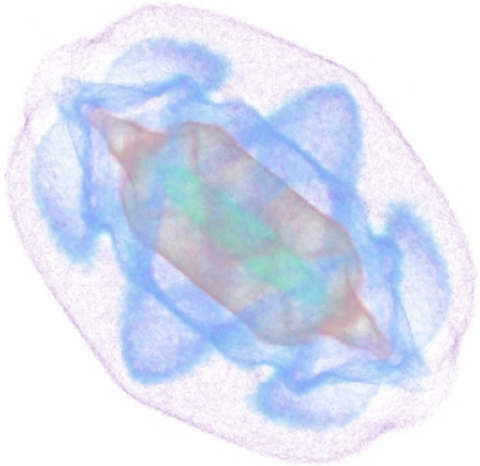
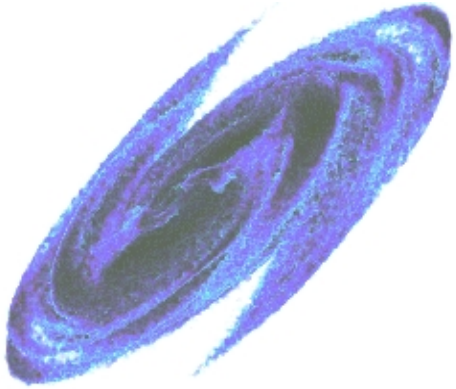
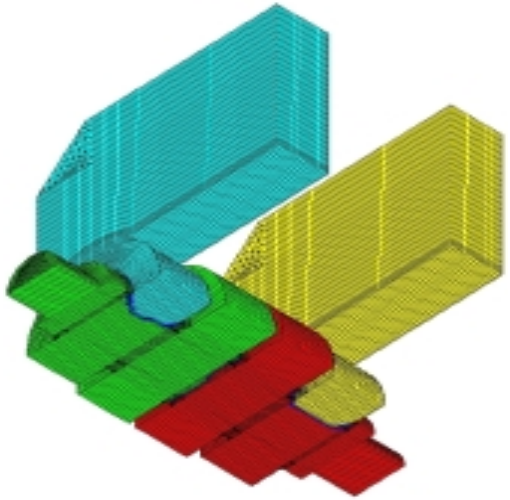
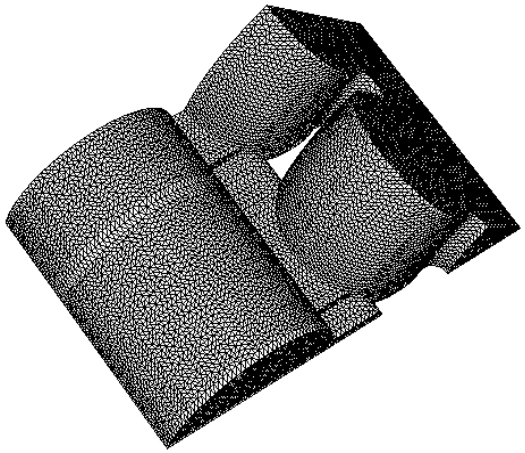
Large-Scale Simulation in the Computational Accelerator Physics Community: Current Activities and Future Plans





Robert D. Ryne





presented to the
High Energy Physics Advisory Panel
Gaithersburg, MD
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with contributions from

Accelerator Grand Challenge Team

R. Ryne[1], K. Ko[2],
J. Ahrens[8], T. Cleland[8], J. Cummings[8], V. Decyk[7], N. Folwell[2],
G. Golub[6], S. Habib[1], W. Humphrey[8],S. Karmesin[8], P. McCormick[8],
A. McPherson[8], E. Ng[9], J. Painter[8], J. Qiang[1], Z. Li[2], B. McCandless[2],
G. Mark[8], W. Mi[6], C.-K. Ng[2], M. Saparov[6], W. Saphir[9], Y. Sun[6], M. Wolf[2]

SSI Accelerator Proposal Team and Participants

R. Ryne[1], J. Irwin[2], K. Ko[2], S. Chattopadhyay[3],
C. Celata[3], P. Colestock[1], E. Esaray[3], S. Habib[1], W. Herrmannsfeldt[2], W. Humphrey[1],
A. Luccio[5], W. Mori[7], P. Spentzouris[4]

[1]Los Alamos National Laboratory
[2]Stanford Linear Accelerator Center
[3]Lawrence Berkeley National Laboratory
[4]Fermi National Accelerator Laboratory
[5]Brookhaven National Laboratory
[6]Stanford University
[7]University of California, Los Angeles
[8]Advanced Computing Laboratory
[9]National Energy Research Scientific Computing Center

Outline

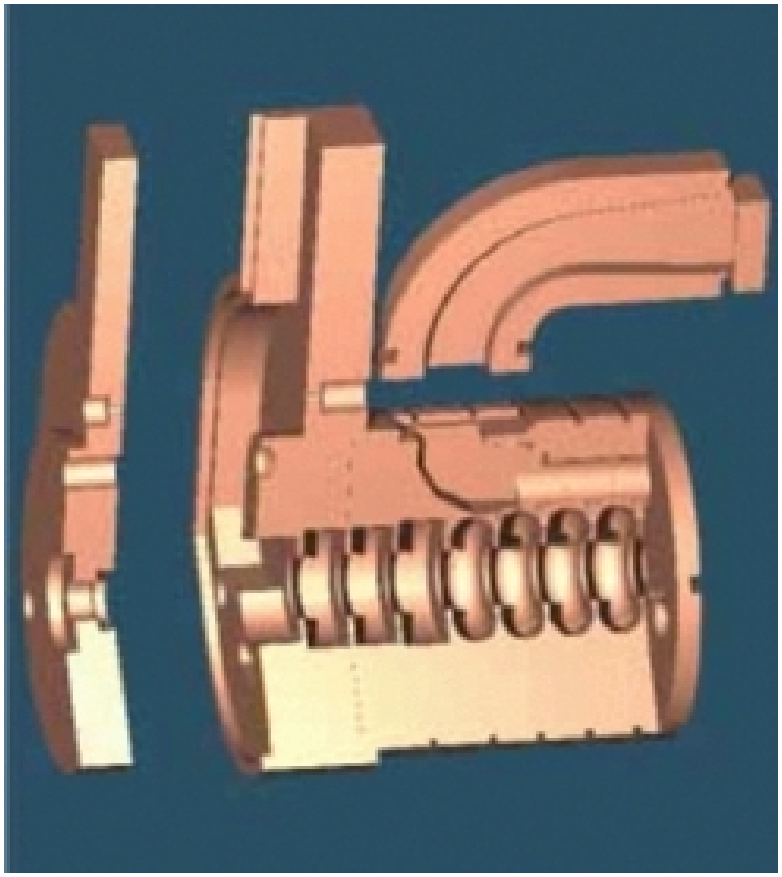
- Why is large-scale accelerator simulation important to future HEP activities?
- How is large-scale (i.e. *terascale*) computing different from ordinary computing?
- What has the accelerator community done in regard to large-scale simulation?
- What resources (e.g. computer time at NERSC and ACL) is the community likely to need?
- What sort of effort is being contemplated based on our pre-SSI activities?

Why is Large-Scale Accelerator Simulation Important to Future HEP and Office of Science Activities?

