Computational Accelerator Physics at NERSC: A User's Perspective

Robert Ryne

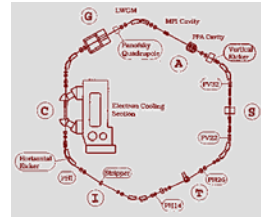Lawrence Berkeley National Laboratory

Outline

- Overview of accelerators and the computational accelerator physics community

- The types of calculations we do at NERSC

- Personal observations about NERSC

- Future challenges in accelerator S&T and the need for HPC

The National Investment in Particle Accelerators is Enormous

Lawrence Berkeley Natl. Lab.
ALS

Indiana Univ.
IUCF

Fermi National Acc. Lab.
Tevatron

Michigan State Univ.
NSCL

Argonne National Lab.
IPNS ATLAS APS

Stanford Linear Acc. Center
SLC PEP-II SSRL

Cornell Univ. **CESR CHESS**

Los Alamos Natl. Lab.
LANSCE/Lujan

Oak Ridge National Lab.
SNS

Thomas Jefferson National
Accelerator Facility: **CEBAF**

Brookhaven National Lab.
RHIC NSLS

Contributions of accelerators have significant economic impact and greatly benefit society

- Medical isotope production
- Electron microscopy
- Accelerator mass spectrometry
- Medical irradiation therapy
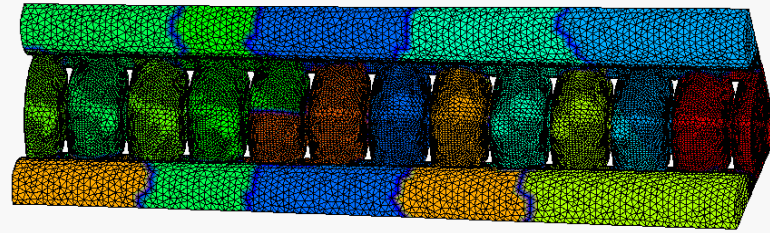- Ion implantation
- Beam lithography
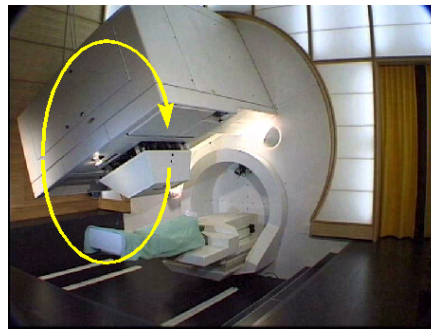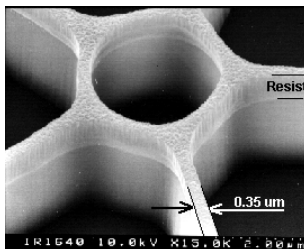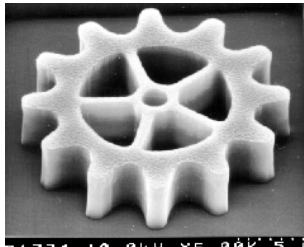
- Transmutation of waste
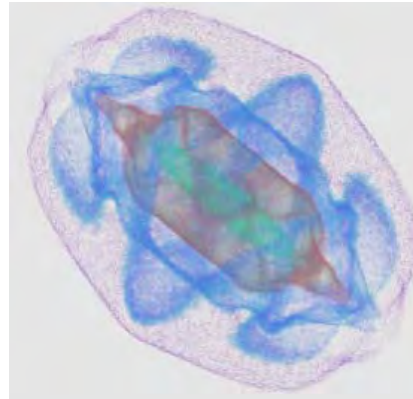- Accelerator-driven energy production
- Hydrodynamic imaging
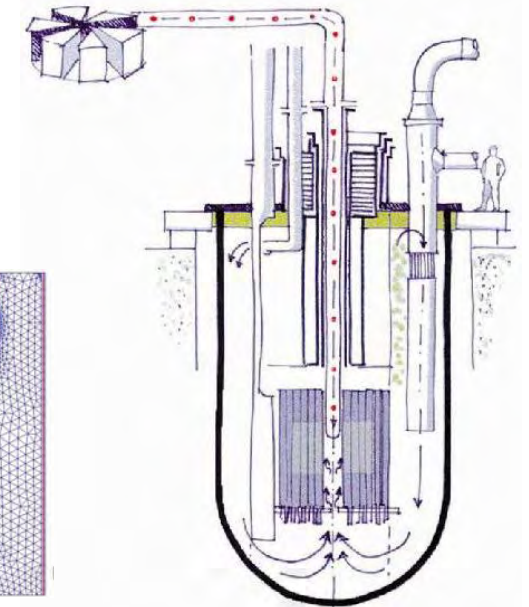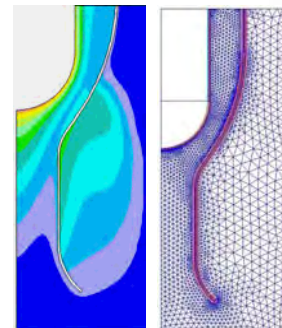
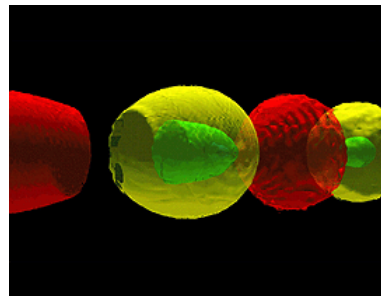# The accelerator community uses high performance computing to tackle of wide range of problems

