The DOE Grand Challenge in Computational Accelerator Physics: A Multi-Disciplinary Success Story

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Schedule of Presentations

- 1:00 pm - Motivation, Grand Challenge Overview (R. Ryne)
- 1:10 pm - Beam Dynamics (R. Ryne)
- 1:30 pm - Electromagnetics (K. Ko)
- 2:00 pm - NERSC Capabilities and Collaboration (E. Ng)
- 2:30 pm - ACL Capabilities and Collaboration (R. Oldehoeft)
- 3:00 pm - Future Plans (R. Ryne)

Why is Large-Scale Accelerator Simulation Important?

- Accelerators critical to scientific research:
  - High energy physics, nuclear physics, materials science, biological science, fusion energy
    - HENP: Next Linear Collider (NLC), isotope accelerator, μ-collider
    - BES: Spallation Neutron Source (SNS), 4th generation light source
    - OFE: Heavy ion fusion accelerators
    - BER: light sources, neutron sources
- New technologies of international importance:
  - accelerator-driven waste transmutation, energy production
- Future accelerators require a new level of simulation

What are the Challenges of Future Accelerators? Why is Large-Scale Simulation Needed?

- Future accelerators:
  - **higher intensity, greater complexity, greater precision**
- Large-scale simulations essential for:
  - design decisions:
    - **evaluate/reduce risk**
    - **reduce cost**
    - **optimize performance**
  - feasibility studies
  - technology advancement

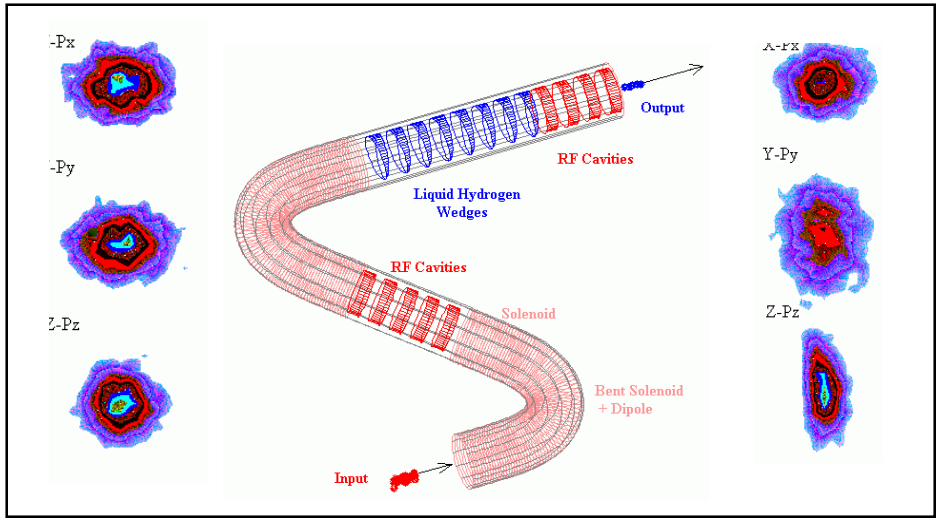
Cost Impacts

- Without large-scale simulation: cost escalation
  - Supercollider: 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

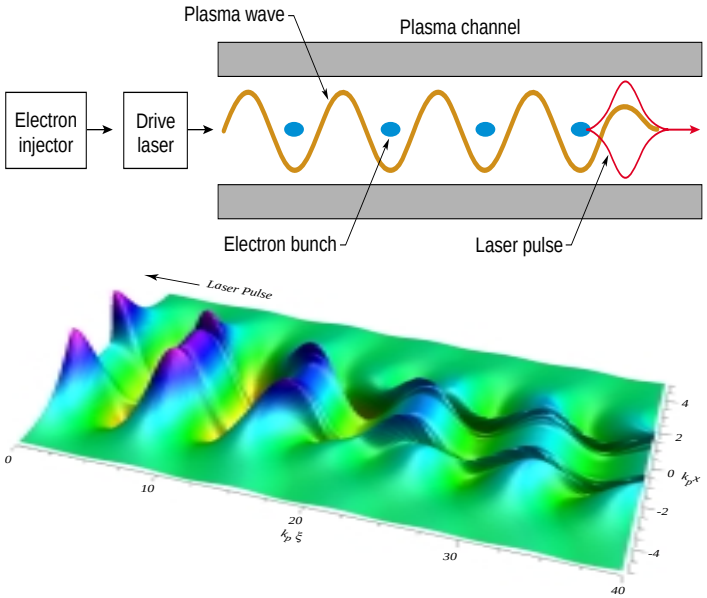
Benefits of Large-Scale Simulation to Accelerator Science and Technology

- *Tool of discovery* to explore beams under extreme conditions

muon cooling channel



ultra-high gradient plasma accelerator



Large-scale simulation, coupled w/ theory & experiment, will help *advance the frontiers* of accelerator technology

Summary: 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

DOE Grand Challenge in Computational Accelerator Physics

- Principal Investigators
  - Kwok Ko (SLAC) and Robert Ryne (LANL)
- Institutions
  - Los Alamos, SLAC, Stanford, UCLA, ACL, NERSC
- Goals
  - Develop a new generation of accelerator modeling tools targeted to high performance computing platforms
  - Apply tools to present and future accelerator applications of national importance

