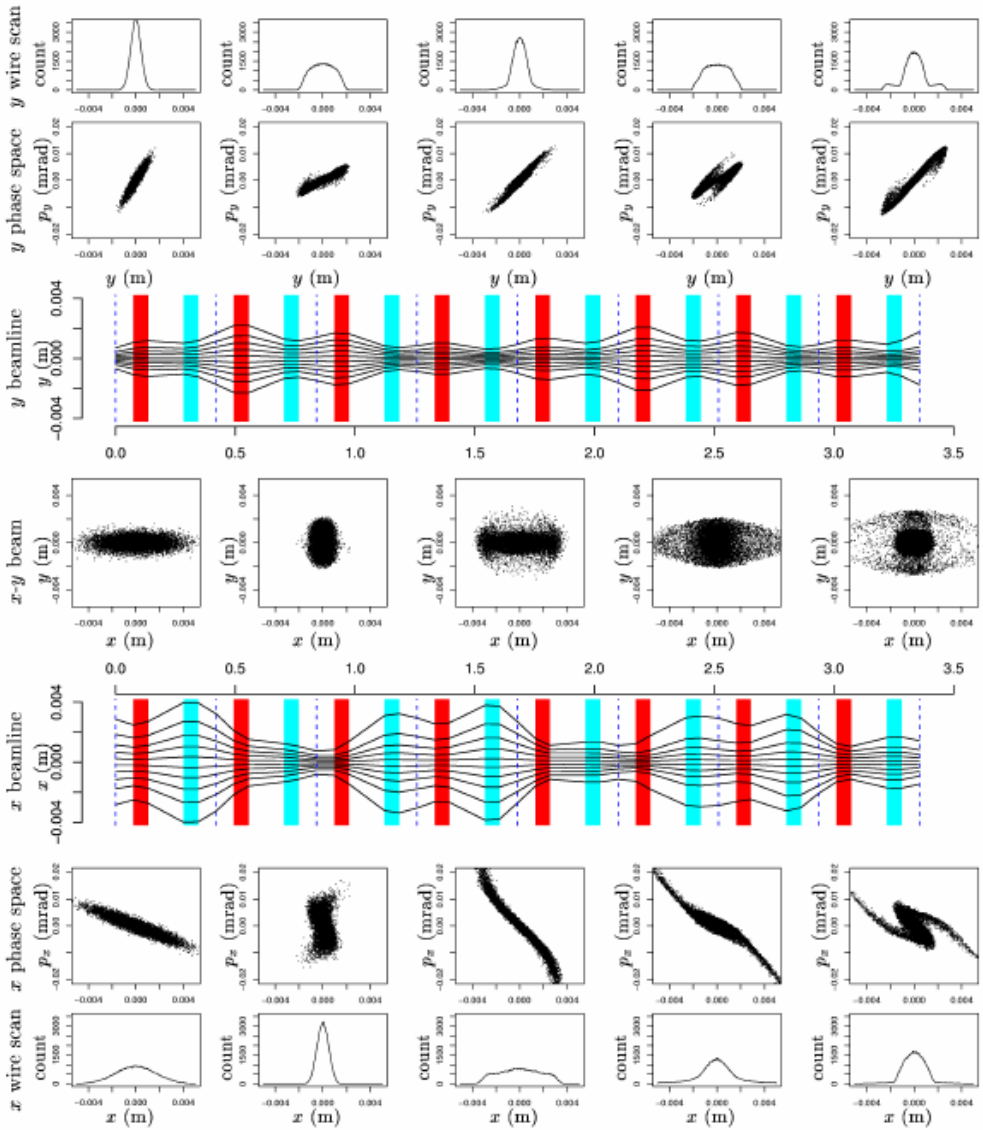


Concluding Thoughts

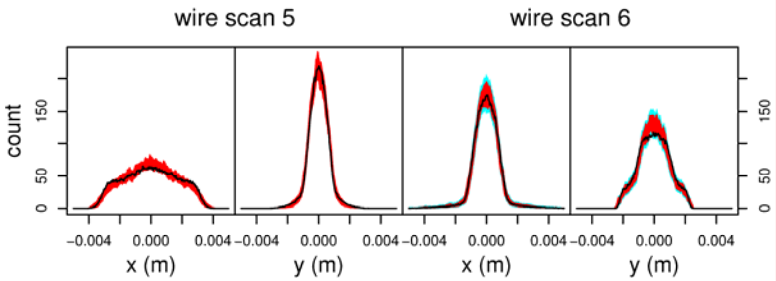
- Much of the computing required to support SNS commissioning and operation is not ultra-high performance. Exceptions are
  - Transverse instabilities, which require a 3D description of space charge, and
  - Electron cloud studies, when the proton beam response is included.
- Most important is to incorporate a broad range of physics models to describe the many issues encountered. The variety and sophistication of our models has increased considerably with time.
- Because of the need for a broad range of models to address the great diversity of phenomena encountered, it is important to develop modular software and a convenient and flexible user interface.
- The main source of inaccuracy/error in simulating hypothetical or measured phenomena is most likely our lack of complete detailed knowledge of the actual operating conditions.

SciDAC collaboration w/ SAPP

Example: Statistical Methods for Calibration & Forcasting



- **Determining initial phase space distribution from 1D wire scan data.**
- **Courtesy D. Higdon (LANL) et al.**