- Designing complicated electromagnetic structures
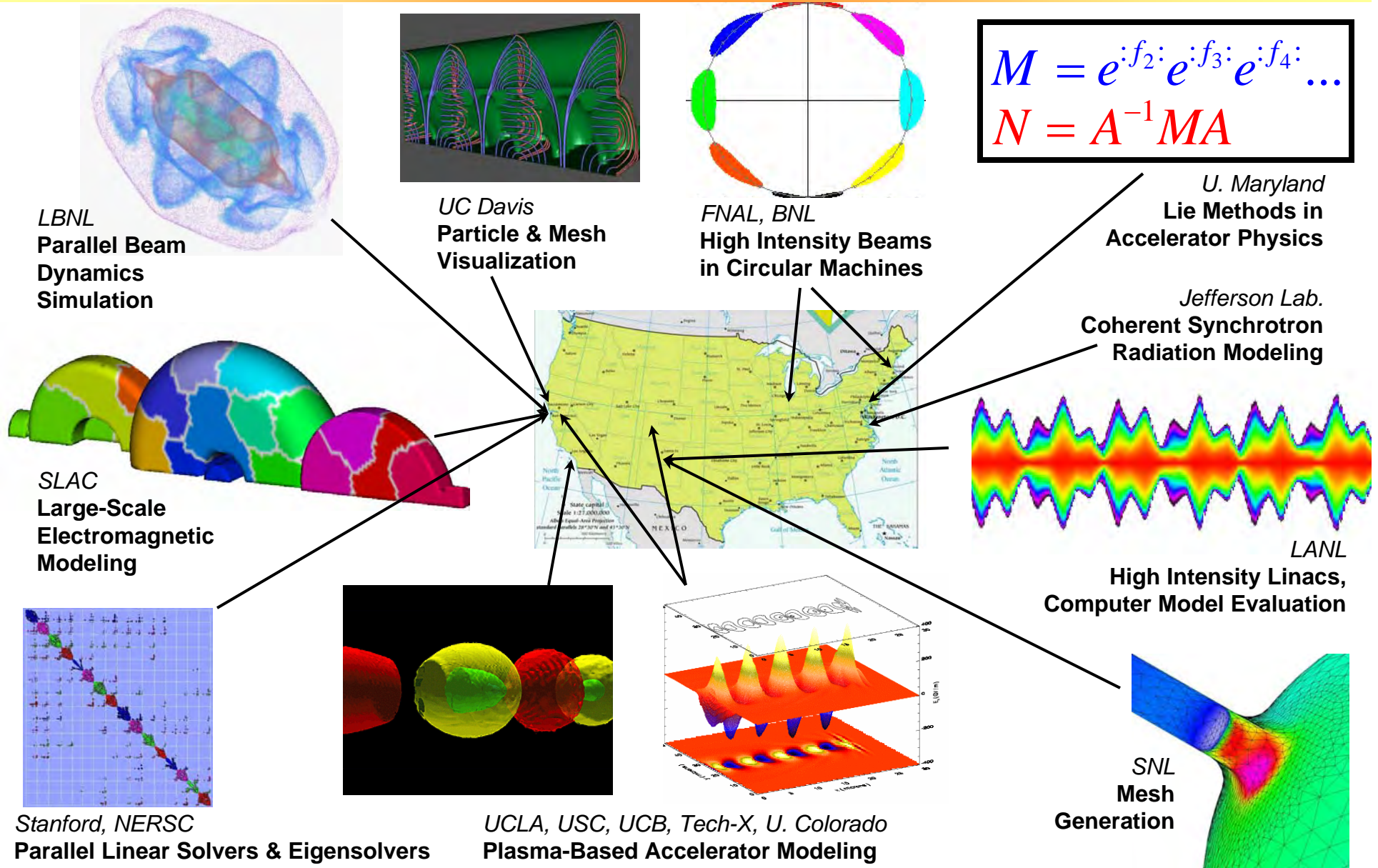
- Modeling high intensity beam dynamics

- Exploring beams under extreme conditions

Why do we need terascale computing for next-generation accelerator design?