Team Members and Collaborators

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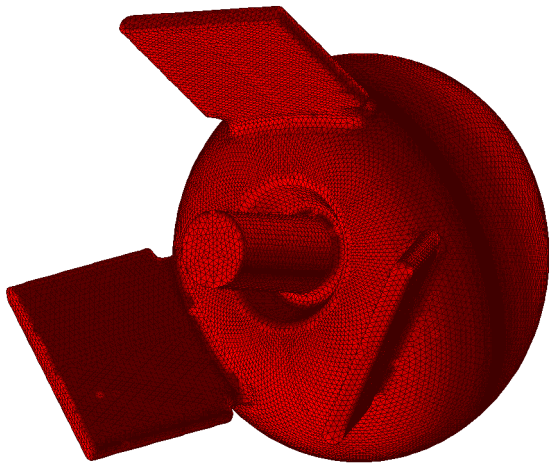
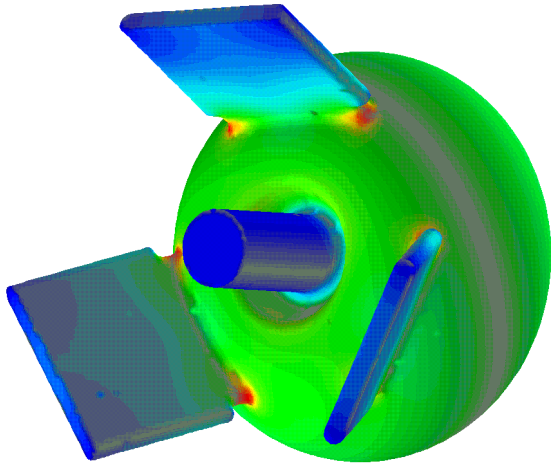
A Multi-Disciplinary Team

- Accelerator physicists and engineers
  - understand/improve existing accelerators; design new ones
  - technology breakthroughs through simulation+theory+experiment
- Applied mathematicians
  - develop methods and algorithms
- Computer scientists and software engineers
  - implementation of algorithms in software
  - develop broad-based frameworks, problem solving environments
- Visualization experts
  - analysis of simulation results
- Collaboration leading to
  - development of large-scale applications codes

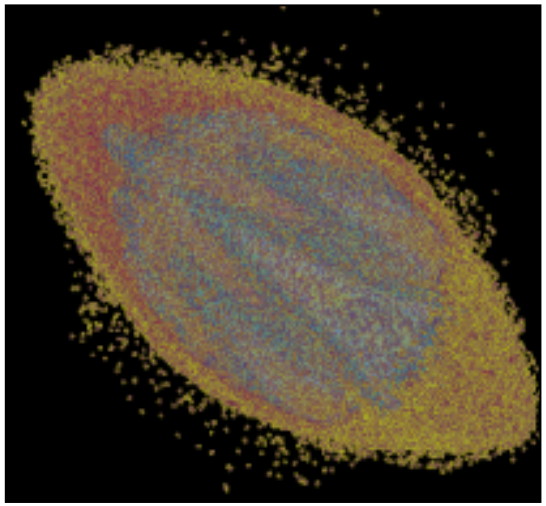
Grand Challenge Focus Areas: Electromagnetics and Beam Dynamics

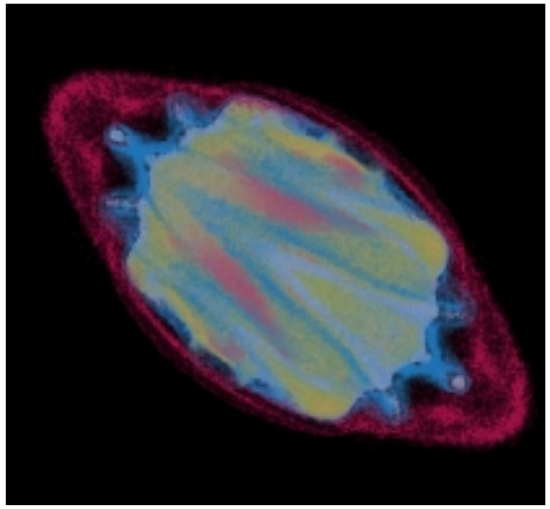




Computational mesh and wall loss for the PEP-II B-factory cavity modeled using Omega3P

Volume renderings of Spallation Neutron Source simulation results modeled using IMPACT





Grand Challenge Bottom Line: "Parallel Computing Works"

- Main deliverables: 3 parallel applications codes
- Electromagnetics:
  - New 3D parallel eigenmode code, Omega3P, models problems with 10's of millions of degrees of freedom
  - Tau3P: New parallel 3D time-domain EM code
- Beam Dynamics:
  - New 3D parallel beam dynamics code, IMPACT, used to perform simulations with up to 800M particles
- Applied to NLC, PEP-II, SNS, APT, ALS projects