- Future accelerators : higher intensity, greater complexity, greater precision, new parameter regimes
  - NLC, μ-systems, hadron colliders, isotope accelerator, SNS, 4th generation light source
- Modeling on parallel computers essential for design decisions
  - evaluate/reduce risk
  - reduce cost
  - optimize performance
- Example problems:
  - designing ***large*** electromagnetic structures for NLC
  - high intensity transport + beam cooling in a μ-system

Example: Need for Large-Scale Electromagnetic Simulations

DDS for the NLC



- Cell Design for the NLC
  - frequency error of 1 part in 10,000.
  - mesh size close to fabrication tolerance (no tuning)

- Wakefield Analysis for NLC
  - needs full-section modeling (206 cells) to verify DDS scheme in suppressing emittance growth

10^6 to 10^9 degrees of freedom

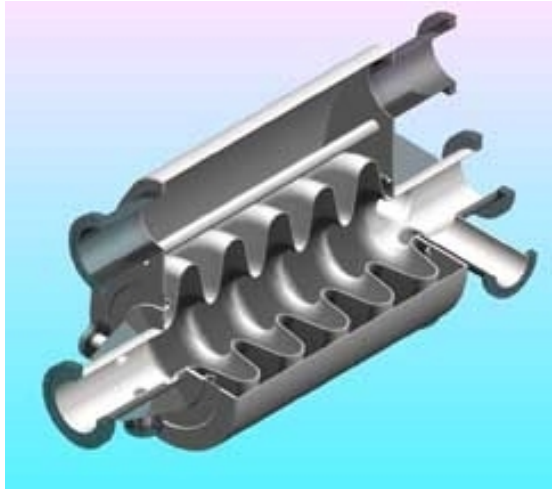
"High-Resolution" design, "System-Scale" analysis only possible on <u>very large scale</u> computers

Use of parallel codes for NLC/DDS design will result in improved designs and ***significant*** cost savings

Example: Need for Large-Scale Intense Beam Simulations

- Future high-average power-accelerators will have to operate with ultra-low losses
- Excess losses ⟶ radioactivation
  - degrade components
  - hinder/prevent hands on maintenance
  - reduce reliability and availability

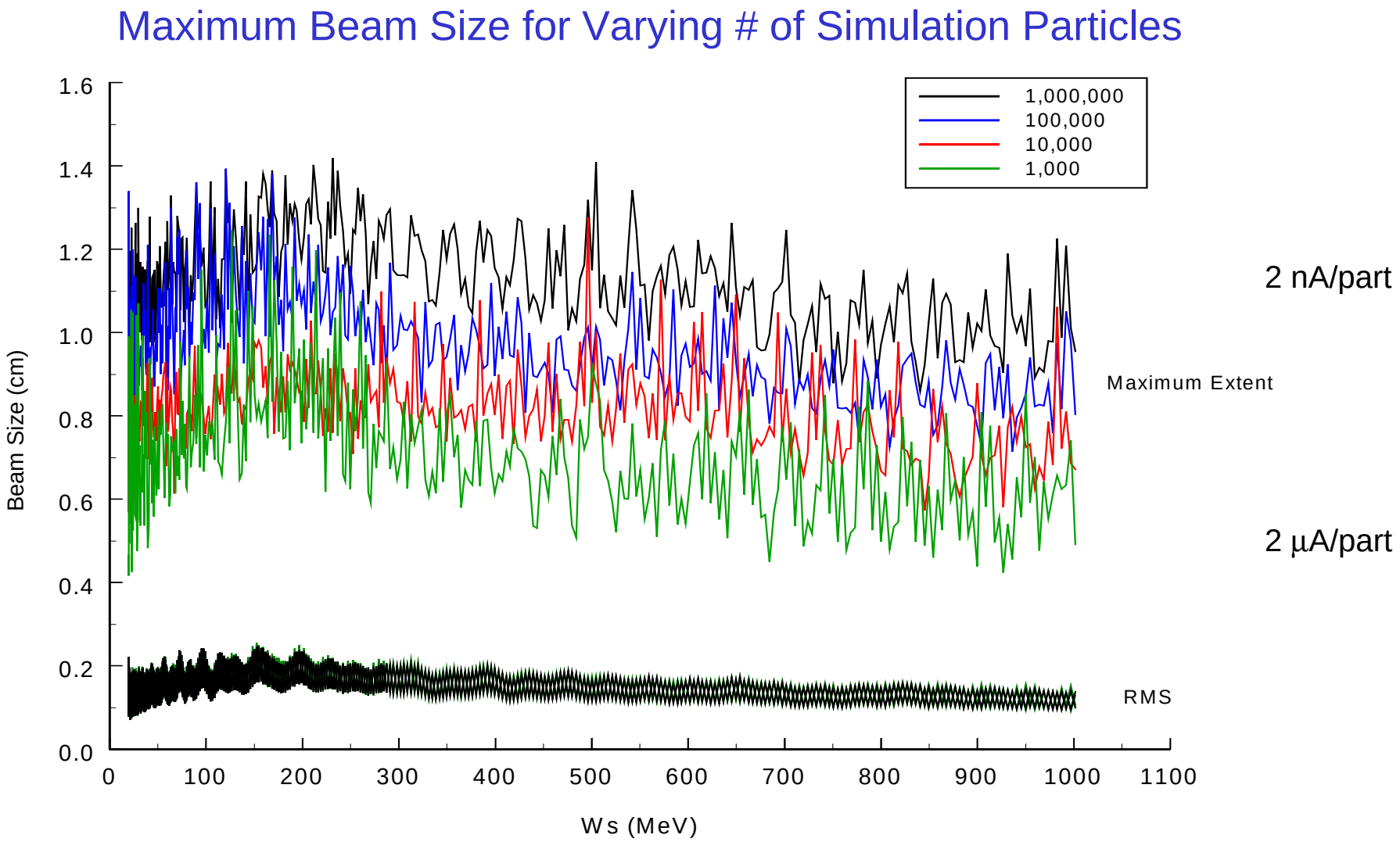
Allowed loss is ~ 0.1-1 nanoampere/meter @ 1GeV



- Major loss mechanism: large amplitude halo particles striking the beam pipe

High-Resolution modeling using 0.1-1 billion particles is needed to make quantitative predictions of beam halo

Large-Scale Simulations are Needed in order for Certain Calculated Quantities to Converge



Benefits of Large Scale Simulation to Accelerator Science and Technology

- ***Tool of discovery*** to explore beams in novel configurations and under extreme conditions
  - plasma accelerators w/ gradients ~ 1-100 GeV/m
  - cooling for muon-based neutrino sources and colliders
  - stripping/separation/reacceleration for production of isotopes

- Large-scale simulation, coupled with theory and experiment, will help advance the frontiers of accelerator technology and lead to major discoveries in beam-driven science.

How is Large-Scale Computing Different from Ordinary Computing?