Simulation of a high intensity proton beam through a series of quadrupole magnets. Statistical techniques were used to combine 1D profile monitor data with simulations to infer the 4D beam distribution. The figure shows the 90% intervals for the predicted profile at scanner #6 (shaded regions), and, for comparison, the observed data (black line). Only data from the odd numbered scanners were used to make the prediction.

Personal thoughts on programming models

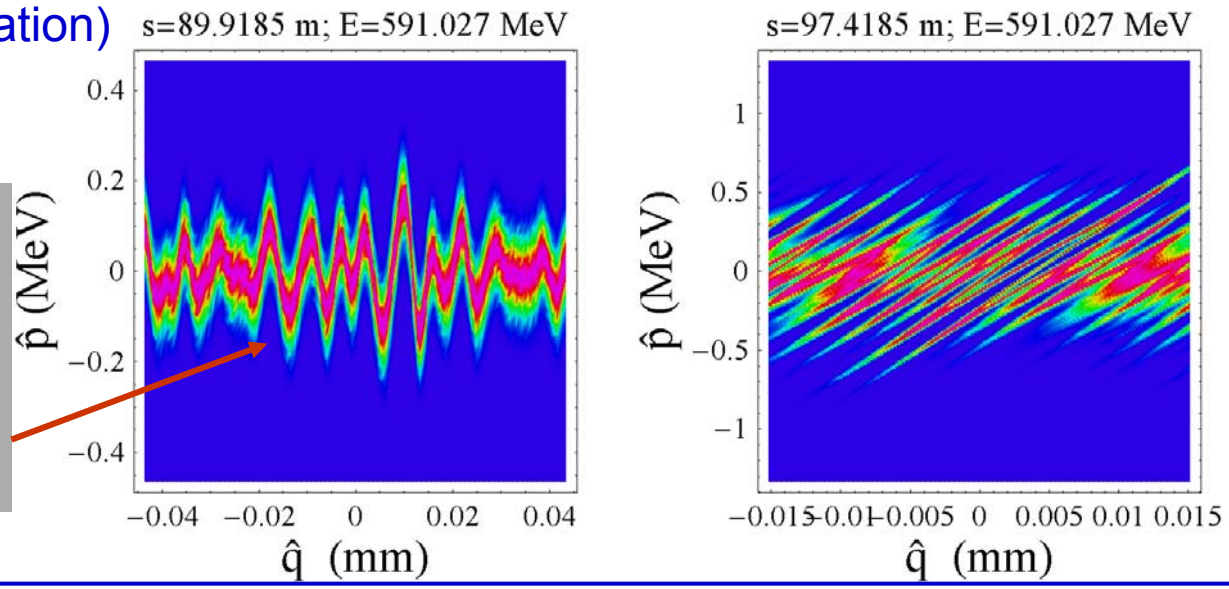
- For maximum performance, need MPI
- For maximum personal productivity, want to take a global view
- Ideally, want to be able to switch between viewpoints in a single code

Direct Vlasov codes represent a promising alternative to particle-based codes

- **Direct Vlasov ideal for study of microbunching instabilities**
  - **not vulnerable to stat fluctuations suffered by macroparticle codes**
  - **due to memory requirements, mainly applicable to 1D and 2D at this time**
- **Previously, Vlasov methods successfully applied to storage-rings**
- **Application to beam dynamics in FEL's is new but very promising**

Longitudinal phase space before and after 2nd bunch compressor in the FERMI FEL. (8000x240 grid calculation)