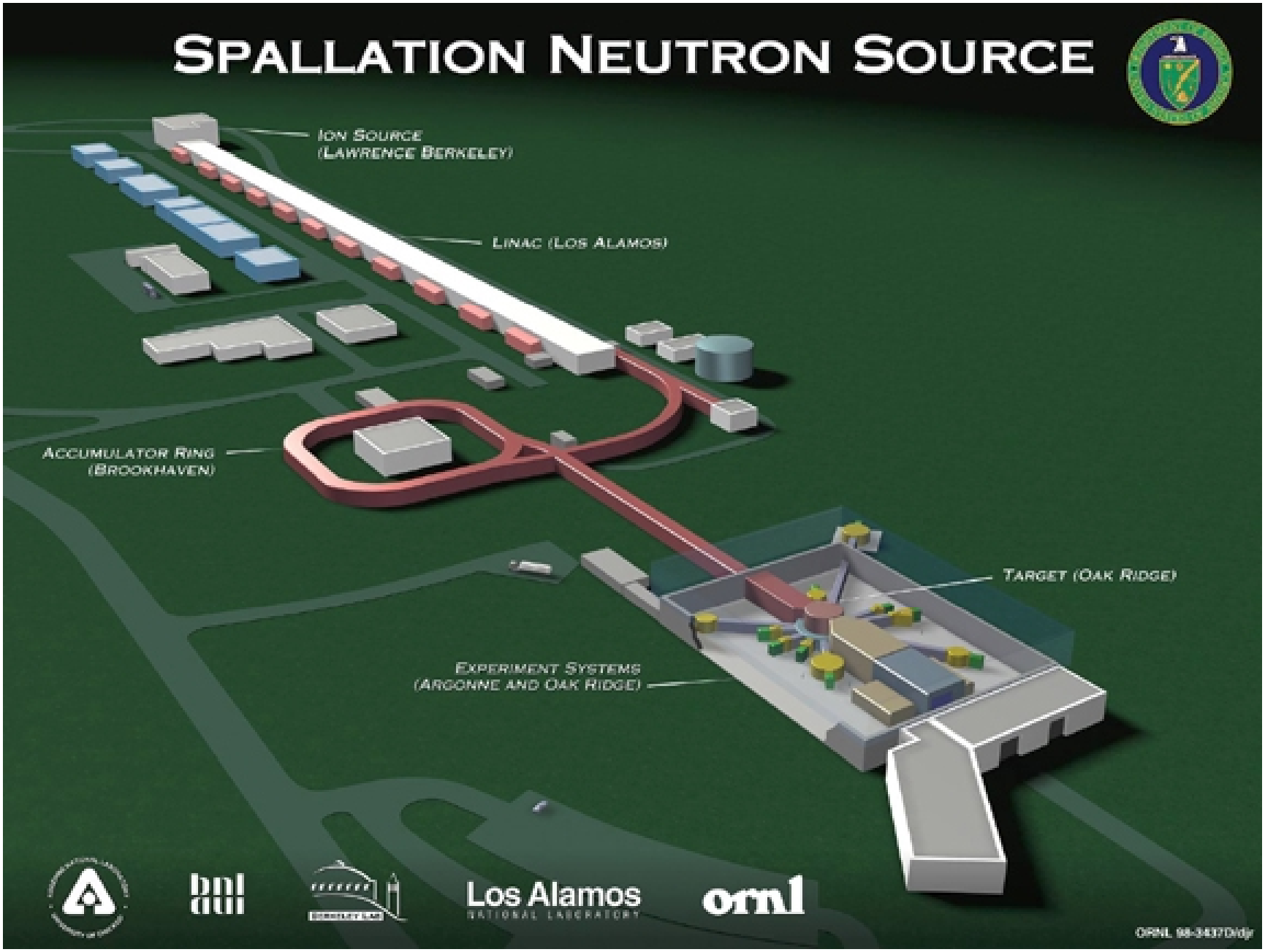
Progress in the Grand Challenge has enabled simulations ***3-4 orders of magnitude*** greater than previously possible

Grand Challenge Support

- Direct MICS funding: $490K
  - LANL: $220K
  - SLAC: $200K
  - UCLA: $50
  - Stanford: $20K
- Leverage
  - Los Alamos Accelerator Code Group: $100K
  - LANL HPCC Postdoc Committee: $35K
  - SLAC Numerical Modeling Group: 2-3 FTE
  - LANL ACL: 1.5 - 2 FTE
- Total effort: ≥ $1M

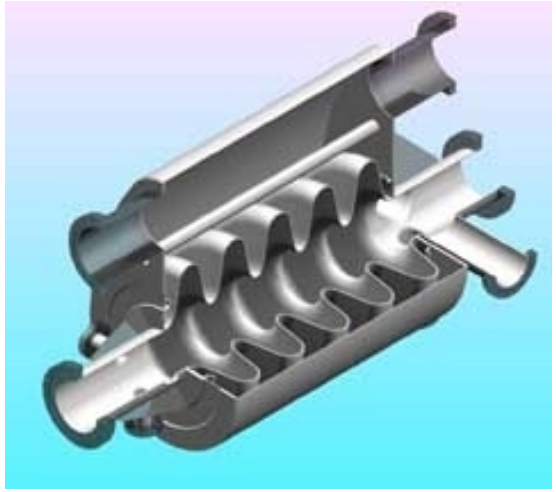
Outline: Beam Dynamics

- Overview: What are we modeling?
- What is our new capability?
  - IMPACT 3D parallel PIC code
- How did we achieve this capability?
  - multi-disciplinary team
  - examples of obstacles encountered and their solution
- IMPACT simulation code
  - algorithms, methods, parallel implementation, results