Architecture:

- Clusters of Symmetric Multiprocessors (SMP's)
  - Deep memory hierarchies
- PC clusters
  - Gaining popularity due to falling cost of networking hardware
  - Ideal for loosely coupled problems
  - Even cost effective for medium-scale tightly coupled problems

SGI Origin 2000 at ACL
IBM SP at NERSC

Programming:

- Complex issues associated w/ programming parallel computers, major differences compared with vector machines
  - *communication, cache*

Complexity & Scale:

- Highly three-dimensional
- 100's of millions of particles and grid points ⟶ data handling

DOE Grand Challenge in Computational Accelerator Physics

Institutions:

- LANL, 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

Status: *"Parallel Computing Works"*

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

- Electromagnetics:
  - New 3D parallel eigenmode code, Omega3P, used to model problems with 10's of millions of degrees of freedom
  - Tau3P: New parallel 3D time-domain electromagnetics code
  - developed by Numerical Modeling Group at SLAC (K. Ko)
- Beam Dynamics:
  - New 3D parallel beam dynamics code, IMPACT, used to perform simulations with up to 800M particles
  - developed at LANL/LANSCE (R. Ryne)
- Codes applied to NLC, PEP-II, SNS, APT, ALS

Brief Tour of Parallel Accelerator Simulations

- Omega3P: NLC cavity design, PEP-II modeling
- Ion Tracking: Parallel particle tracking for NLC
- IMPACT: Intense beam dynamics

<u>Preamble:</u>
What is needed to successfully develop large-scale parallel applications codes?

Development of large-scale parallel applications involves the integration of many pieces

Electromagnetics

- Parametric Geometry - CAD models to facilitate optimization
- Mesh Generation - impacts matrix conditioning/time-stepping
- Adaptive Refinement - improve accuracy/optimize resources

Beam Dynamics

- Frameworks - accelerator system geometry, models of beamline elements,...
- Transfer Map Methods -Symplectic maps corresponding to beamline elements
- Particle Managers - to minimize communication in parallel PIC codes

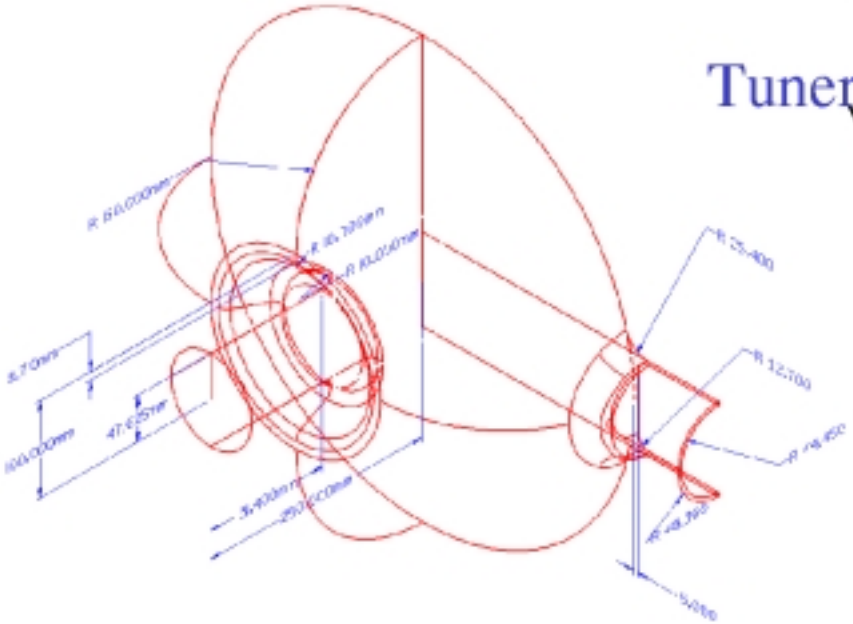
Both

- Parallel Solvers - scalable algorithms with fast convergence
- Domain Decomposition - partitioning tools for load balancing
- Visualization - efficient post-processing of large data sets; feature extraction and scientific discovery in simulation results
- Performance/Error Analysis - computer science/applied math

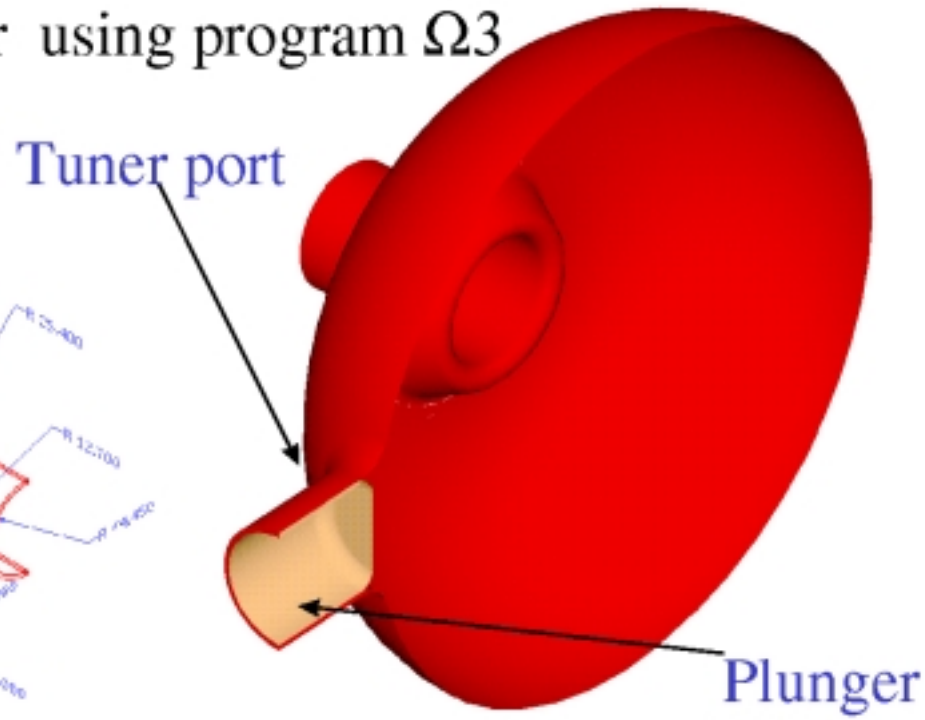
Success depends on integrating the combined efforts of a multi-disciplinary team including physicists, applied mathematicians, statisticians, computer scientists, software engineers, geometry builders, visualization experts,...

Parameterized solid model

– Analyze cavity with tuner using program Ω3



Engineering drawing

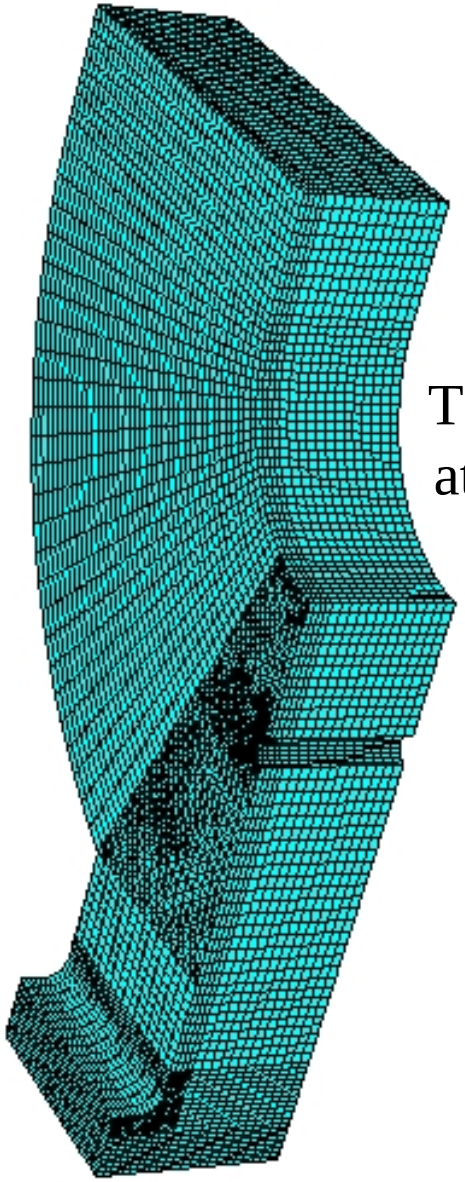


Parametric Solid model

- Interface to a variational solid modeler EMS/Intergraph
- Can resolve necessary features (e.g., small distance between the tuner port and the plunger)
- Easy to change plunger position