Energy modulations result from amplification of initial shot noise due to space charge and coherent synchrotron radiation effects



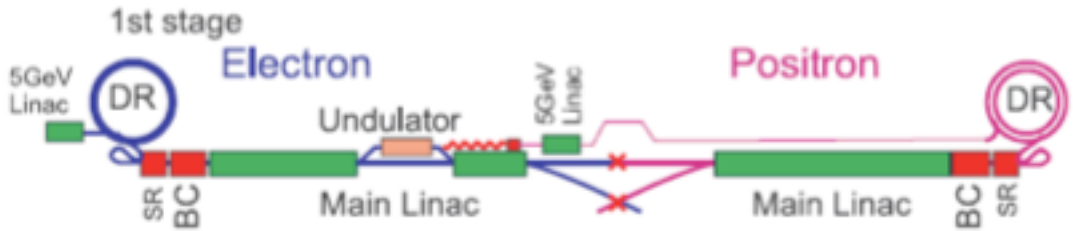
M. Venturini, LBNL

Planned/Proposed future accelerator facilities

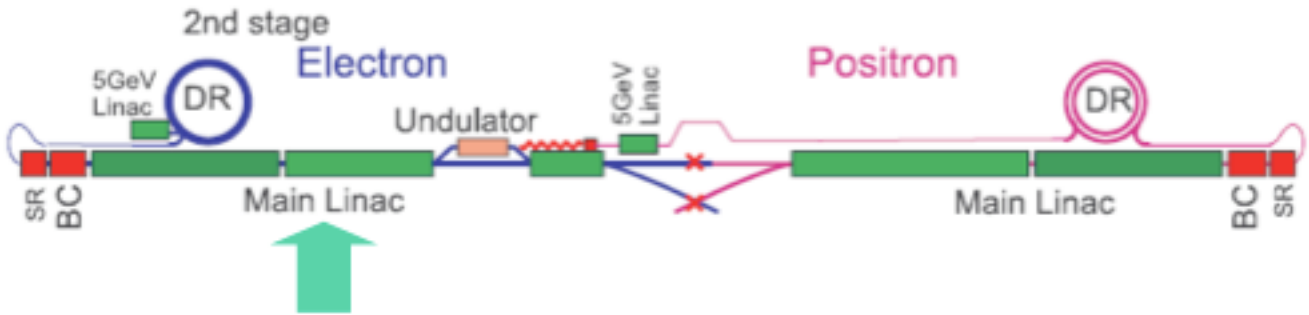
- International Linear Collider (ILC)
- Neutrino facilities
- Exotic beam facilities
- Electron-ion colliders (eRHIC,ELIC)
- 4th generation light sources