SPALLATION NEUTRON SOURCE
ION SOURCE
(LAWRENCE BERKELEY)
LINAC (LOS ALAMOS)
ACCUMULATOR RING
(BROOKHAVEN)
TARGET (OAK RIDGE)
EXPERIMENT SYSTEMS
(ARGONNE AND OAK RIDGE)
Los Alamos
NATIONAL LABORATORY
ornl
ORNL 98-3437D/dj/r

What are we Modeling?

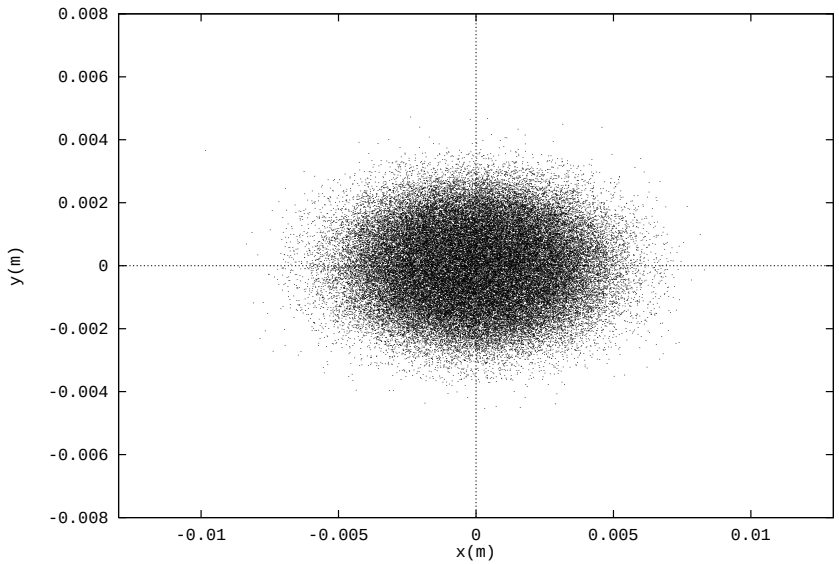
- Propagation and acceleration of intense charged particle beams through a variety of accelerator systems
  - extremely complex nonlinear external fields
  - intense, nonlinear self-fields



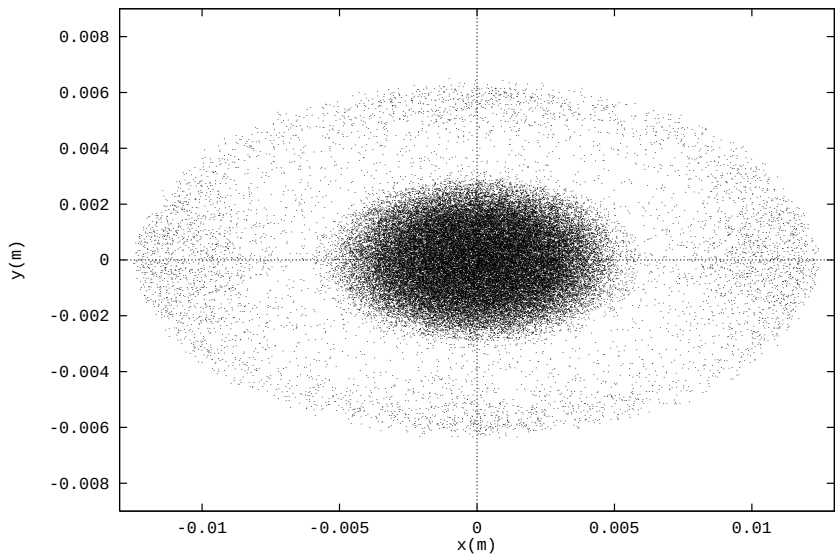
Large-Scale Simulation is Needed to Accurately Model Beam Halo

- Future high-average-power accelerators will operate with ultra-low losses
  - excess losses cause radioactivity
  - hinders or prevents hands-on maintenance
  - reduces availability, reliability, maintainability
- Allowed loss of 1-10 particles per billion
- A major source of beam loss: beam halo
- Small-scale simulations with ~1M particles insufficient to predict tails of beam distribution
- **Large-scale simulation needed to facilitate aperture decision, balance risk vs. cost**