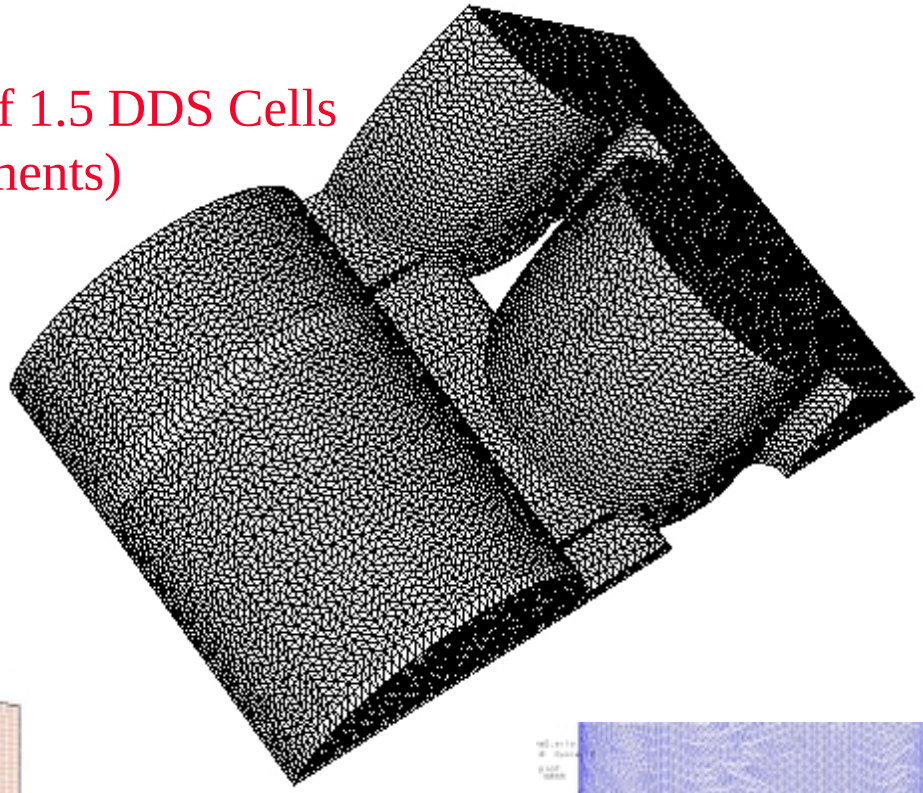
Mesh Generation for Omega3P and Tau3P Simulations

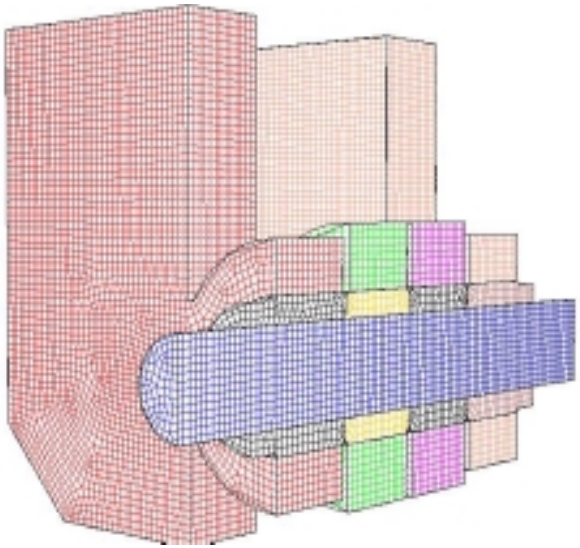
Size of meshes limited by workstation memory - <u>Parallel Mesh Generation</u>



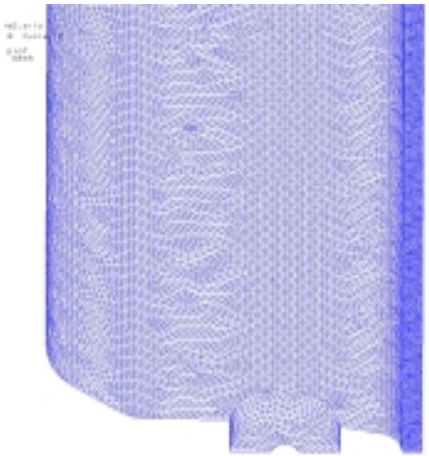
T-Junction
at X-Band

One octant of 1.5 DDS Cells
(500,000 elements)