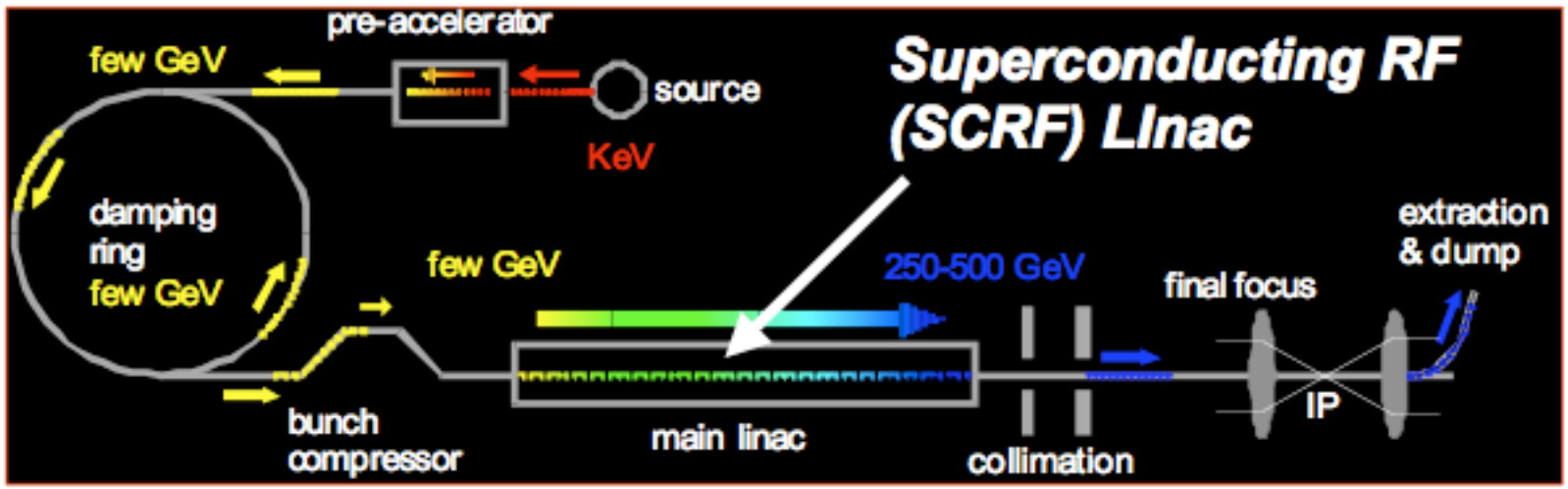
The ILC Machine Design

500 GeV

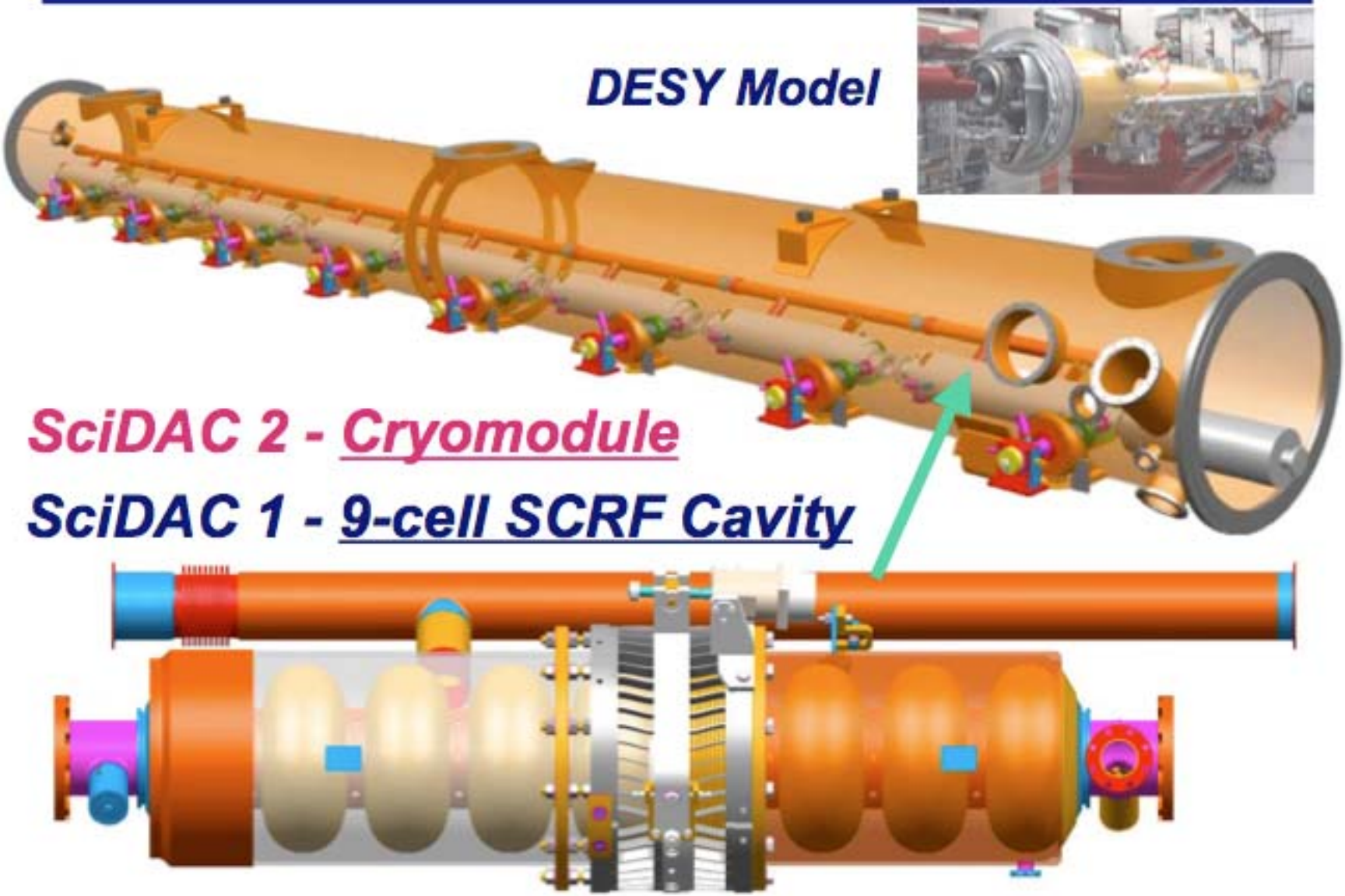


1 TeV



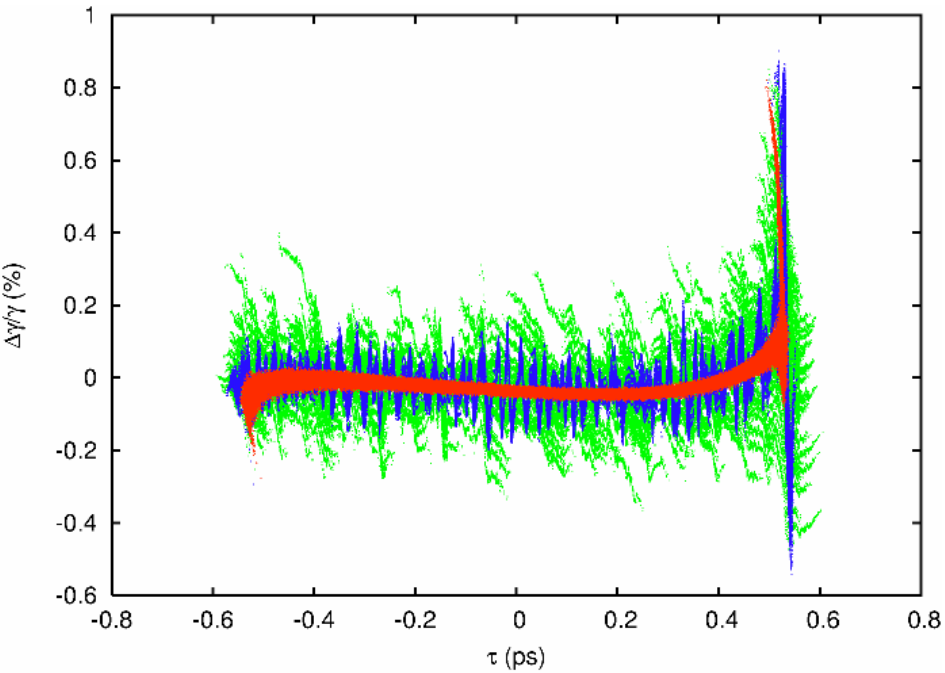