Example of a Beam with/without Halo



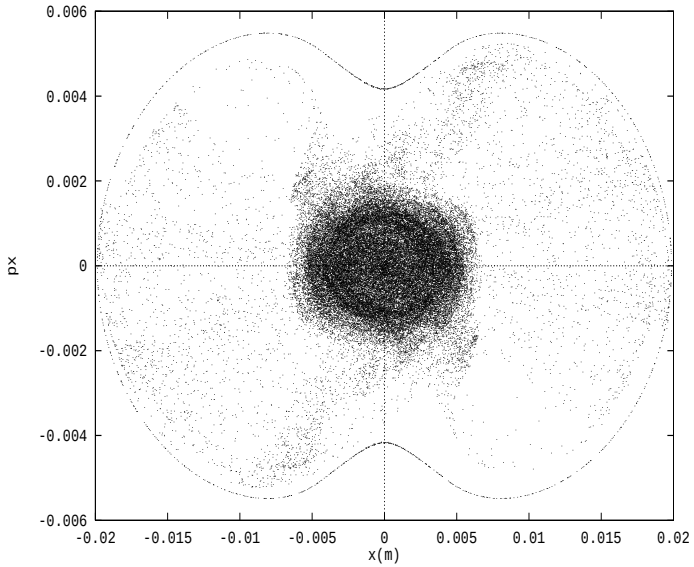
Matched beam (properly injected into accelerator)



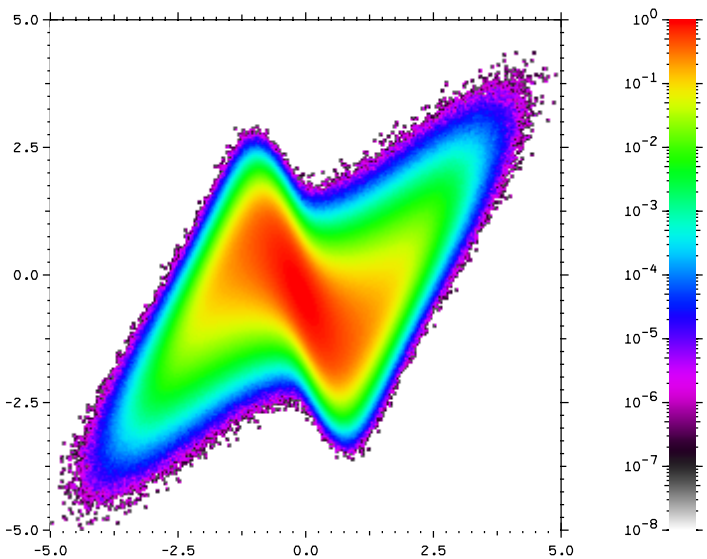
Mismatched beam (improperly injected) exhibits a beam halo

Old and New Capability

- 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.

IMPACT: Integrated Map and Particle Accelerator Tracking Code

3D parallel beam dynamics code developed "from the ground up"

- POOMA, F90/MPI, and HPF implementation
- Reuse of existing parallel problem solving environments and libraries (e.g. POOMA, PLIB)
- *Particle managers* to minimize communication
- Dynamic load balancing
- Optimized cross-box FFTs on Origin 2000
- Used in 48 hr, 2048 PE run during Nirvana acceptance
- Submitted to vendors for 30 T-op procurement
- 100M particle production runs *routine* on Nirvana
- 1 billion particle test runs performed on Blue Mountain

New Capability Required Assembling a Multi-Disciplinary Team

- Development of coherent accelerator simulation environment requires the latest developments in:
  - computer science and software engineering
    - object-orientation
    - design for change and extensibility
    - frameworks and problem solving environments
    - parallel implementation
    - scripting
  - computational science and applied mathematics
    - methods and algorithms

Beam Dynamics Collaborating Institutions

- LANL/LANSCE and Theoretical Divisions
  - intense beam dynamics theory (Vlasov/Poisson)
  - Collisions (Fokker-Planck)
- LANL/ACL
  - POOMA, Nirvana support, Viz support, PAWS,...
- SLAC, NERSC
  - Parallel tracking on PC cluster
- UCLA Dept. of Physics
  - PLIB: parallel library for particle simulation

International Beam Dynamics Collaboration with PSI/ETH Zurich

- Parallel tree-solver implemented in POOMA
- Combining modern European accelerator frameworks with POOMA
- Builds on Grand Challenge accomplishments, design philosophy

Goal: Ability to model cyclotrons, synchrotrons, and linacs in a single simulation environment

International Collaboration on Modeling Stochastic Systems

- Developed parallel Langevin code
  - damping/diffusion known apriori
- New 2nd order stochastic leap-frog algorithm
- Effect of noise on classical and quantum dynamics
  - w/ K. Shizumi, Tsukuba Japan

Goals:

- Self-consistent Fokker-Planck modeling
- Hard collisions via hybrid Fokker-Planck + direct simulation monte carlo