- ## High accuracy requirements
  - Design of 3D electromagnetic components
    - frequency accuracy to 1:10000

- ## Large-scale requirements
  - Designing 3D electromagnetic components
    - system-scale modeling
  - Modeling 3D intense beam dynamics
    - Halos, beam-beam effects, circular machines
  - Modeling 3D advanced accelerator concepts
    - laser- and plasma-based accelerators

- ## More physics
  - collisions, multi-species, surface effects, ionization, CSR, wakes,…

Accelerating Scientific Discovery in Accelerator Technology and Beam Physics: A SciDAC Multi-disciplinary, Multi-institutional Collaboration

$$M = e^{:f_2:}e^{:f_3:}e^{:f_4:}\ldots$$
$$N = A^{-1}MA$$

LBNL
Parallel Beam Dynamics Simulation

UC Davis
Particle & Mesh Visualization

FNAL, BNL
High Intensity Beams in Circular Machines

U. Maryland
Lie Methods in Accelerator Physics

Jefferson Lab.
Coherent Synchrotron Radiation Modeling

SLAC
Large-Scale Electromagnetic Modeling

LANL
High Intensity Linacs, Computer Model Evaluation

Stanford, NERSC
Parallel Linear Solvers & Eigensolvers

UCLA, USC, UCB, Tech-X, U. Colorado
Plasma-Based Accelerator Modeling

SNL
Mesh Generation

Noteworthy computations that we have performed at NERSC

- First successful 3D eigenmode calculation of ~50 cell Next Linear Collider (NLC) structure including accelerating cells and damping manifold
- First self-consistent 3D Fokker-Planck simulation
- Simulations identified possible heating mechanism in PEP-II B-factory interaction region
- Simulations in support of SLAC E-157 plasma wakefield accelerator experiment
- Simulations in support of Spallation Neutron Source linac design effort
- Simulations in support of CERN/SPL design effort (similar to US neutrino factory design effort)

Challenges in Electromagnetic Systems Simulation: Example – NLC Accelerator Structure (RDDS) Design


1 inch (approx.)

- Start w/ cylindrical cell geometry
- adjust geometry for maximum efficiency
- add micron-scale variations from cell-to-cell to reduce wakefields
- stack into multi-cell structure
- Add damping manifold to suppress long-range wakefields, improve vaccum conductance, but preserve RDS performance. *Highly 3D structure*.
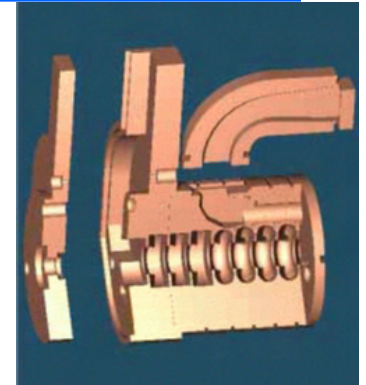
**Require 0.01% accuracy** in accelerating frequency to maintain structure efficiency (**High resolution modeling**)

Verify wake suppression in entire 206-cell section (**System scale simulation**)
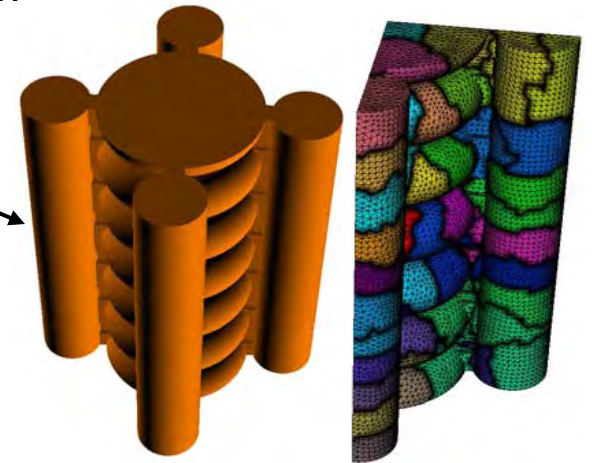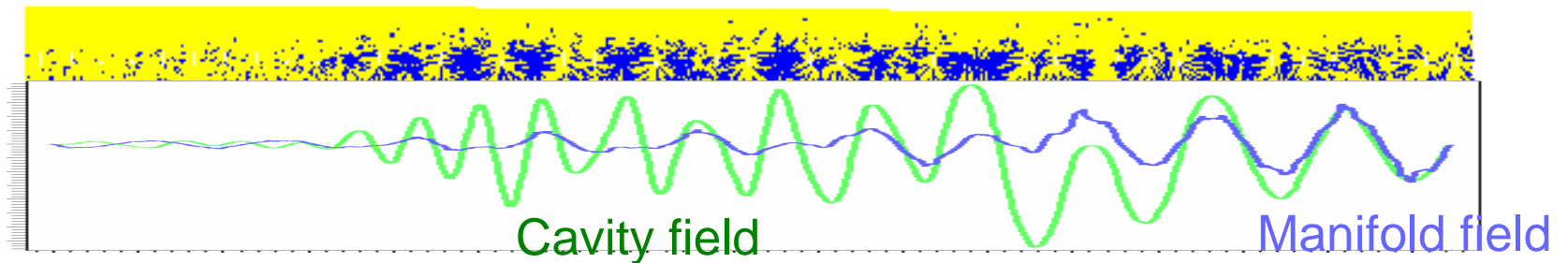
__Parallel__ solvers needed to model large, complex 3D electromagnetic structures to **high accuracy**