Input Coupler for NLC



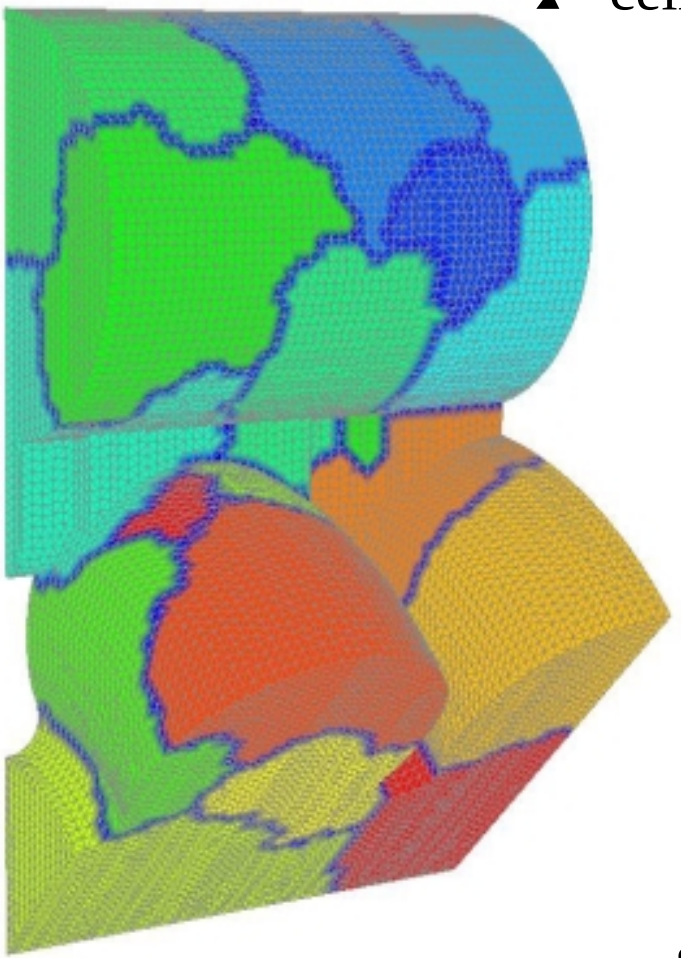
RFQ Cavity for SNS

Domain Decomposition

Partitioning to optimize load balance & minimize communication

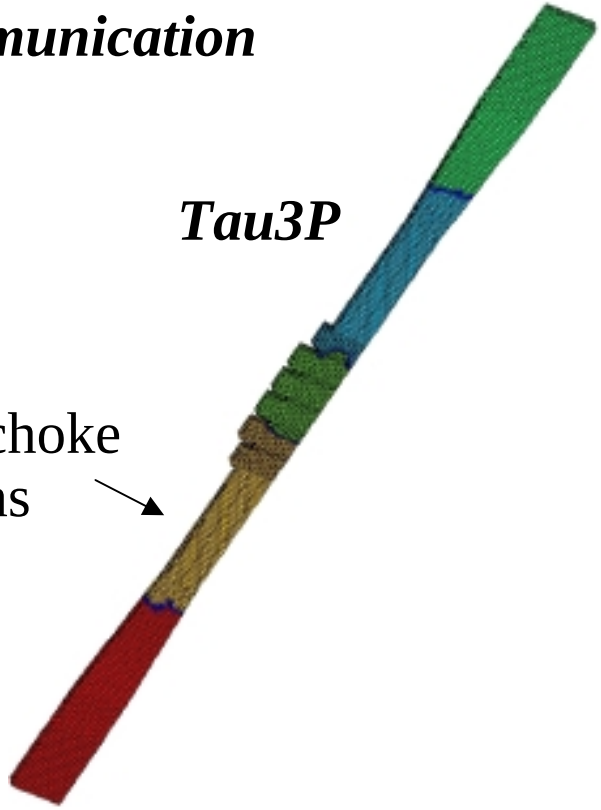
Omega3P

Octant of 1.5 DDS cells in 16 domains

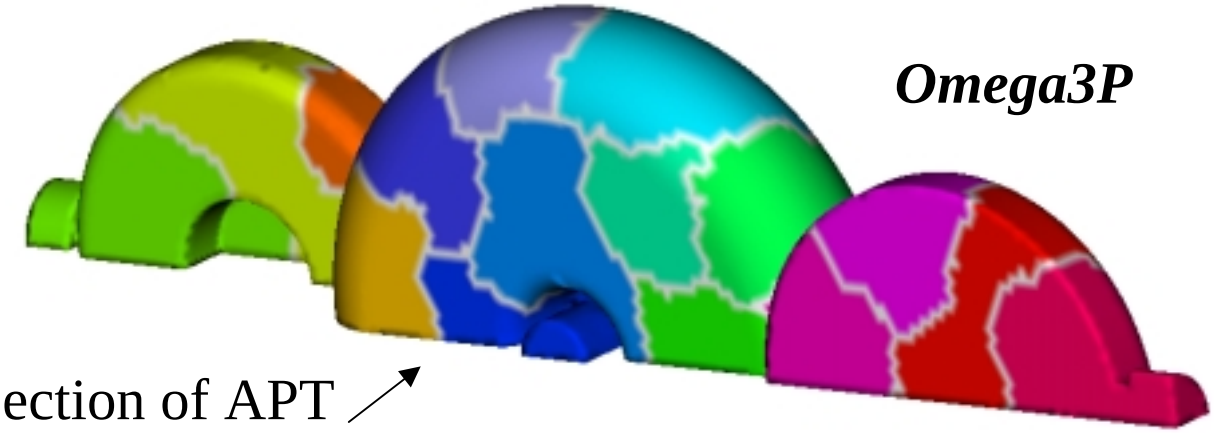


Tau3P

Quarter of RF choke in 4 domains



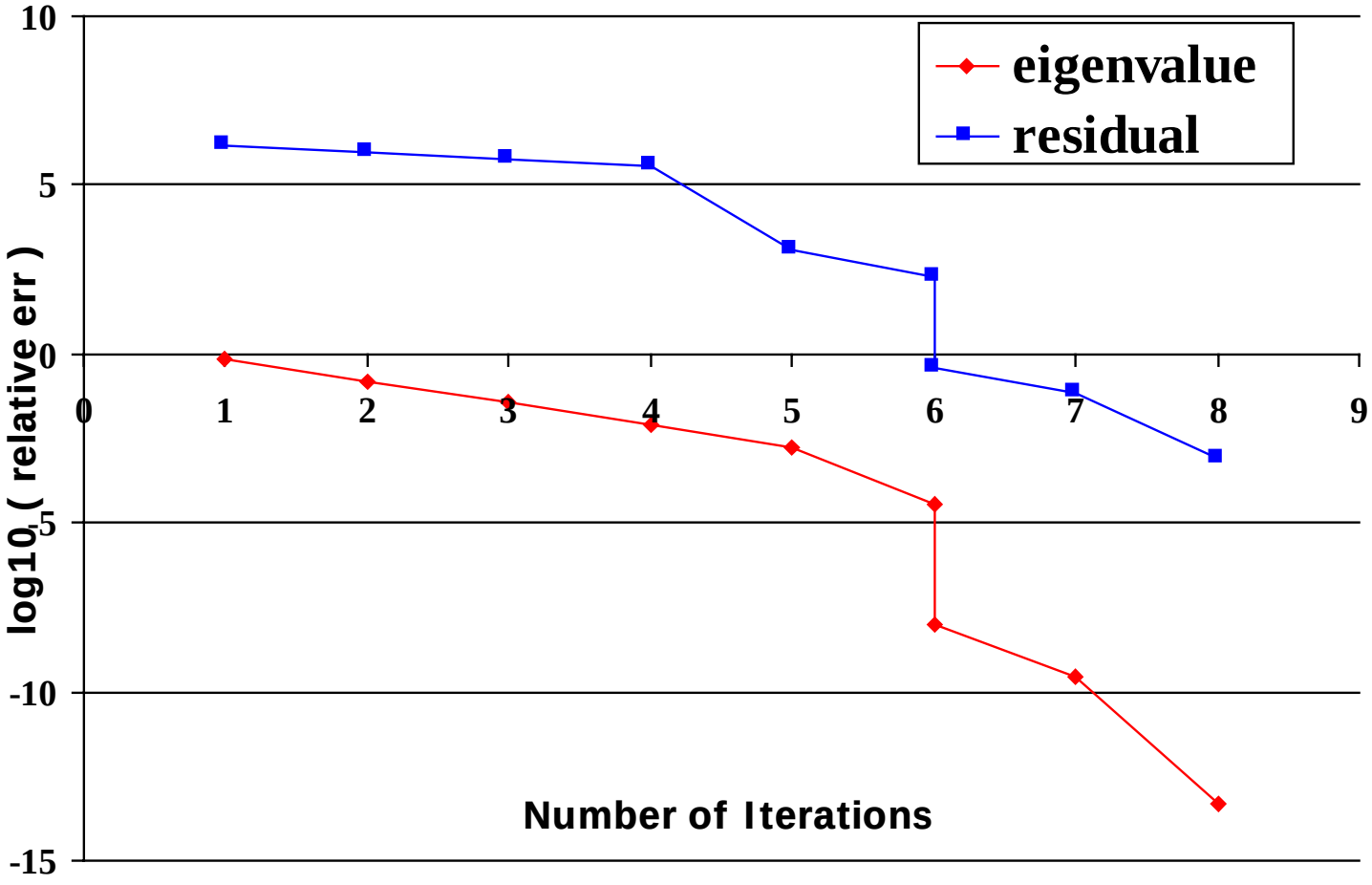
Omega3P



Section of APT side-coupled linac

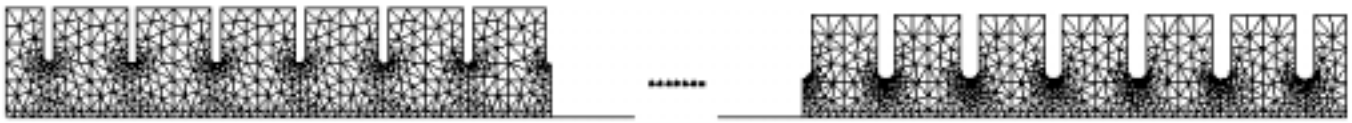
Parallel Fields Solver

Omega3P *convergence on DDS example with 500K DOF's*

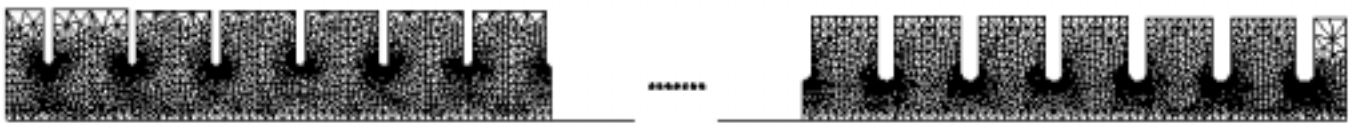


Simulation Results for NLC Detuned Structure

- initial mesh:



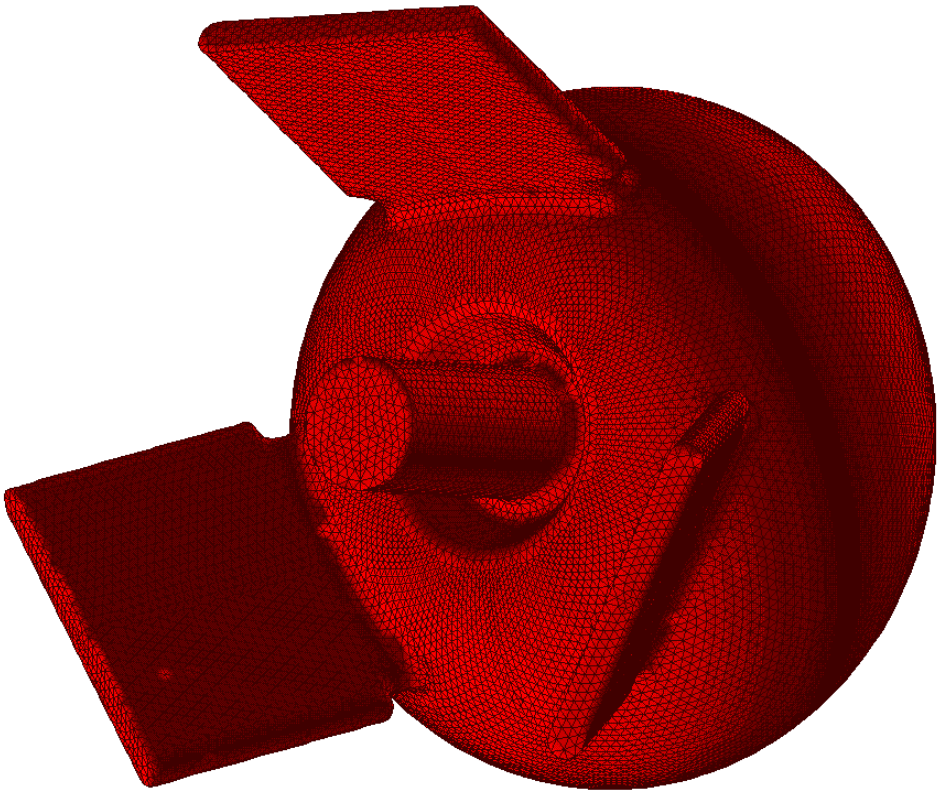
- adaptive refinement:



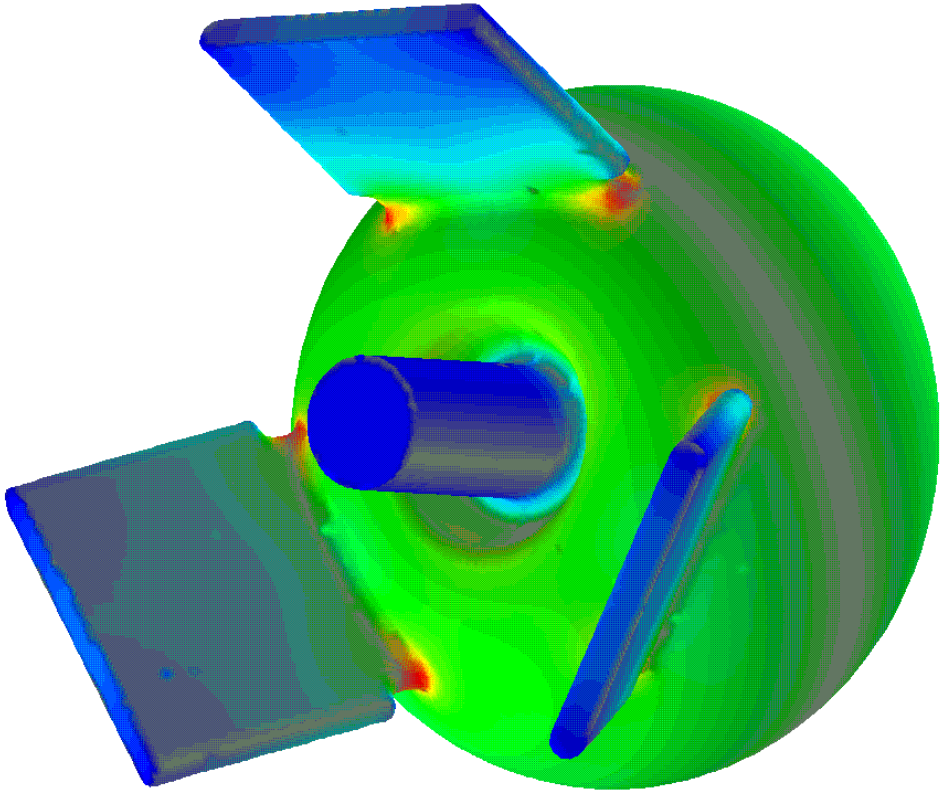
Mesh level	DOF	Solution time	Memory
0	227,769	25 minutes	4.0 GB
1	651,194	98 minutes	6.2 GB

(30)

