Advanced Computing for Accelerator Science & Technology

Robert Ryne
Los Alamos National Laboratory

Outline

- Publications and invited talks
- Scientific impact
- Significant achievements in FY00
  - Algorithms
    - realistic boundary conditions; self-consistent treatment of soft Coulomb collisions; for beams in circular systems
  - Software
    - 4 new space-charge solvers in IMPACT -- more physics, wider applicability
    - LANGEVIN3D code for self-consistent simulation of Fokker/Planck equation
    - extension of IMPACT to circular systems
  - Applications
    - SNS linac, LEDA expt, NLC structure design
  - Future plans (ACAST)

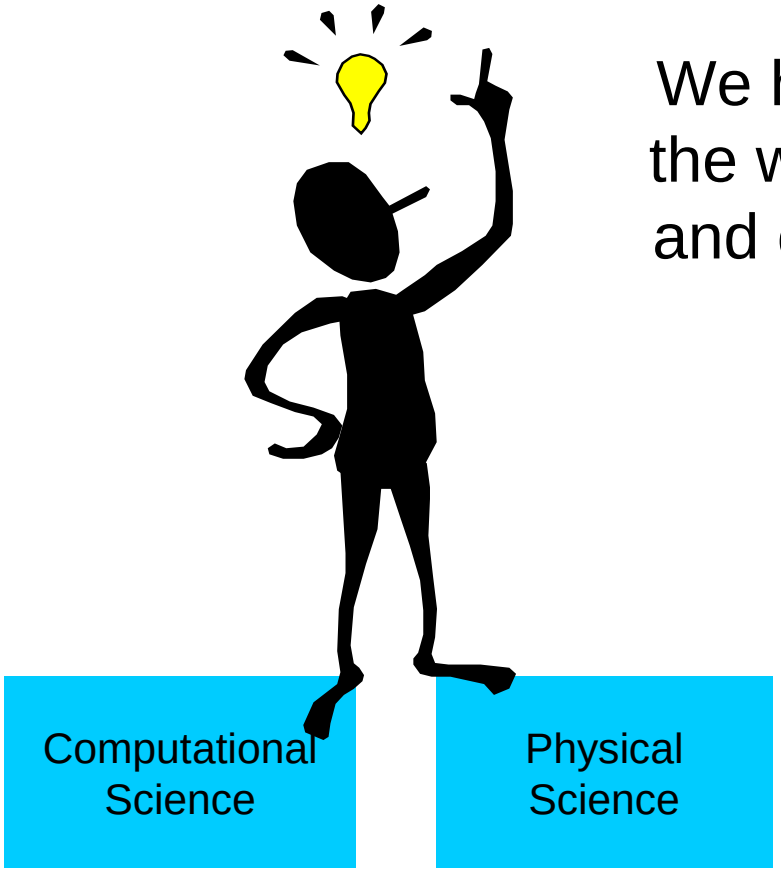
Selected Publications

- J. Qiang, R. Ryne, S. Habib, and V. Decyk, "An Object-Oriented Parallel Particle-In-Cell Code for Beam Dynamics Simulation in Linear Accelerators," accepted by J. Comp. Phys., 1999. Also in proceedings of SC'99 (technical program), Portland, Oregon, Nov. 13-19, 1999.
- J. Qiang, R. Ryne and S. Habib, "Self-Consistent Langevin Simulation of Coulomb Collisions in Charged-Particle Beams," extended abstract accepted for SC'2000; to be published in the proceedings of SC'2000 (technical program), November 4-10, 2000, Dallas, TX.
- J. Qiang, R. Ryne, and S. Habib, "Fortran Implementation of Object-Oriented Design in Parallel Beam Dynamics Simulations," accepted by Comp. Phys. Comm.
- J. Qiang and S. Habib, "A Second-Order Stochastic Leap-Frog Algorithm for Multiplicative Noise Brownian Motion," accepted by Physical Review E.

Selected Publications, cont.

- J. Qiang and R. Ryne, “Beam Halo Studies Using a Three-Dimensional Particle-Core Model,” Phys. Rev. ST Accel.Beams. **3**, 064201, (June 2000).
- J. Qiang, R. Ryne, B. Blind, J. Billen, T. Bhatia, R. Garnett, G. Neuschaefer, H. Takeda, "High Resolution Parallel Particle-In- Cell Simulations of Beam Dynamics in SNS Linac," accepted by Nuc. Inst. Meth. A.
- R. Ryne, J. Qiang and S. Habib, "Computational Challenges in High Intensity Ion Beam Physics," proceedings of the 2nd ICFA Advanced Accelerator Workshop on the Physics of High Brightness Beams, November 9-12, 1999. Los Angeles, CA.
- I. Hofmann, J. Qiang, and R. Ryne, "Thresholds of Energy Equipartition in 3D Bunched Beams," submitted to Phys. Rev. Lett.
- S. Habib et al., “The Quantum-Classical Transition in Nonlinear Dynamical Systems,” to be submitted to Phys. Rev. Lett.

Multi-disciplinary Activity



We have one foot planted firmly in the world of computational science and one planted firmly in the world of physical science

Invited Talks

- R. Ryne, “Applications of Large-Scale Simulation to Problems in Accelerator Physics,” International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT’2000), FNAL, Oct. 2000
- J. Qiang, “Large-Scale Simulation of High-Intensity Beams,” International Computational Accelerator Physics Conference (ICAP’2000), Darmstadt, Germany, Sept. 2000
- A. Adelmann, “Parallel Computing in the Design of Accelerators,” ICAP’2000
- K. Ko, “High Performance Computing in Accelerator Physics,” International Linear Accelerator Conference (Linac’2000), Monterey, CA, August 2000.
- K. Ko, "Large Scale Electromagnetic Modeling of Accelerator Structures and Components using High Performance Computers,” 1999 Particle Accelerator Conference, New York, NY, March 1999.
- R. Ryne, “The US DOE Grand Challenge in Computational Accelerator Physics,” Linac’98, Chicago, IL, August 1998.

Collaboration/impact beyond accelerator physics

- Modeling collisions in plasmas
  - new Fokker/Planck code
- Modeling astrophysical systems
  - starting w/ IMPACT, developed astrophysical PIC code
  - also used to test scripting ideas
- Modeling stochastic dynamical systems
  - new leap-frog integrator for systems w/ multiplicative noise
- Simulations requiring solution of large eigensystems
  - new eigensolver developed by SLAC/NMG & Stanford SCCM
- Modeling quantum systems
  - Spectral and DeRaedt-style codes to solve the Schrodinger, density matrix, and Wigner-function equations

We are publishing papers but...

…are we making a difference?