NLC RDDS 47 Cell Stack - *Omega3P*

*Calculation of modes in entire structure has begun*
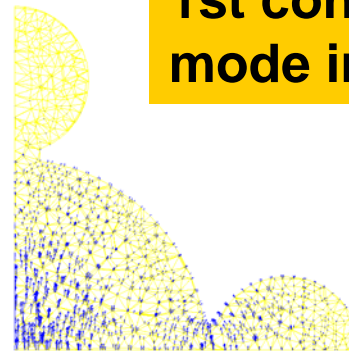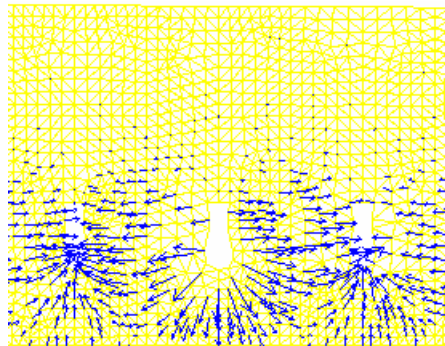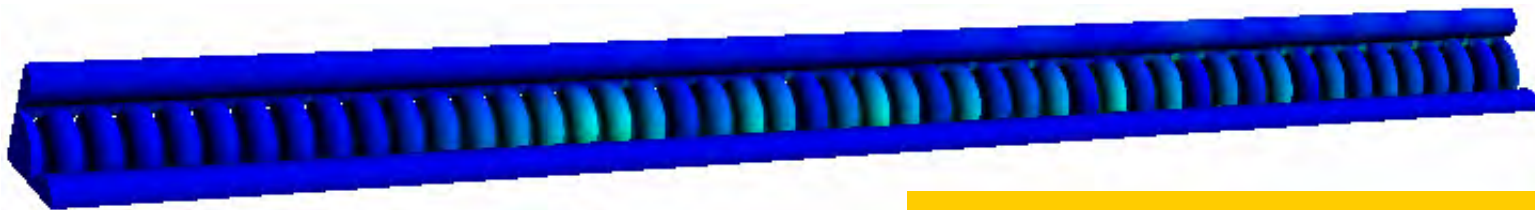
**1st convergence of a
mode in a dense spectrum**

Cavity field   Manifold field

3D First-Principles Fokker-Planck Simulation

- Requires analog of 1000s of space-charge calculations/step
  - "…it would be completely impractical (in terms of # of particles, computation time, and statistical fluctuations) to actually compute [the Rosenbluth potentials] as multiple integrals" J.Math.Phys. 138 (1997).

- Feasibility demonstrated!
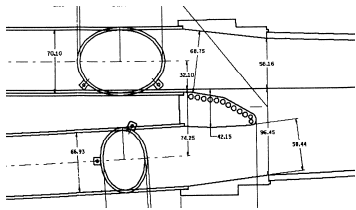
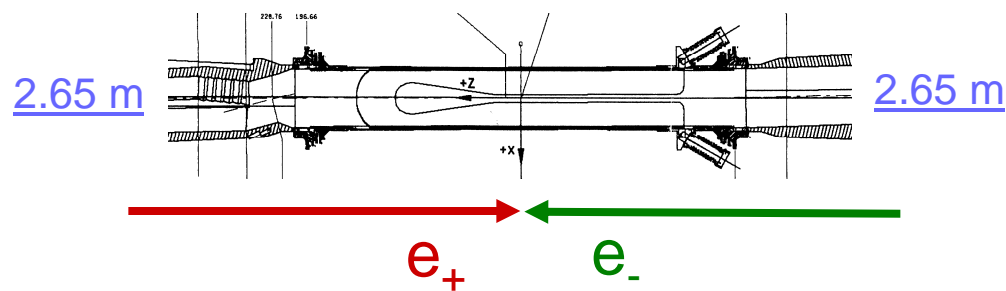Self-Consistent Diffusion Coefficients
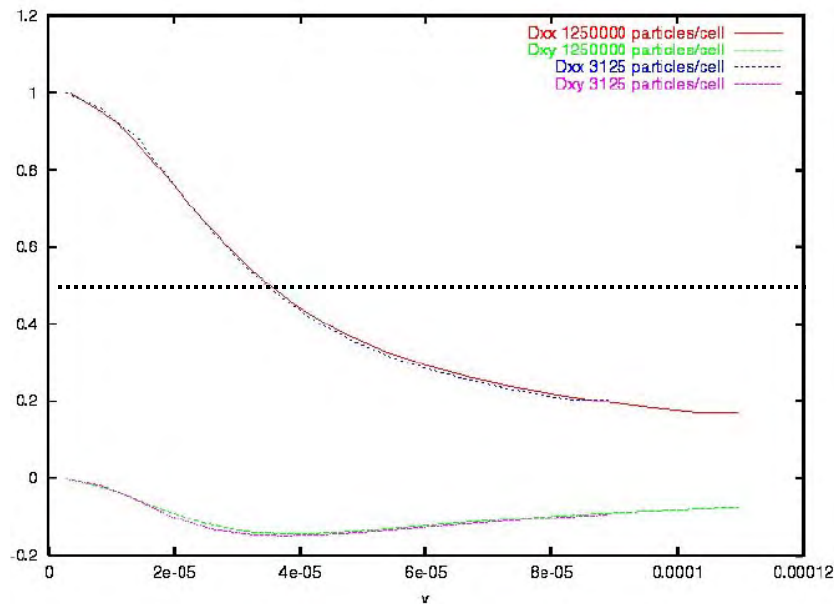
Spitzer approximation