Example: PEP-II Cavity Simulation

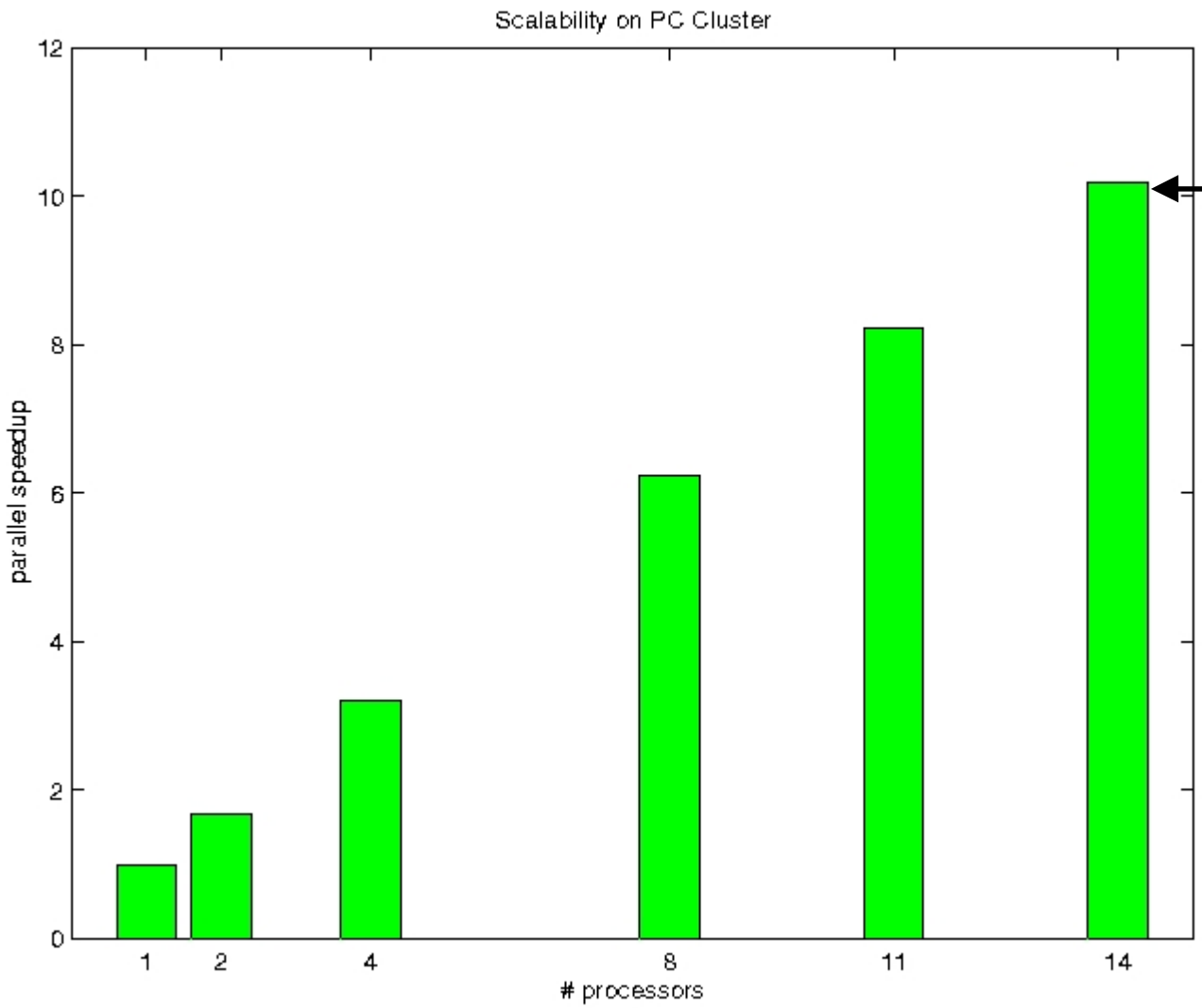


Computational Mesh



Wall Loss

Scaling of Ion Tracking Code on SLAC PC Cluster



3-hour single processor job requires 18 min on 14 processors

10x speedup with 72% parallel efficiency

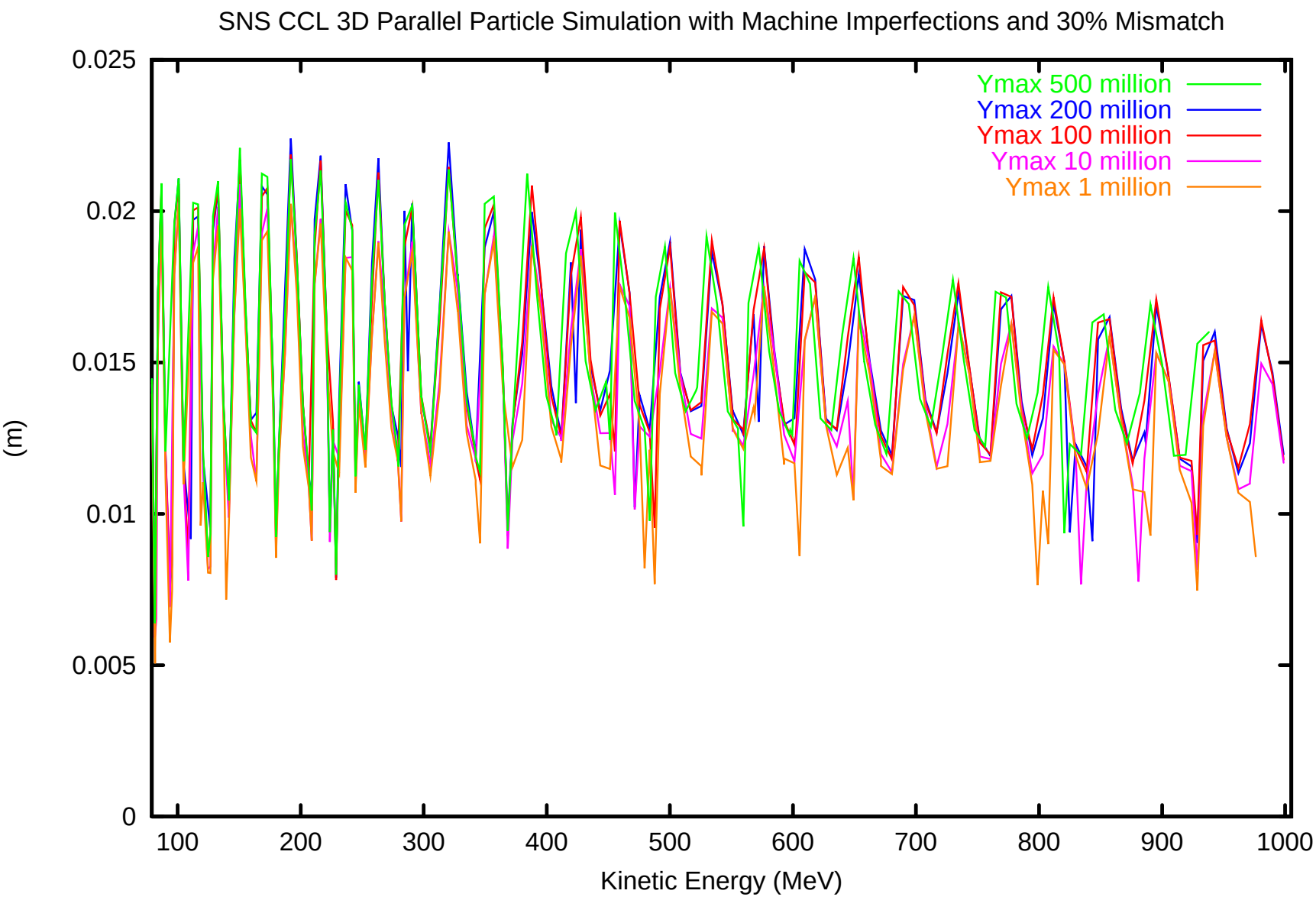
Large-Scale Beam Dynamics Simulations using IMPACT

- 100M particle simulations require ~5 hours on 256 processors
- Simulations have been performed with 800M particles
  - Approaching real-world number of particles (900M for SNS)

Compare:

- 1M particle, 2D simulation using legacy code on a PC: weekend
- 100M particle, 3D IMPACT simulation on 256 processors : 5 hrs