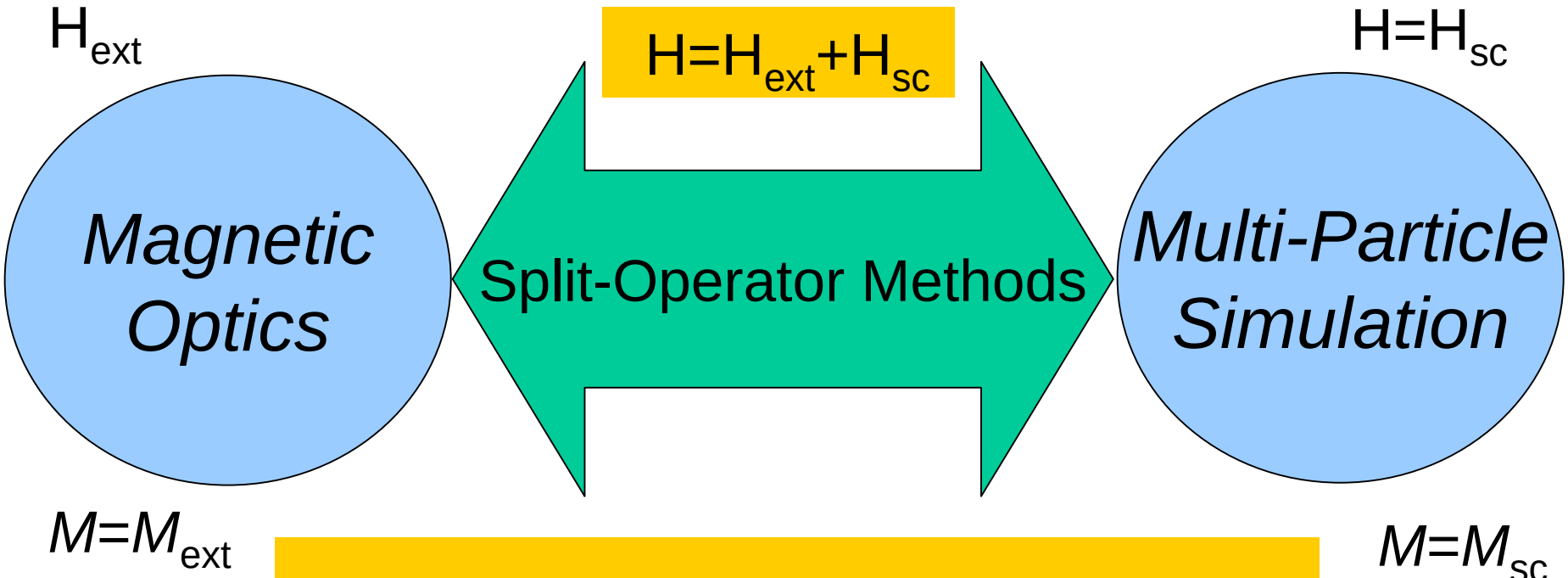
Unexpected Obstacles Encountered During Code Development and Their Solution

- Performance: major improvement through use of optimized parallel particle managers (ACL & UCLA)
- Computer science support for multi-box runs
  - MPI settings: critical to using HIPPI effectively
  - FFT performance: modification of FFT routines in POOMA
- Code initialization
  - on-processor initial-particle generation essential
- Visualization and data handling
  - ACL viz team built 1.2 TB file system for large runs
  - required parallel data analysis between simulation and viz
  - parallel volume rendering to explore structure of 3D data

Description of Methods and Philosophy used in IMPACT

- Parallel Particle-In-Cell (PIC) + Magnetic Optics capability
- Uses split-operator methods with $H=H_{ext}+H_{space\ charge}$
- Philosophy:
  - Do not take tiny steps to push ~100M particles
  - Do take tiny steps to compute maps; then push w/ maps
- Realistic treatment of beamline elements
  - rapidly varying s-dependence of beamline elements decoupled from slowly varying space charge
- 3D parallel space charge capability
  - FFT-based, open boundary conditions