Previous approximate calculations performed w/out parallel computation were not self-consistent
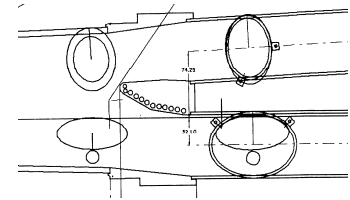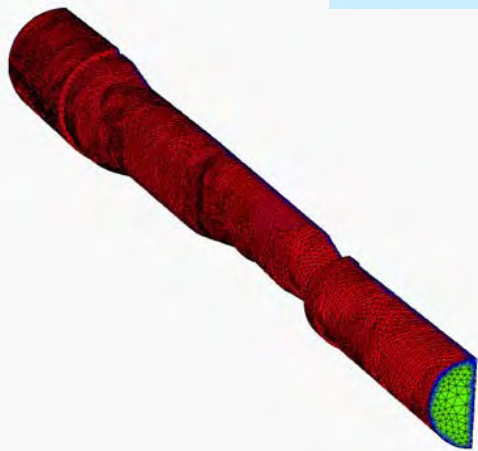
PEP II - IR Beamline Complex
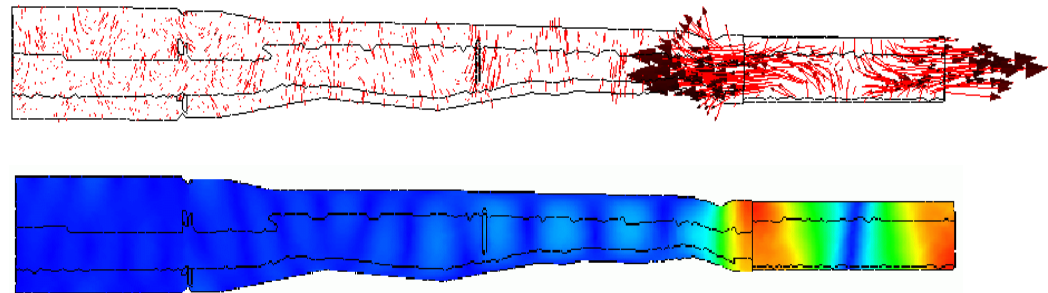

Left crotch

Center beam pipe

Right crotch

2.65 m

2.65 m

e_+

e_-

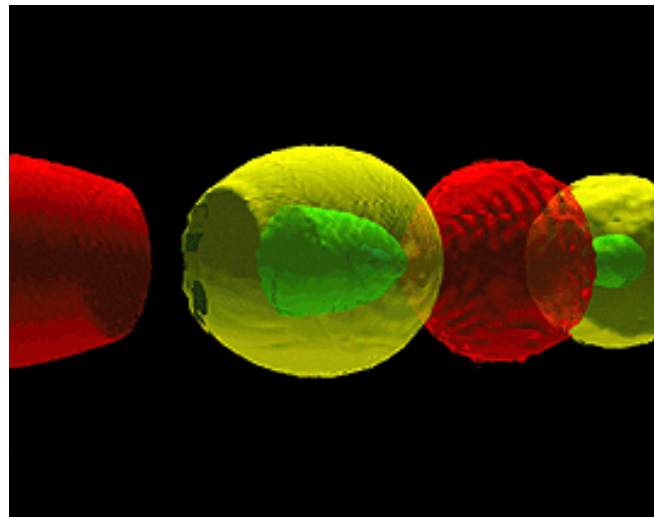*Identify localized modes to understand beam heating*

Short section from IP

# Laser/Plasma-based acceleration can produce gradients ~ 100 GeV/m

- High gradients measured in the lab over short distances
  - 100s to 1000s times greater than conventional technology
- Plasma wakefield accelerator (PWFA) concept uses extremely high fields in plasmas

- Challenge is to control & stage high-gradient sections to produce a high quality, high energy beam
- Simulation of 1-10 GeV PWFA would require ~ 10K-100K CPU-hours

Direct comparison between expt and full-scale PIC simulation using OSIRIS of the refraction of a 30 GeV e- beam at a plasma vacuum interface