YES

- Our codes are being used by several major projects
- We are impacting project cost
- People are seeking us out for help

New parallel applications codes have been applied to major accelerator projects

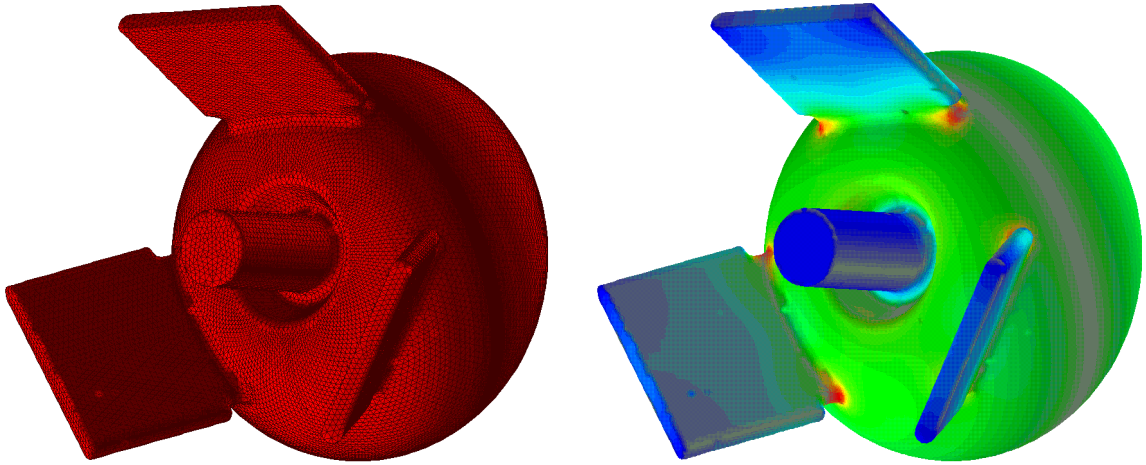
- Main deliverables: 5 parallel applications codes
- Electromagnetics:
  - 3D parallel eigenmode code Omega3P
  - 3D parallel time-domain EM code Tau3P
  - New 3D electrostatics code Phi3P under development
- Beam Dynamics:
  - 3D parallel Poisson/Vlasov code, IMPACT
  - 3D parallel Fokker/Planck code LANGEVIN3D
- Applied to SNS, NLC, PEP-II, APT, ALS, CERN/SPL

New capability has enabled simulations ***3-4 orders of magnitude*** greater than previously possible

Importance of Accelerators & Accelerator Simulation

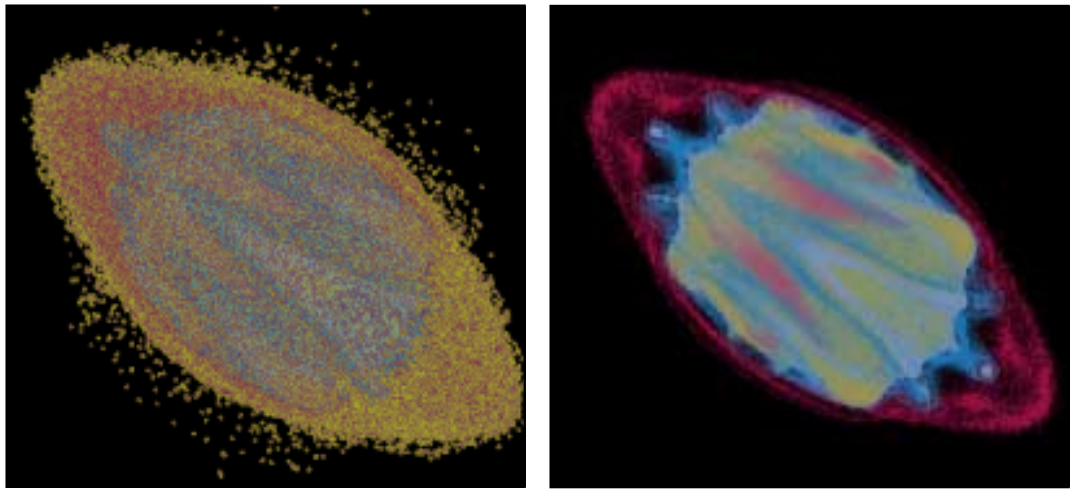
- Accelerators critical to scientific research:
  - HEP, NP, BES, BER, FE
    - linear collider (NLC), ν-factory/ μ-collider, rare isotope accelerator
    - spallation neutron source, 4th generation light source
    - heavy ion fusion accelerators
- New technologies of international importance:
  - accelerator-driven waste transmutation, energy production
- Large-scale simulations essential for
  - design decisions & feasibility studies:
    - **evaluate/reduce risk, reduce cost, optimize performance**
  - accelerator science and technology advancement

Grand Challenge Example Applications in Electromagnetics and Beam Dynamics



Computational mesh and wall loss for the PEP-II B-factory cavity modeled using Omega3P

Volume renderings of Spallation Neutron Source simulation results modeled using IMPACT



Development of IMPACT has Enabled the Largest, Most Detailed Linac Simulations ever Performed

- Model of SNS linac used 400 accelerating structures
- Simulations run w/ up to 800M particles on a 512^3 grid
- Approaching real-world # of particles (900M for SNS)

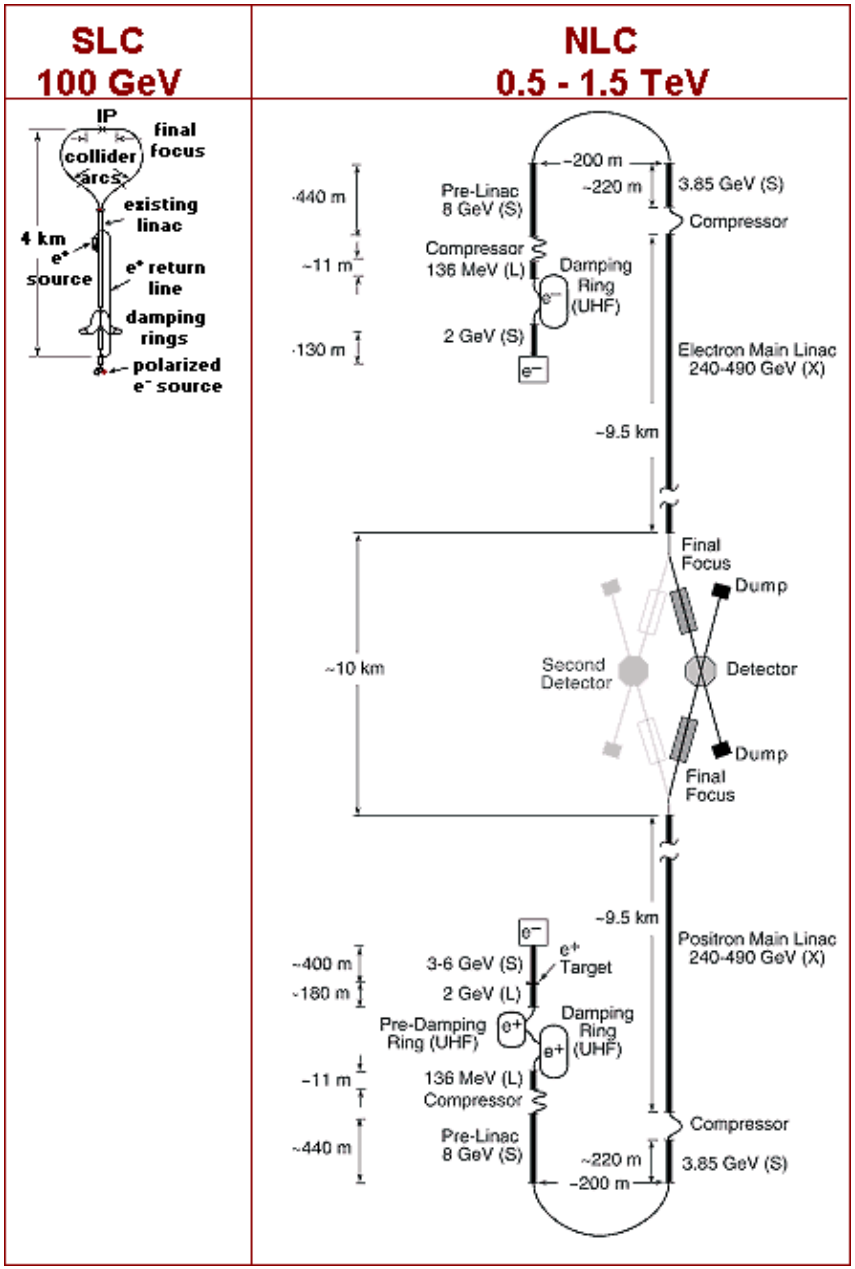
- 100M particle runs now ***routine*** (5-10 hrs on 256 PEs)
- Analogous 1M particle simulation using legacy 2D code on a PC requires weekend
  - 3 order-of-magnitude increase in simulation capability