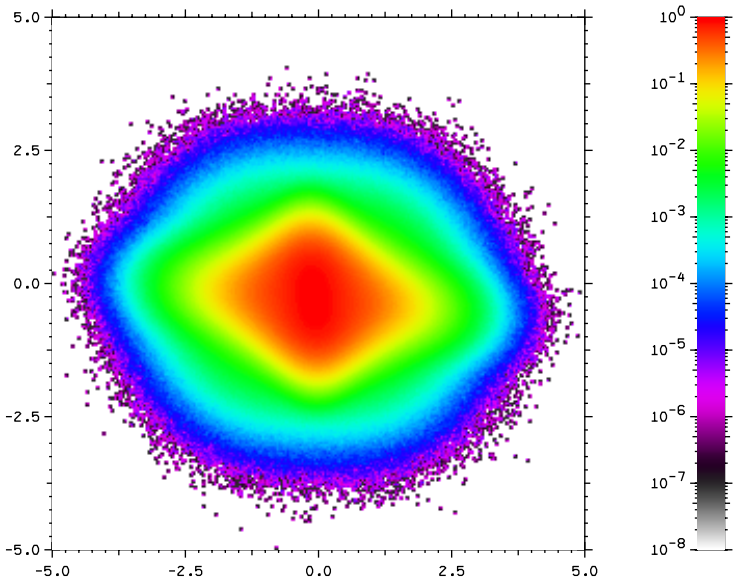
Split-Operator Approach



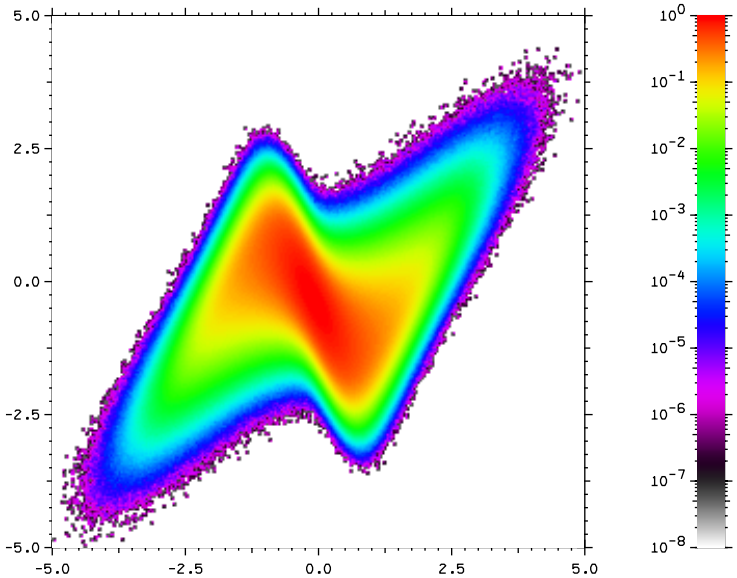
$$M(t)= M_{ext}(t/2)\, M_{sc}(t)\, M_{ext}(t/2) + O(t^3)$$