Experiment

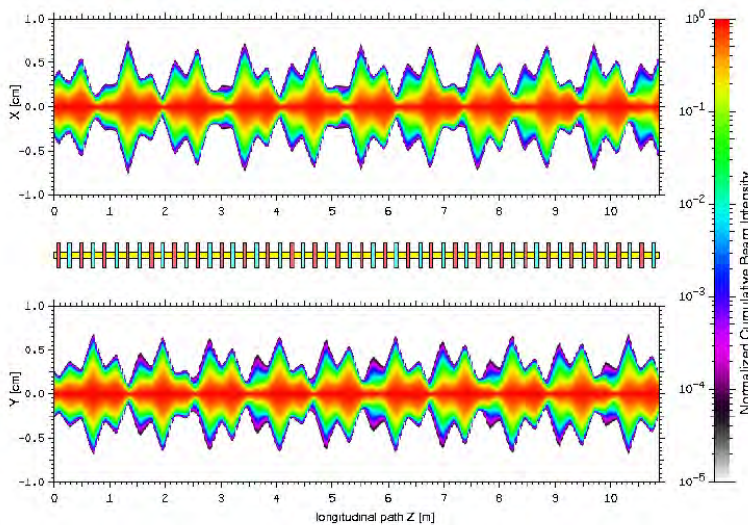(a)

Laser off

(b)

Laser on

PIC Simulation

(c)

(d)
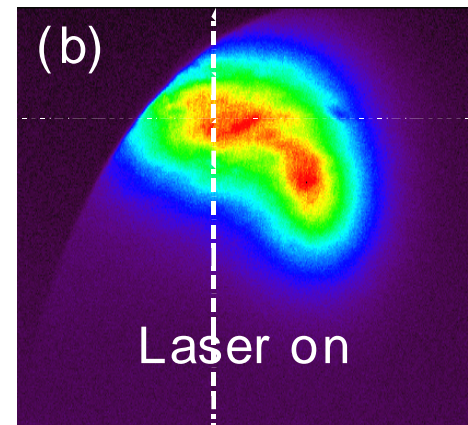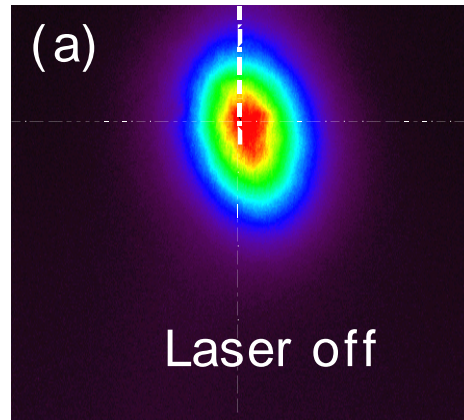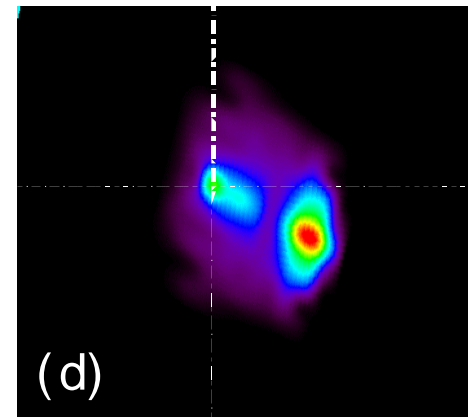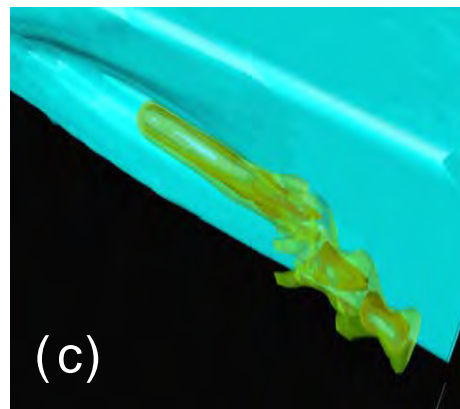
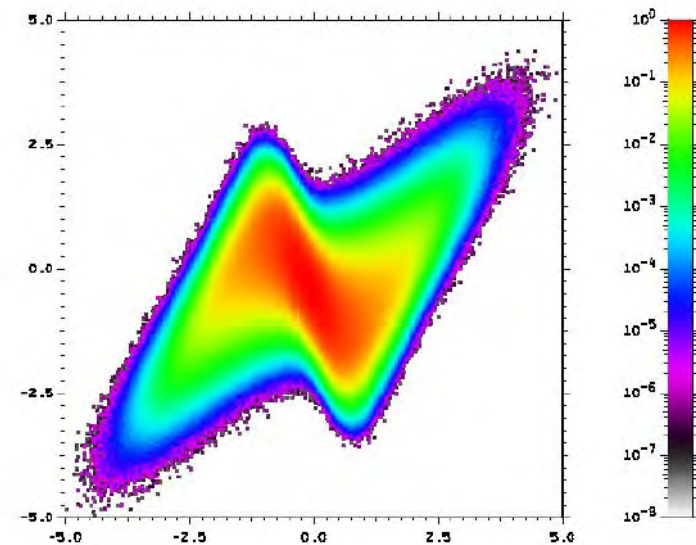# Linac Modeling: Old vs. New Capability

- 1980s: 10K particle, 2D serial simulations
- Early 1990s: 10K-100K, 2D serial simulations
- 2000: 100M (~10 hrs on 256 PEs); *more realistic model*