ILC – Cryomodule (8 Cavities)

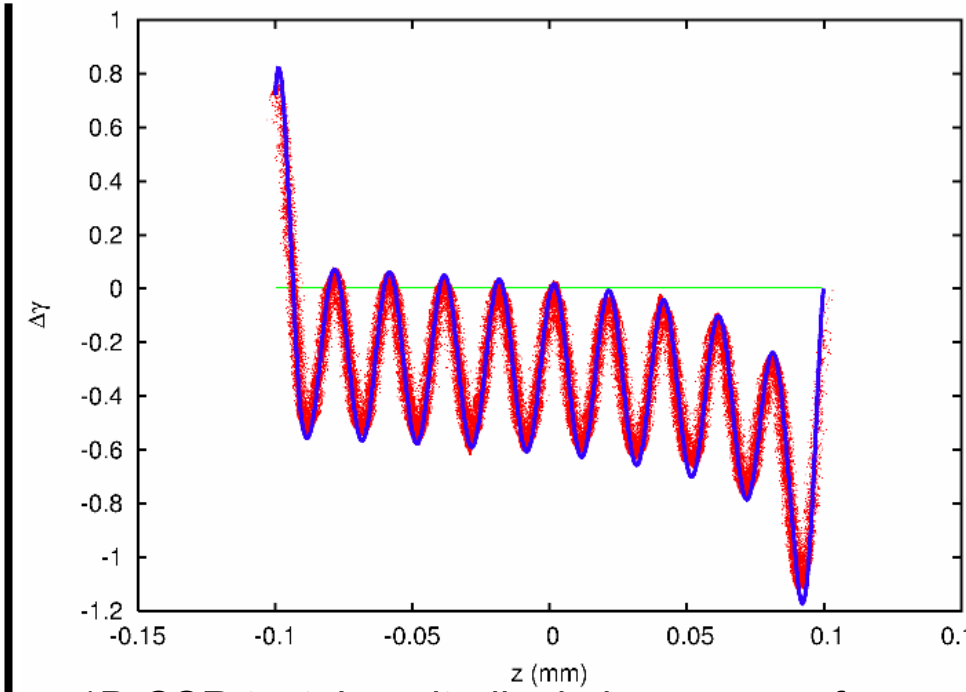


Future light sources

Example IMPACT simulations relevant to x-ray light source modeling (I. Pogorelov, LBNL)