100x larger simulations performed in 1/10 the time

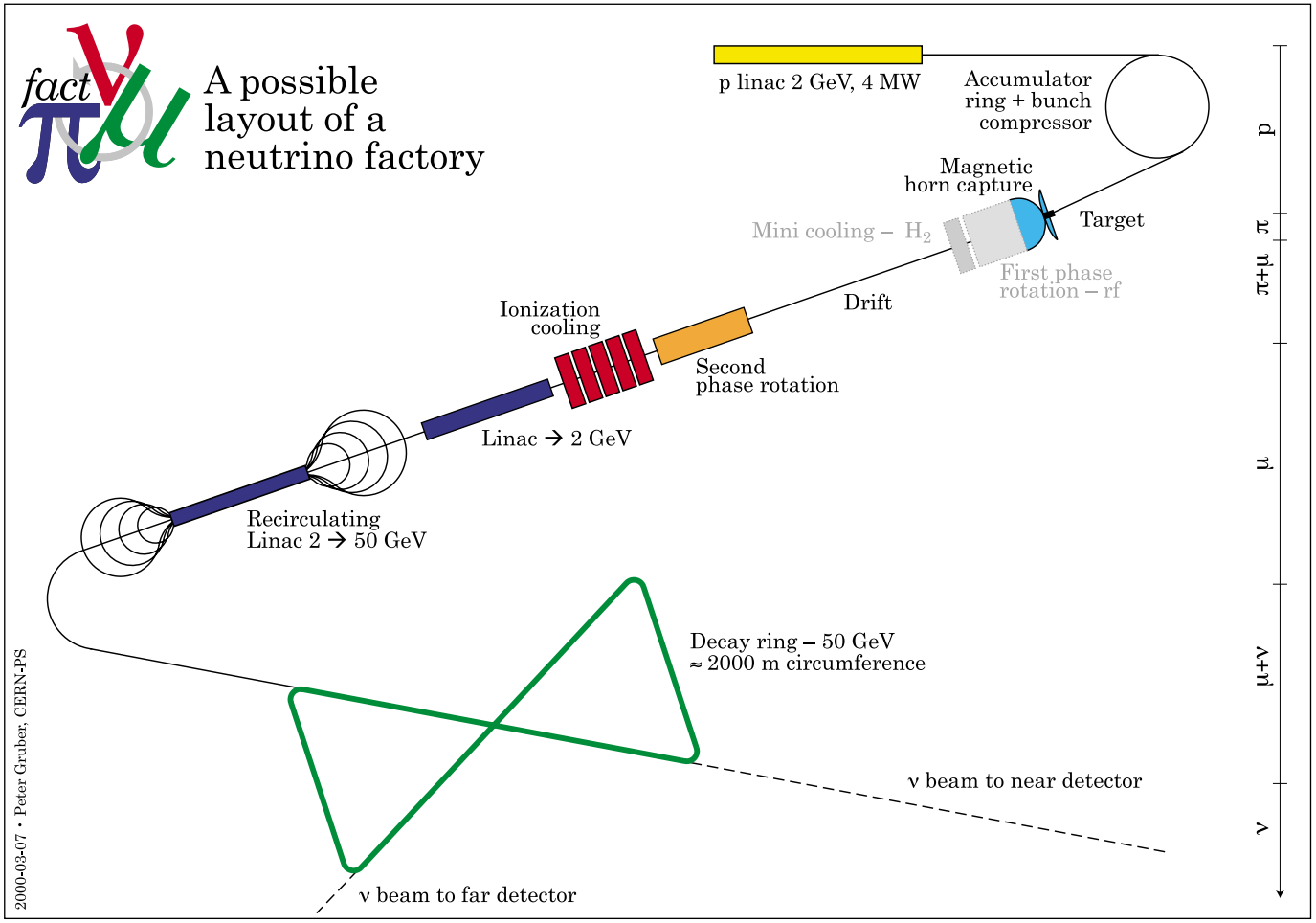
Cost Impacts

- Without large-scale simulation: cost escalation
  - SSC: 1 cm increase in aperture due to lack of confidence in design resulted in $1B cost increase
- With large-scale simulation: cost savings
  - NLC: Large-scale electromagnetic simulations have led to $100M cost reduction

Example: Comparison of Stanford Linear Collider and Next Linear Collider



Neutrino Factory Complex



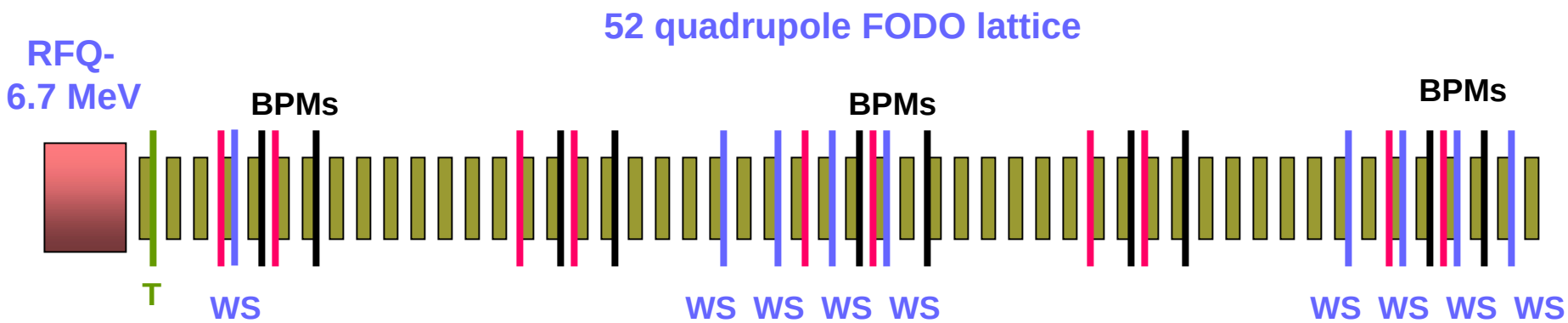
Cost impact of new accelerator modeling codes

- Next Linear Collider (NLC)
  - design of rounded damped-detuned accelerating structure has resulted in ~$100M cost reduction
- Proton radiography
  - large-scale simulations will be used to validate design changes leading to ~$100M cost reduction

FY00 Accomplishments: Algorithms and Software

- New Poisson solvers in IMPACT code
  - existing: open transversely + open/periodic longitudinally
  - new: round/rectangular pipe + open/periodic longitudinally
    - needed for LEDA beam halo experiment
- Self-consistent solution of Fokker/Planck (LANGEVIN3D code)
  - damping/diffusion coefficients via convolution in velocity space
  - solved by modeling associated Langevin equation
- Treatment of beams in circular accelerators
  - new algorithm for conversion from $(X,P_x,Y,P_y,T,P_t)(s) \rightarrow (x, y, z)(t)$