LEDA halo expt; 100M particles

SNS linac; 500M particles
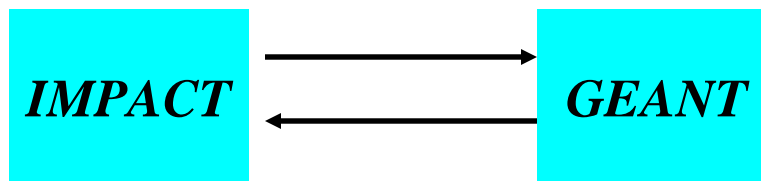
Future Challenges in Beam Dynamics Modeling

- **Intense beams in circular machines** is a major challenge:
  - 100 to 1000 times more challenging than linacs
- Additional physics adds further complexity
  - Intense beams in bending magnets
  - Collisions
  - Wakefields
  - Radiation
  - Ionization
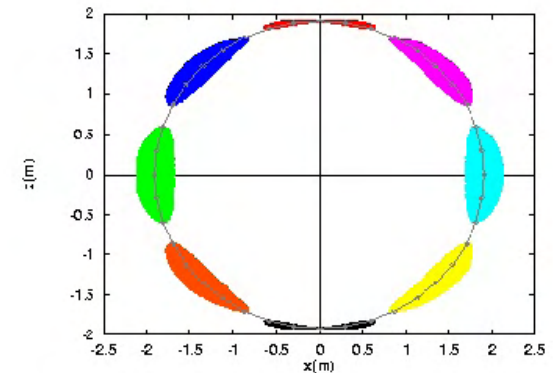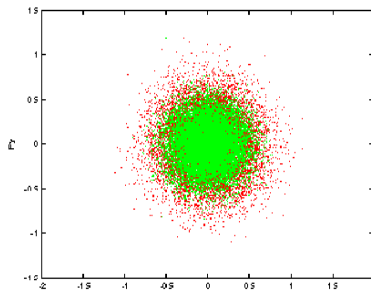
"banana" effect in circular machine code

IMPACT → GEANT

Personal Observations

Personal observations about NERSC

- Outstanding support by User Services
  - Reliable, timely, friendly
  - Great phone support
  - Excellent web pages
  - Ease of adding new users
- Science-enabling resources
  - Seaborg, HPSS
  - ESnet
  - Auxiliary systems (viz, math servers)
  - Stable environment
- Algorithm and software development
  - Linear solvers, eigensolvers, cluster development,…
- Outstanding support staff
  - Event coordinators, training, publications,…

Personal observations, cont.

- NERSC does an excellent job of serving the needs of both a large user community and a small number of power users/projects

- NERSC has made the right choices in hardware. The staff has been very successful at procuring systems that are high-end yet with the stability and reliability to serve its large community of users

- NERSC provides enhanced support to selected projects
  - P.O.C. for the SciDAC accelerator modeling project
  - Server support, cvs, software requests, technical support,…

# Future Activities in Accelerator S&T and the Need for HPC

Particle accelerators are among the most broadly applicable, most important scientific instruments in the world

We may be on the brink of major new discoveries

Given the complexity and importance of accelerators, it is imperative that the most advanced HPC tools be brought to bear on their design, optimization, commissioning, and operation

Accelerators are Crucial to Scientific Discoveries in High Energy Physics, Nuclear Physics, Materials Science, and Biological Science


"Starting this fall, a machine called RHIC will collide gold nuclei with such force that they will melt into their primordial building blocks"
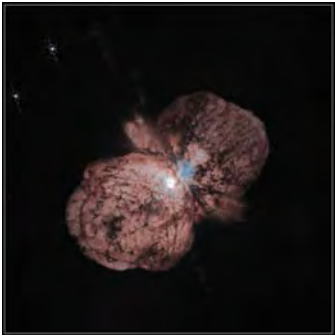
"A new generation of accelerators capable of generating beams of exotic radioactive nuclei aims to simulate the element-building process in stars and shed light on nuclear structure"

"Muon Experiment Challenges Reigning Model of Particles"
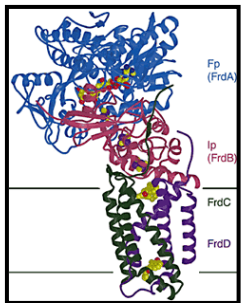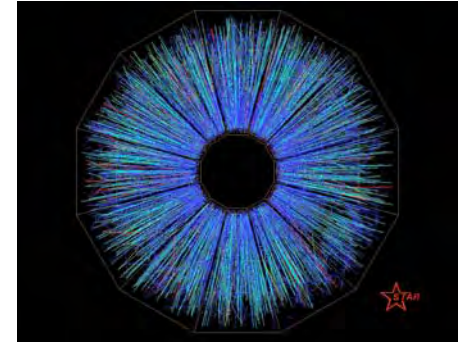
"Biologists and other researchers are lining up at synchrotrons to probe materials and molecules with hard x-rays"
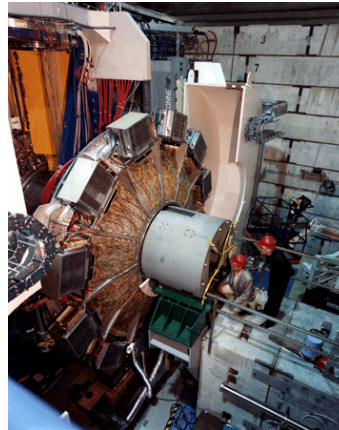
"Violated particles reveal quirks of antimatter"