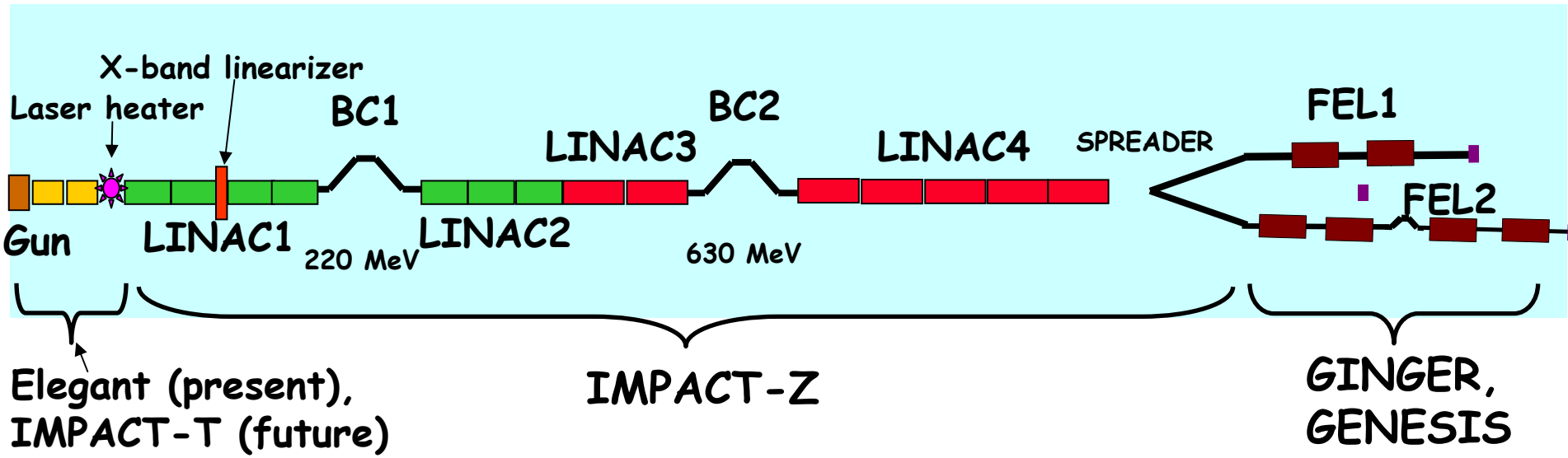


Microbunching instability seen in 2Mp space-charge simulations (green) and 100Mp space-charge simulations (blue) with CSR turned off;
Comparison with the no-space-charge, no-CSR result (red).



1D CSR test: Longitudinal phase space for a relativistic electron bunch ($\gamma \sim 450$) before (green) and after (red) a single bend magnet. The solid blue line is the analytic prediction. Run performed with 2M particles on a 64x64x2048 mesh with an initial distribution that has no uncorrelated energy spread, but a 20% sinusoidal density modulation on top of an otherwise flattop distribution.