Application: LEDA Halo Experiment



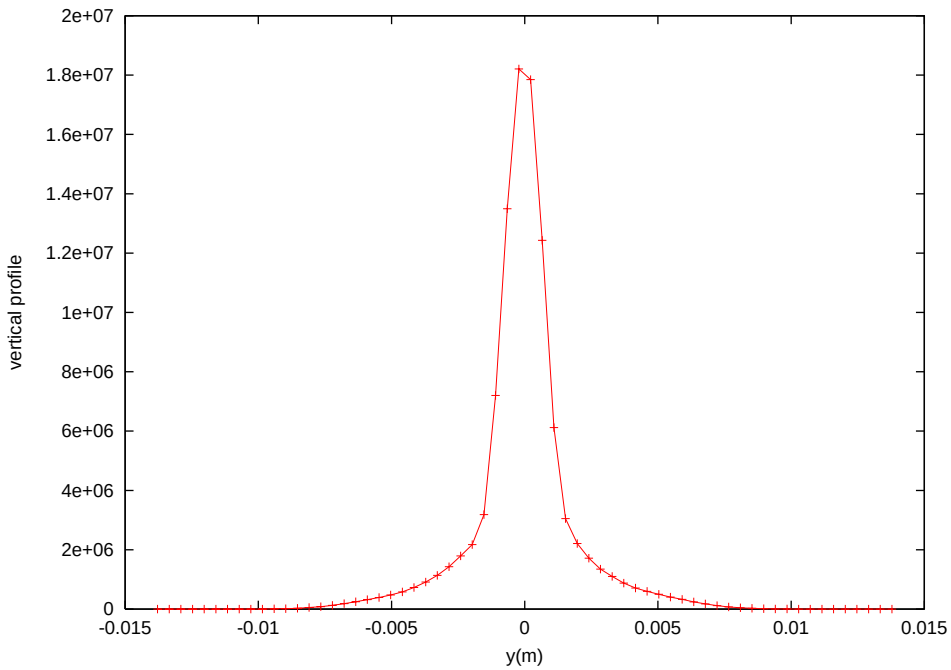
52 Quadrupoles
10 Steering Magnets
9 Wire Scanners
1 Toroid
10 Beam Position Monitors

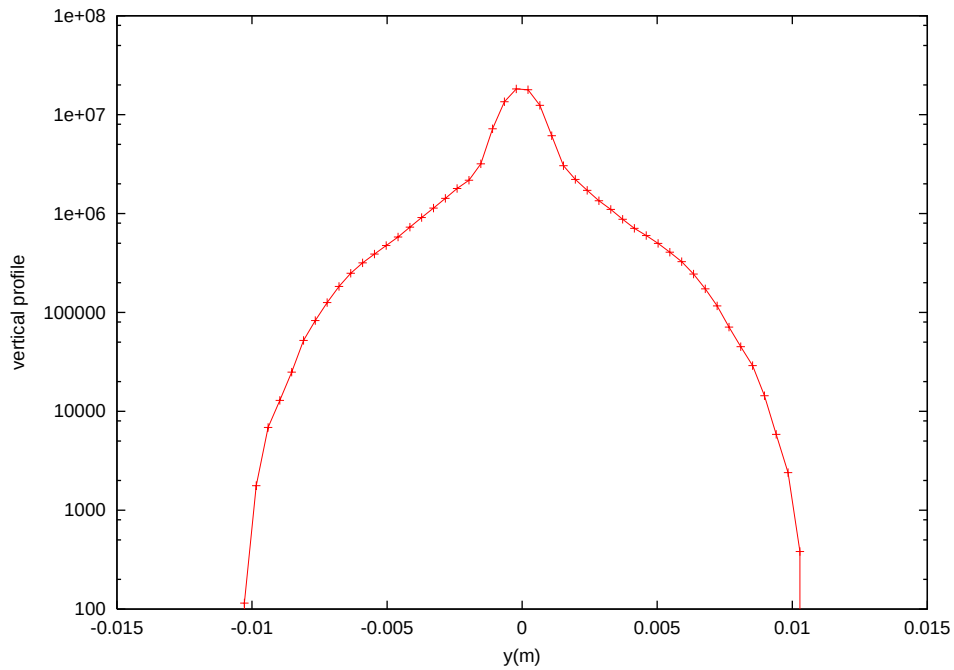
LEDA Goals

- Evaluate/Assess (“Validate”):
  - computer models (IMPACT, LINAC)
    - halo
    - emittance
  - physical models of intense beam dynamics
    - particle-core model