Large-Scale Parallel Simulation Enables Unprecedented Accuracy

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



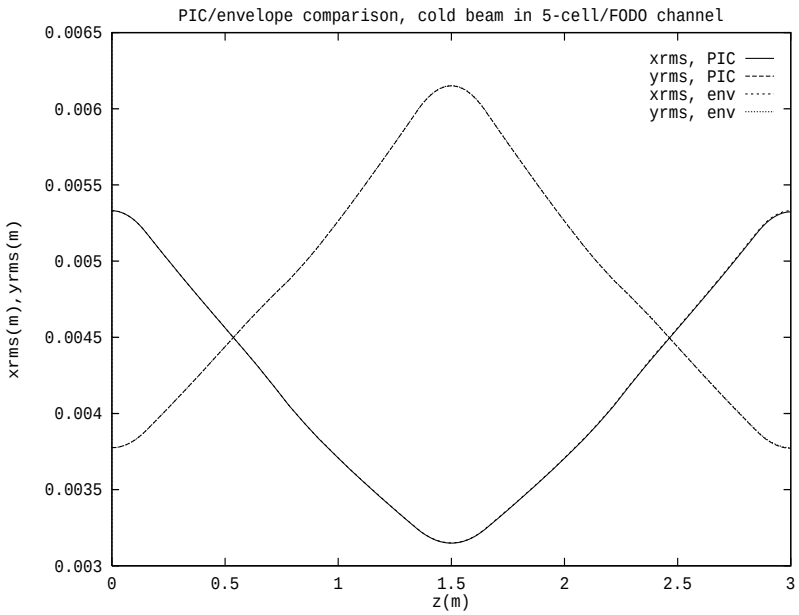
X-Y Plot

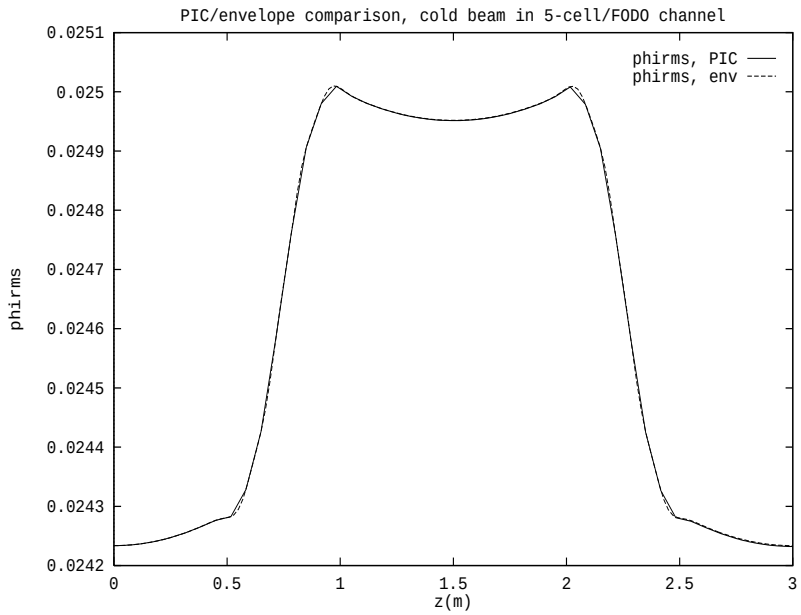


X-P_X Plot

IMPACT Test Case: Comparison with Exact Solution of 3D Envelope Equations

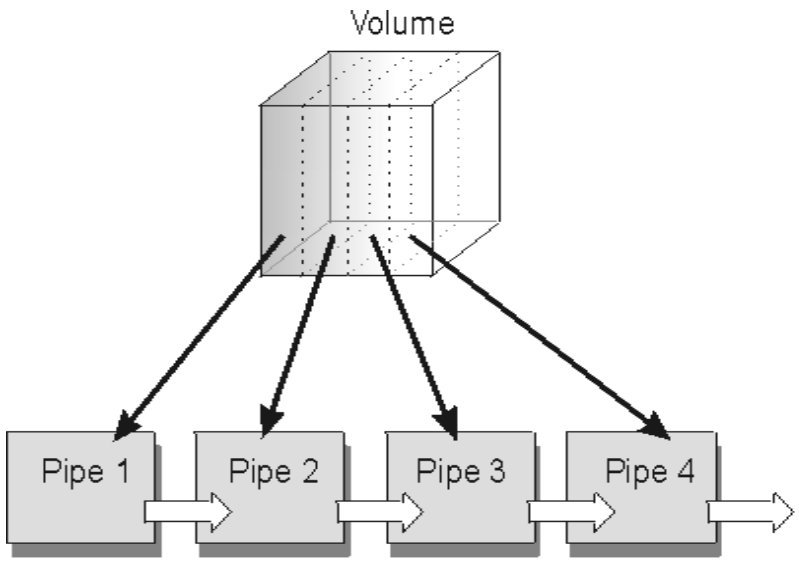
Transverse, longitudinal envelopes obtained from IMPACT particle simulation agree w/ analytical envelope equations

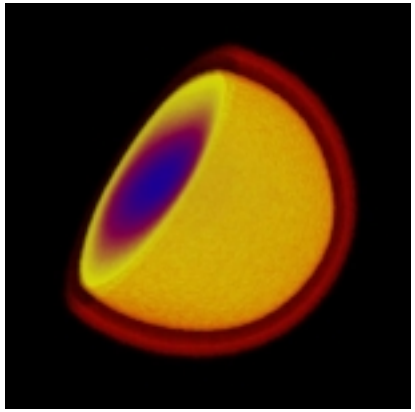


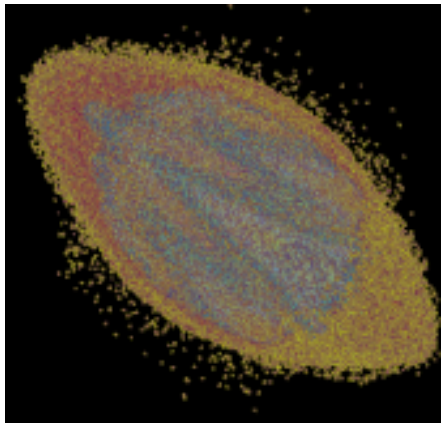


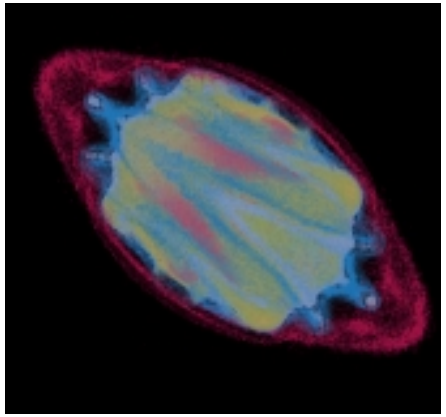
High Performance Volume Rendering

- High performance computing and advanced visualization needed to ***reduce, render & explore*** huge data sets
  - 100M-1B particles, 5-50 Gbytes/step, TB/simulation
- Example: parallel volume rendering









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

- Physical model used 400 distinct accelerating structures
- Simulations run with up to 800M particles on a 512^3 grid
- Approaching real-world # of particles (900M for SNS)
- 100M particle runs of 500 m linac 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

Beyond the Accelerator Grand Challenge

- "Core" activities (existing team)
  - Complex version of Omega3P for lossy structures
  - Tau3P w/ rigid beam for wakefield calculations
  - IMPACT
    - extension to circular systems; additional structures (e.g. RFQs); field solvers w/ realistic boundary conditions; collisions; wakes
  - Combined beam dynamics and electromagnetics
    - use of hybrid grids (regular + unstructured)
    - *self-consistent* treatment of beam/cavity interaction
- New activities
  - beams under extreme conditions (plasma accelerators, phase space cooling); beam-beam; coherent synchrotron radiation

More Breadth, Broader Inclusion of Accelerator Community

- Accelerator Grand Challenge provides foundation
  - community-wide effort to develop a comprehensive, coherent accelerator simulation environment
- Added institutions bring new expertise to existing team
  - LBNL: laser/plasma accelerators
  - FNAL: high energy hadron colliders; muon systems
  - BNL: high intensity rings; muon systems
  - TJNAF: high power FELs; coherent synch. radiation

Proposed Funding Scenario under SSI

	FY2001	FY2002	FY2003	FY2004	FY2005
Core Activity	$1.5M	$1.8M	$2.0M	$1.8M	$1.8M
New Activity	$1.0M	$1.2M	$1.5M	$1.2M	$1.2M
Total	$2.5M	$3.0M	$3.5M	$3.0M	$3.0M

- Due to Grand Challenge close-out in mid FY2000, bridge funds needed for remainder of year
- Additional funding appropriate in FY2000 to augment core effort and bring new partners on board
  - smooth ramp-up to SSI-scale effort starting in FY2001