Particle accelerators are among the largest, most complex, most expensive scientific instruments in the world

Cost of leading-edge high energy accelerators: several billion $

Design decisions may have huge consequences

Example: Impact of Simulation

- Without large-scale simulation: cost escalation
  - Superconducting Super Collider (SSC): 1 cm increase in aperture due to lack of confidence in design resulted in $1B cost increase

- With large-scale simulation: cost savings
  - $100M reduction is estimated cost due to improved accelerator structure design for the Next Linear Collider (NLC)

Ongoing/Planned Simulation Activities

- PEPII (heating)
- FNAL booster, BNL AGS, LANL PSR (beam loss)
- PEPII, Tevatron, RHIC (beam-beam effect, luminosity)
- Next Linear Collider
- Neutrino factory/muon collider
- SLAC E162 (plasma wakefield accelerator)
- Laser driven accelerators (l'OASIS, UMichigan, UCLA, NRL, UTexas, LLNL,…)
- Next-generation light source

Opportunities at Next-Generation Accelerator Facilities

Exploring physics beyond the Standard Model. Are there new particles? New interactions?
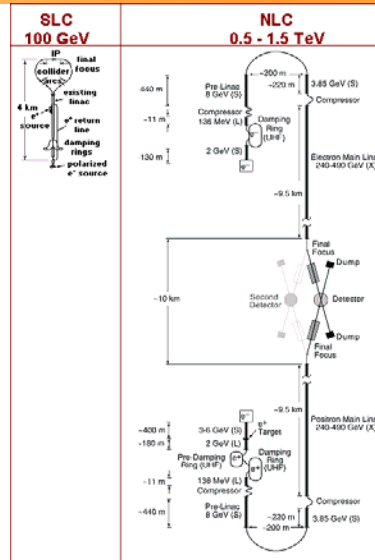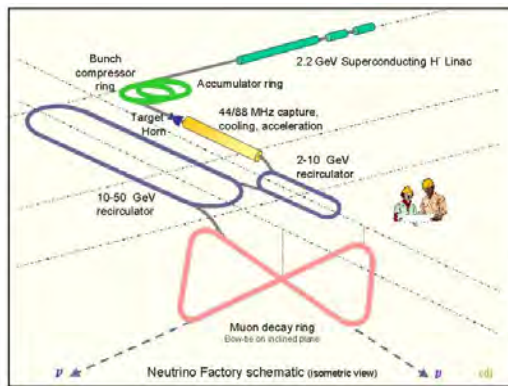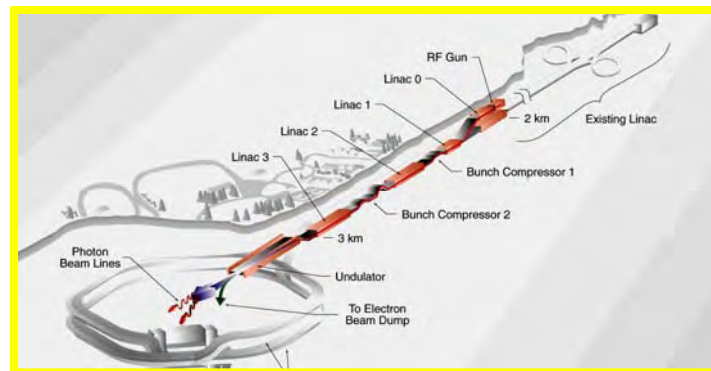

Research with exotic nuclei: The nature of nucleonic matter; origin of the elements; tests of the Standard Model
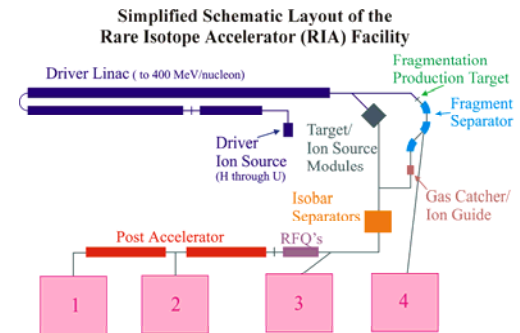
Research using intense, ultra-short pulses of x-ray radiation (4th generation light source): fundamental quantum mechanics; atomic, molecular, and optical physics; chemistry; materials science; biology

HPC will play a major role

- **Present accelerators:** Maximize investment by
  - optimizing performance
  - expanding operational envelopes
  - increasing reliability and availability

- **Next-generation accelerators**
  - better designs
  - feasibility studies
  - Facilitate important design decisions
  - completion on schedule and within budget

- **Accelerator science and technology**
  - help develop new methods of acceleration
  - explore beams under extreme conditions