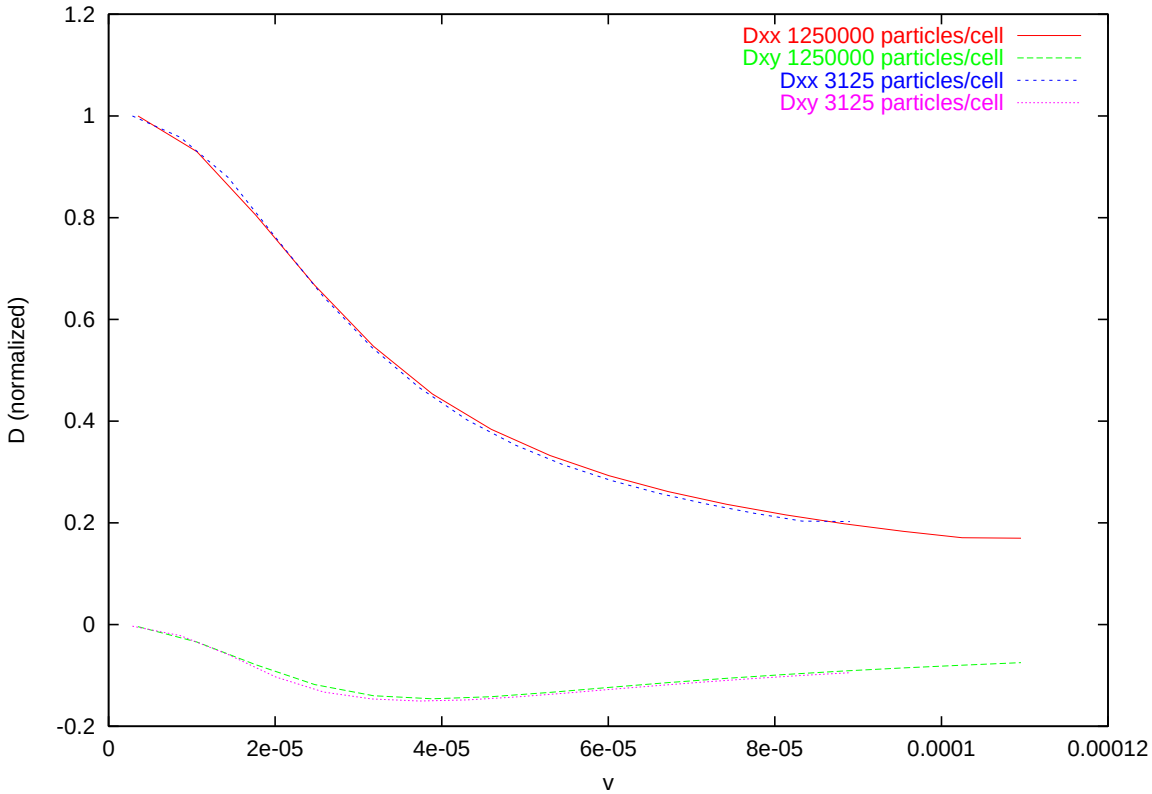
IMPACT Simulation of LEDA w/ 100Mp

Vertical profile at quad 49



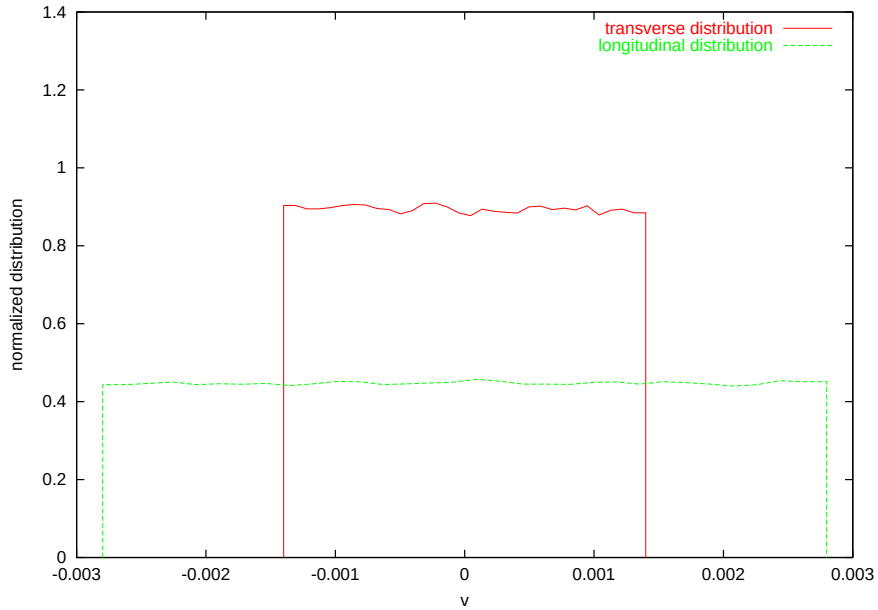


First-ever self-consistent Fokker/Planck

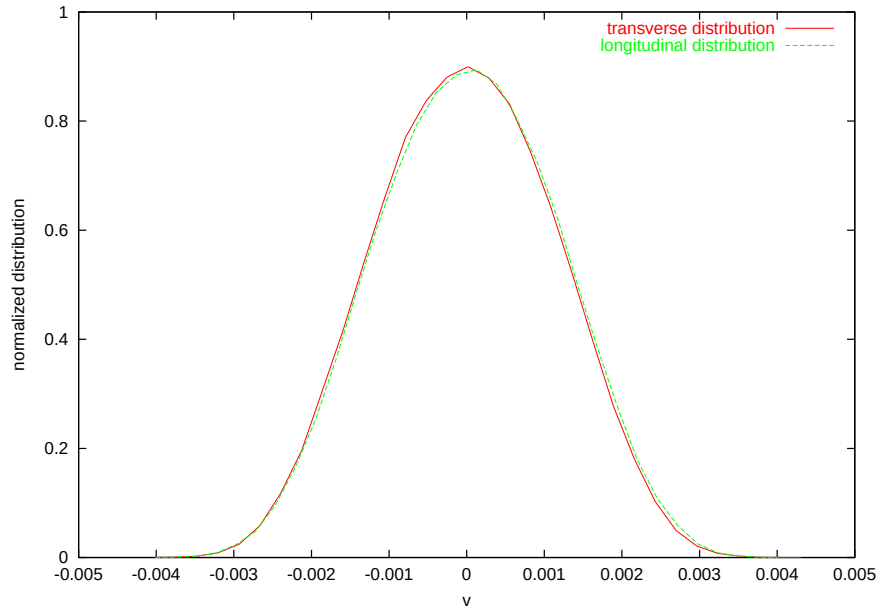


Diagonal and off-diagonal diffusion coefficients for a Maxwellian distribution as a function of velocity.