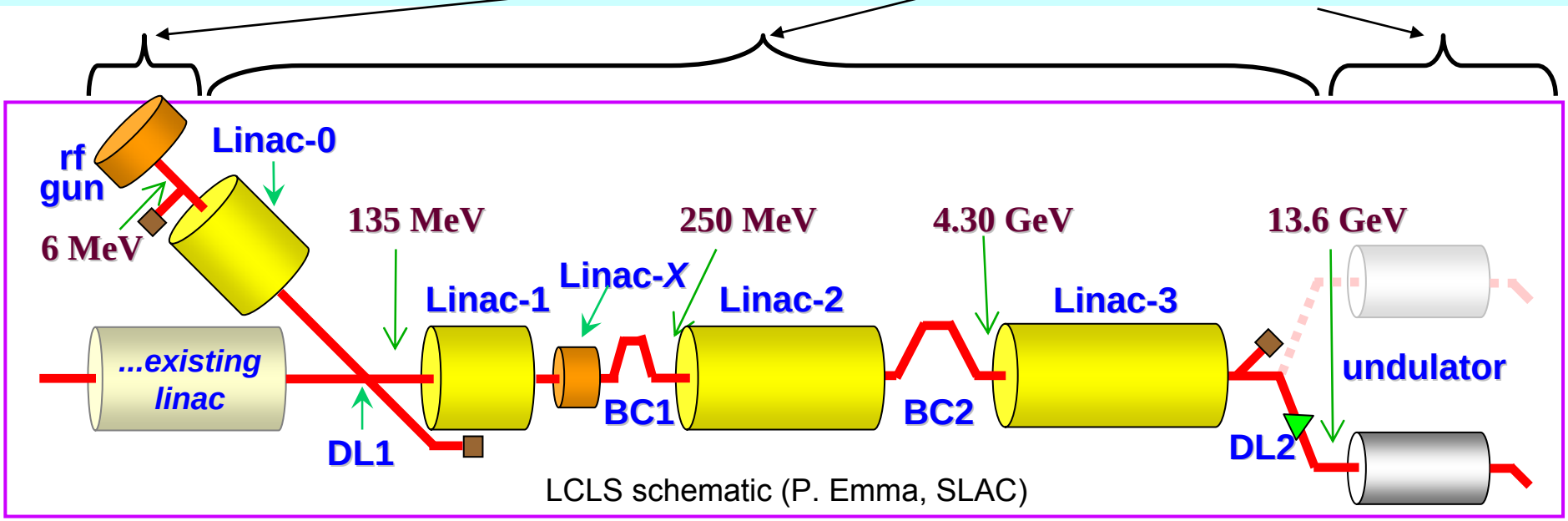
IMPACT-Z simulations of an X-ray light source: FERMI@Elettra



- Control of numerical particle sampling noise is essential to faithfully simulate microbunching instability in the linac and accurately model radiation production in the FEL
- We have performed IMPACT-Z driver linac simulations using 100Mp
- By further developing and combining parallel tools, we are on the verge of being able to perform start-to-end parallel modeling of future x-ray light sources
  - IMPACT (J. Qiang), Elegant (M. Borland), GINGER (W. Fawley), GENESIS, SPUR (S. Reich)

Thanks to SciDAC1, LBNL/LDRD, FERMI, & LBNL/UCB expertise, LBNL has unique capabilities to apply to BES future light sources

- LBNL Center for Beam Physics maintains IMPACT-Z, IMPACT-T, GINGER
- We're entering an era when we will be able to do start-to-end parallel simulation from photoinjector (IMPACT-T) to linac (IMPACT-Z) to FEL (GINGER)



LCLS schematic (P. Emma, SLAC)

- Under proposed BES SciDAC2 project, we would
  - collaborate w/ code developers at ANL (M. Borland, Elegant) and UCLA (S. Reiche, GENESIS & SPUR) to further develop and establish a comprehensive suite of parallel codes & capabilities for BES x-ray light source design
  - collaborate w/ LCLS (P. Emma, Z. Huang) toward performing large-scale (100Mp) simulations for independent assessment of LCLS design & optimization
  - collaborate with BES-supported researchers designing other future light sources to ensure that the parallel codes serve the needs of the community

The Future:
Petascale computing will help enable design and construction of new facilities to explore the frontiers of physics

- **Enabling frontier physics**
  - **—Energy frontier**
  - **—Intensity/brightness frontier**
  - **—Gradient frontier**
  - **—Ultra-fast frontier**
  - **—Precision frontier**

Built on multi-physics foundation laid by SciDAC1

- **Emphasis on optimization**
- **Emphasis on close coupling to control rooms**

Acknowledgements

- J. Cary, K. Ko, W. Mori, C. Ng, J. Qiang, P. Spentzouris
- J. Holmes
- And many, many others

Papers presented at SC'06

- **Performance Modeling and Optimization of a High Energy Colliding Beam Simulation Code**
  - —Hongzhang Shan, Erich Strohmaier, Ji Qiang, David H. Bailey, Kathy Yelick
  - —Tues Nov 14, 4:30-5:00pm, Particles & Continuum session
- **25 Years of Accelerator Modeling**
  - —Robert D. Ryne
  - —Wed Nov 15, 2:15-3:00pm, Masterworks session