Approach to Thermal Distribution

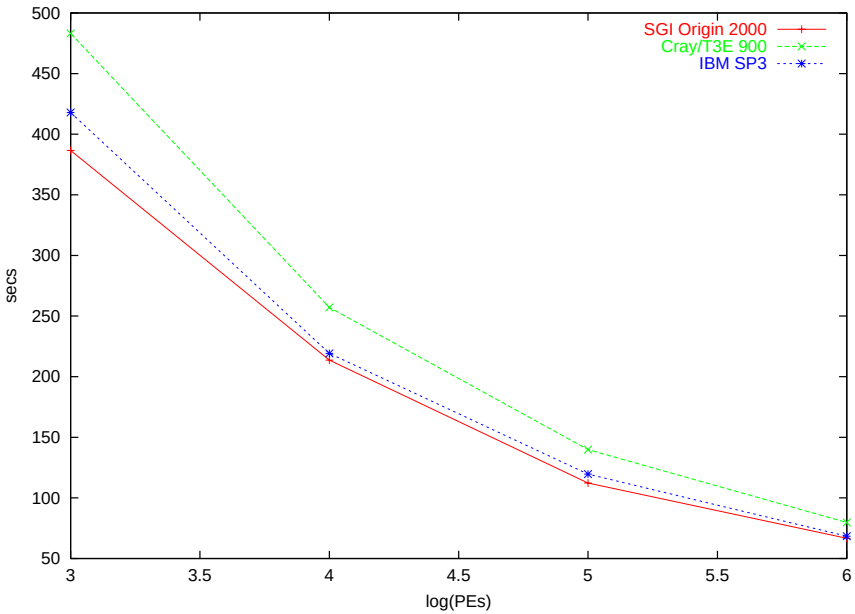


Initial velocity distribution

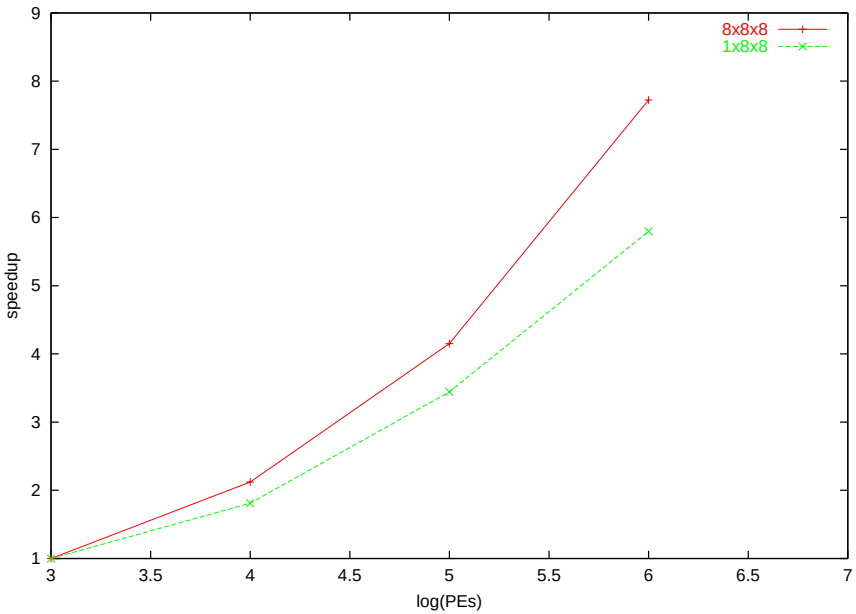


Final velocity distribution

Speedup



Speedup on
T3E, SP3, O2K



Speedup for two problem sizes
on O2K

Intense Beams in Circular Accelerators

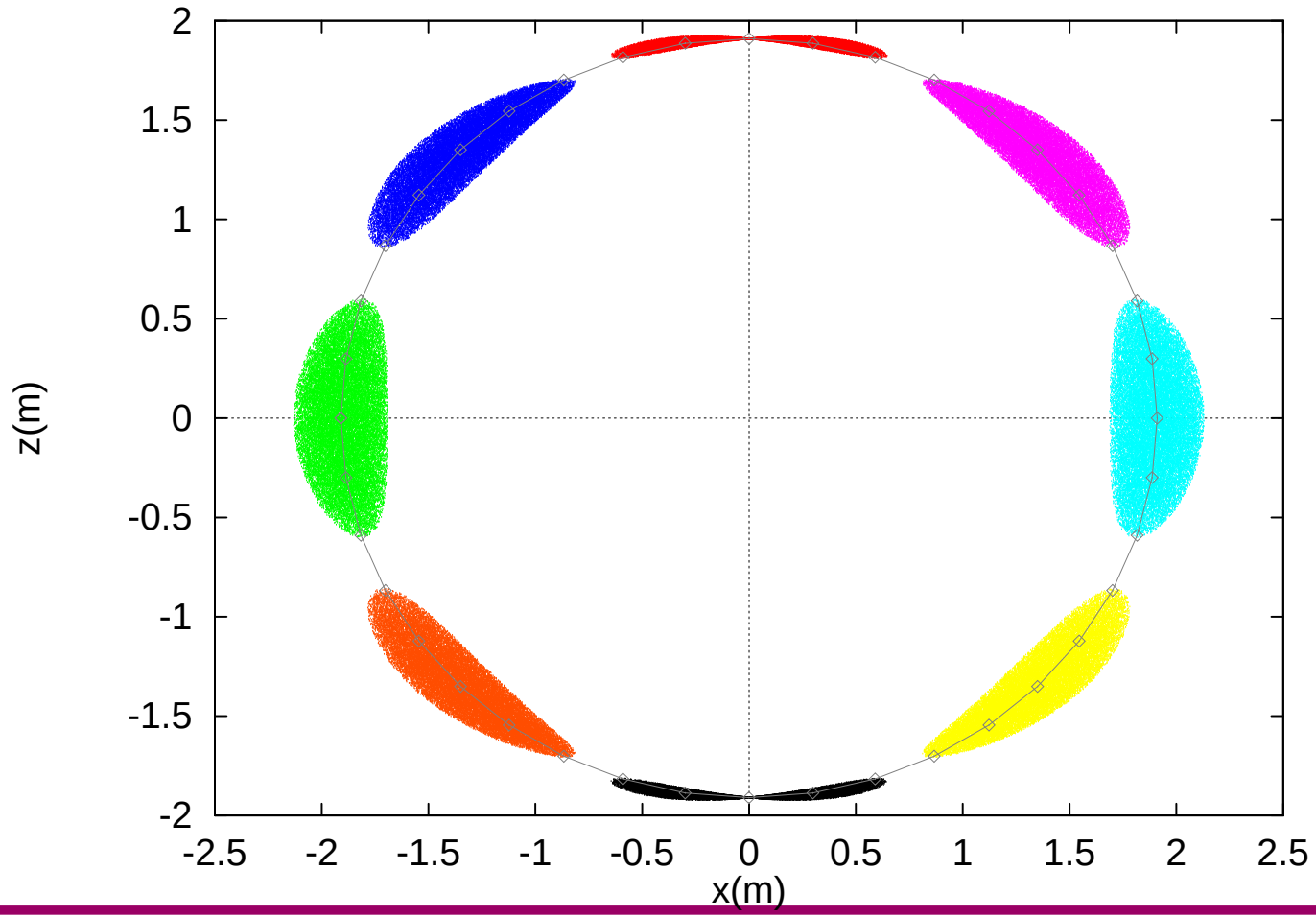
- Previous years' work emphasized high intensity *linear* accelerators
- New work extends this capability to treat intense beams in bending magnets
- Additional effort was needed to treat circular systems
  - vast majority of accelerator codes use the arc length ("z" or "s") as the independent variable, not time. (facilitates design/analysis)
  - Simulation of intense beams requires solving $\nabla^2\phi=\rho$ at *fixed time*

We are approaching a situation where users will be able to "flip a switch" to turn space charge on/off in the major accelerator codes

Kinematics in bends can lead to non-trivial behavior as a result of conversion to fixed time

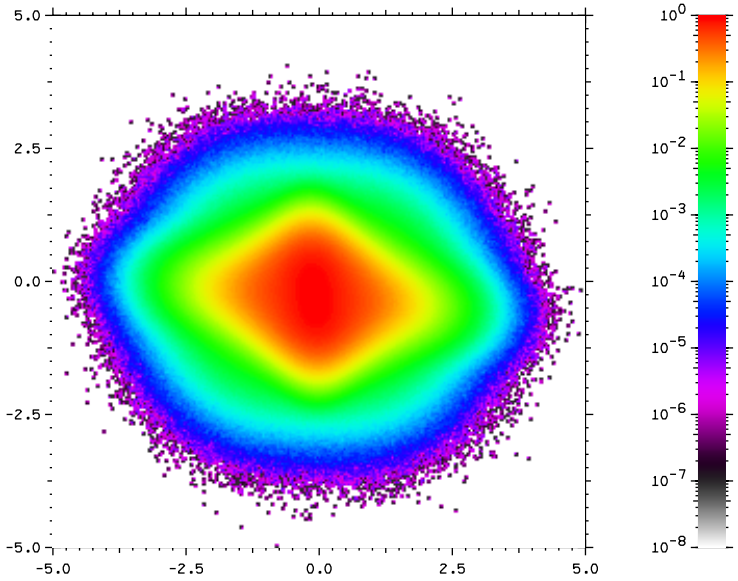
x-z plots based on x-ϕ data from an s-code.

Data shown in a bend at different 8 times

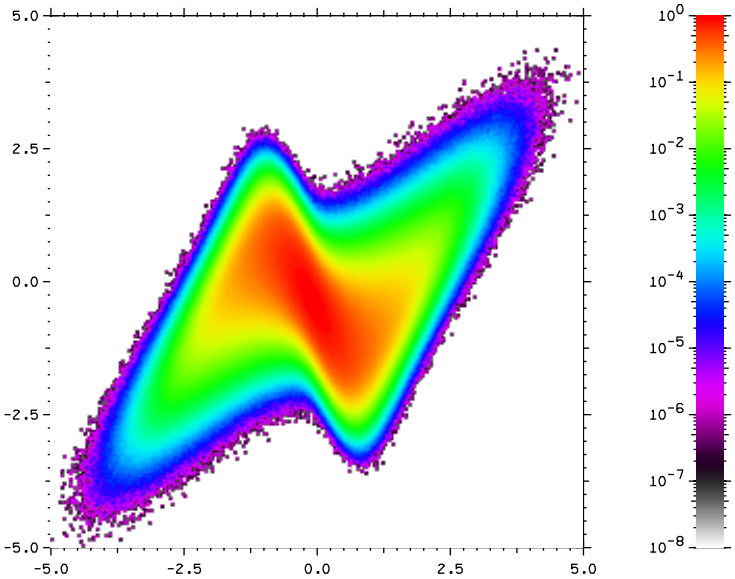


Large-Scale Parallel Simulation Enables Unprecedented Accuracy

- **Log scale shows integrated charge density obtained from 500M particle simulation on parallel supercomputer**
- **Approaching part-per-million accuracy**



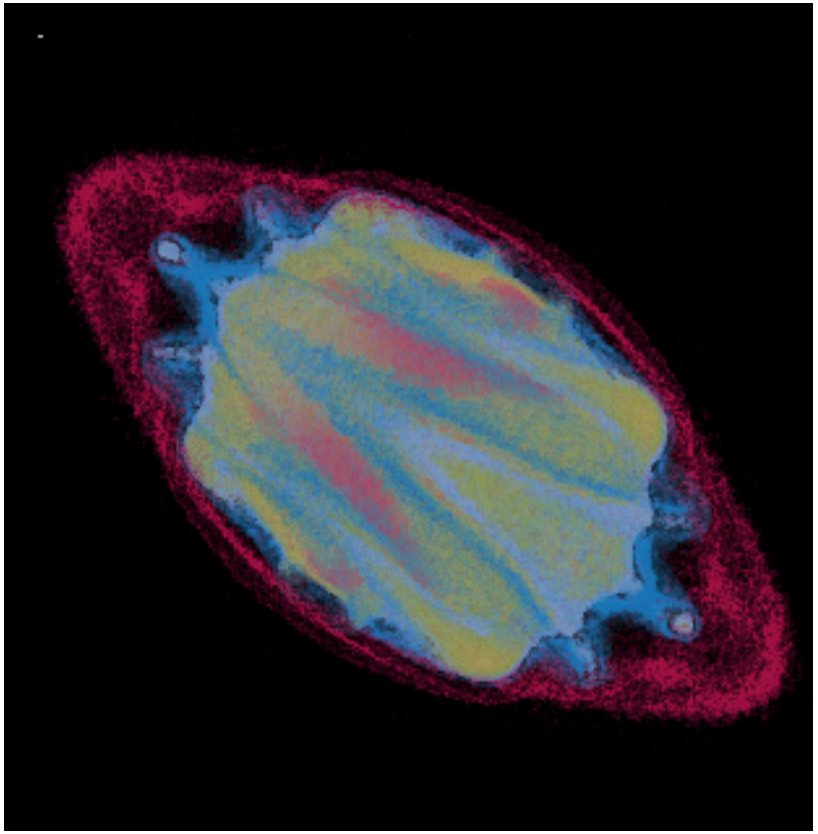
X-Y Plot



X-P_X Plot

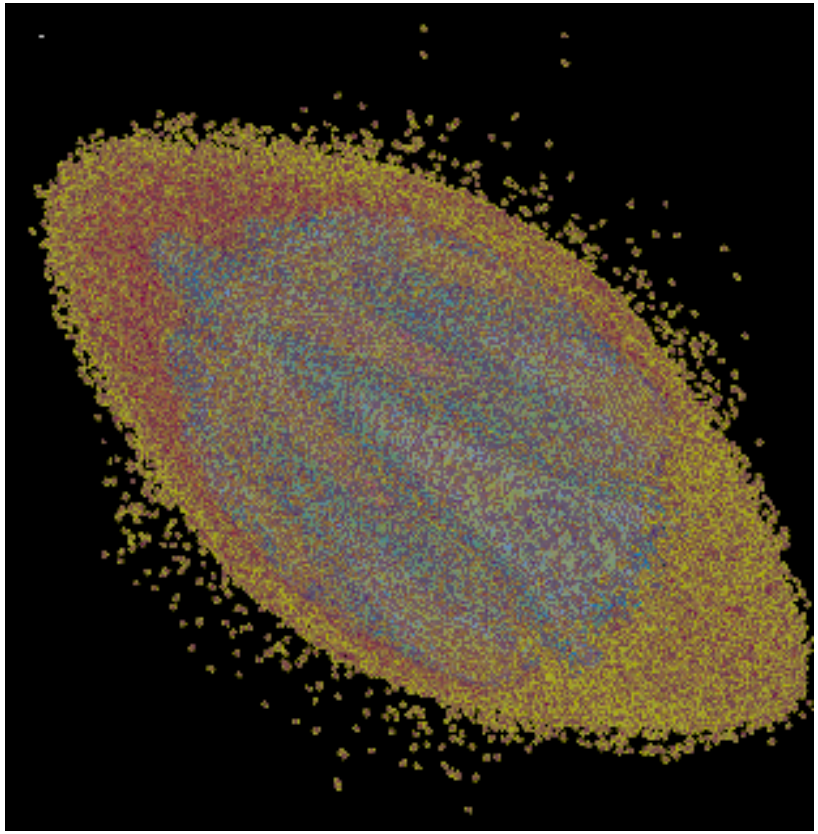
Volume Rendering of SNS Results

Transparency to see inside volume



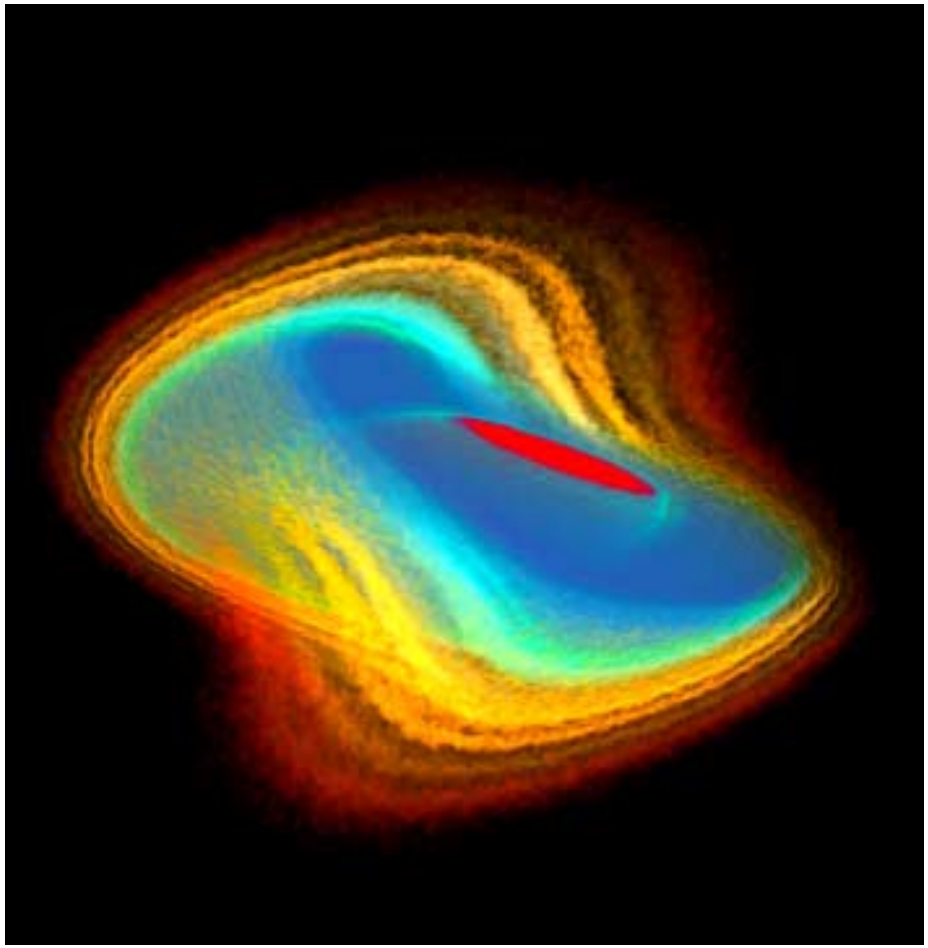
x-p_x-z space

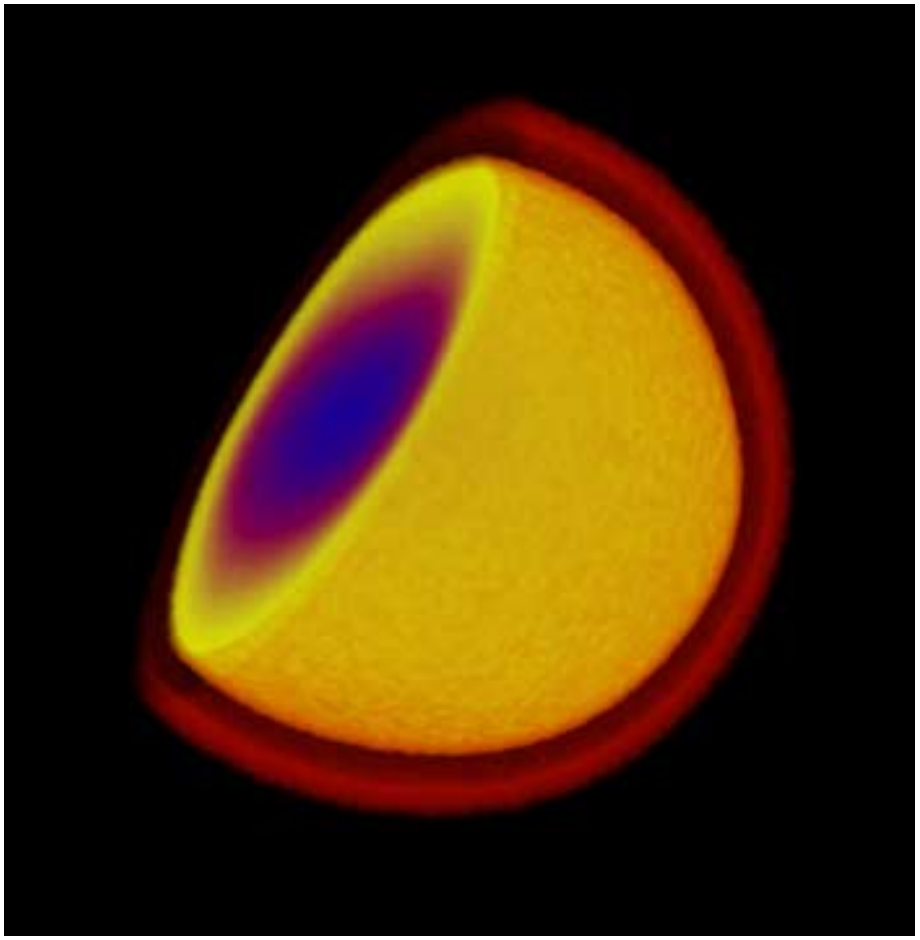
Opacity to accentuate halo



x-p_x-z space

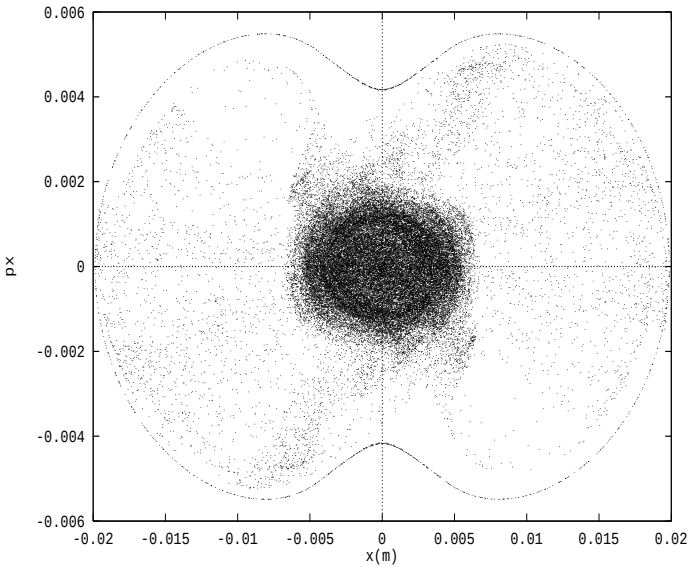
Volume Rendering of APT Results



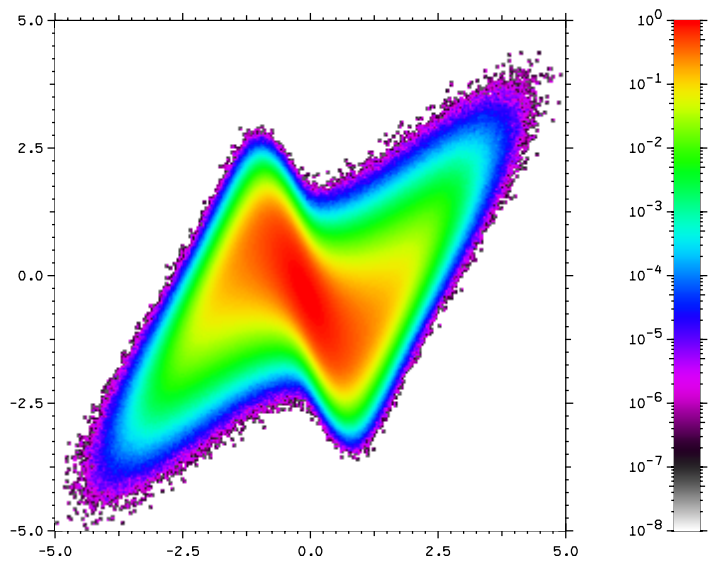


How far has the accelerator community come?

- 1980s: 10K particle, 2D serial simulations typical
- Early 1990s: 10K-100K particle, 2D serial simulations typical



1994: 2M particle simulation on CM5. 2D space charge. Idealized transport system.



1999: 500M particle simulation on Nirvana. 3D space charge. Realistic model of SNS linac.

Where are we going as a Community?
ACAST: Advanced Computing for Accelerator S&T

- National R&D effort to establish a comprehensive terascale capability in accelerator systems simulation
- Participants:
  - LANL, SLAC, LBNL, FNAL, BNL ,TJNAF, Stanford , UCLA, ACL, NERSC
- Budget:
  - $1M through end of FY00
- Focus Areas:
  - Beam Systems Simulation (BSS)
  - Electromagnetic Systems Simulation (ESS)
  - Beam/Electromagnetic Systems Integration (BESI)
- See http://public.lanl.gov/ryne/proposal.html

Large-scale simulation will play a key role in 3 areas

- Present accelerators: Maximize investment by
  - optimizing performance
  - expanding operational envelopes
  - increasing safety, reliability and availability
- Next-generation accelerators
  - facilitate important design decisions
  - help ensure success
  - help ensure completion on schedule and within budget
- Accelerator science and technology
  - advance the frontiers of accelerator technology
  - new developments and discoveries in beam-driven science