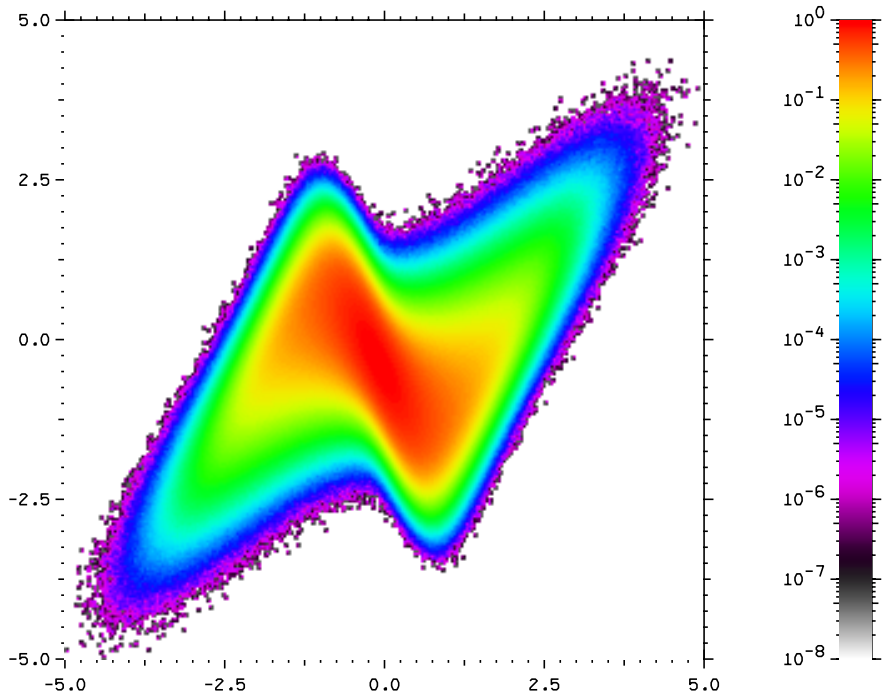
- Parallel simulation is 100x larger and requires 1/10 the time
- Parallel computing results in a ***3 order-of-magnitude*** increase in simulation capability



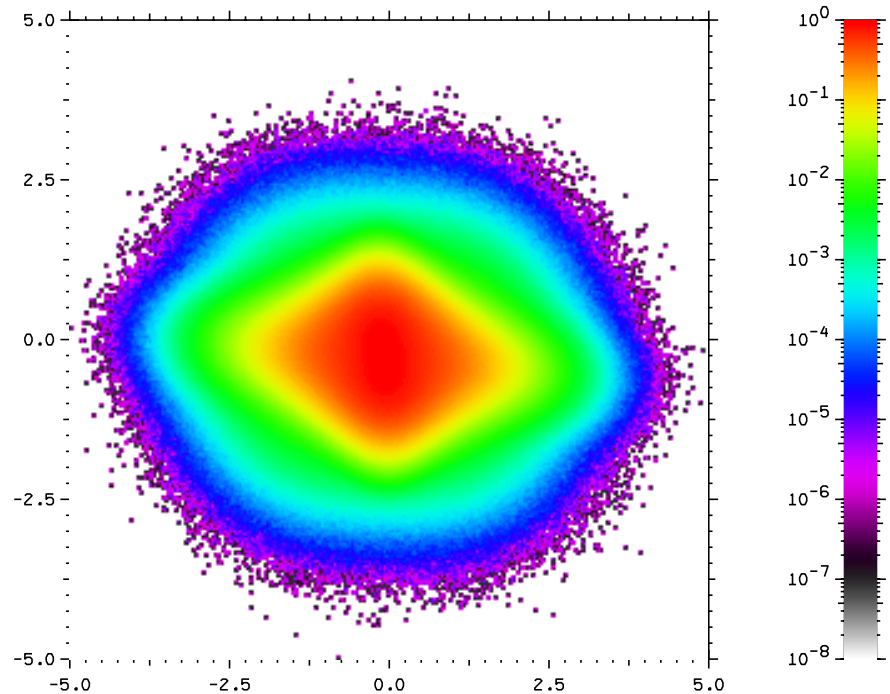
Maximum particle amplitude with varying # of simulation particles, run on the ACL Nirvana system using 32-1024 processors

Plots of "Integrated Density" from a 500 million particle linac simulation

X-P_X Plot



X-Y Plot



Major NERSC Allocations for Accelerator Science by Year

- FY99: 180K processor-hours
- FY00: 532K processor-hours
- FY01: ???

Large-Scale Accel. Simulation Efforts at NERSC in FY00

"Computational Accelerator Physics Grand Challenge"

Robert Ryne (LANL) and Kwok Ko (SLAC) [200K hours]

Involves NERSC and ACL

"Continuing Studies of Plasma Beat Wave Accelerators"

Warren Mori (UCLA)

Reached "class A" status at NERSC for FY00 [250K hours]

"Simulation of Advanced Acceleration Techniques and Applications"

Eric Esarey/N. Birdsall (LBNL/UCB) [52K hours]

"Effects of CSR on Accelerator Performance"

Rui Li (TJNAF) [30K hours]

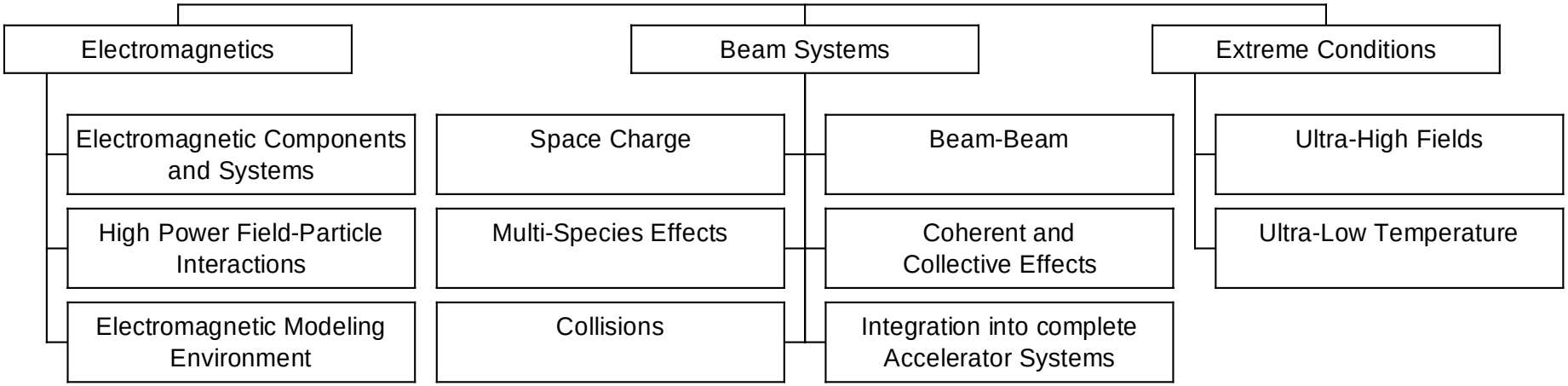
List of NERSC Class A Awards in FY00

PI	# req	Office	Science	MPP hrs
Cohen	1	FES	fusion	650,000
Olson	1	HENP	nuclear	210,000
Joshi	1	HENP	accel.	250,000
Washington	1	BER	envir.	375,000
Sinclair	3	HENP	hep	115,000
Jardin	9	FES	fusion	231,500
Stocks	1	BES	matsci	325,000
Liu	1	HENP	nuclear	51,000
Soni	1	HENP	hep	240,000
Wehner	4	BER	envir.	96,200
Bell	1	ASCR	app math	175,000
Schnack	2	FES	fusion	192,000
Ryne	1	HENP	accel.	200,000
Gupta	1	HENP	hep	120,000
				3,230,700

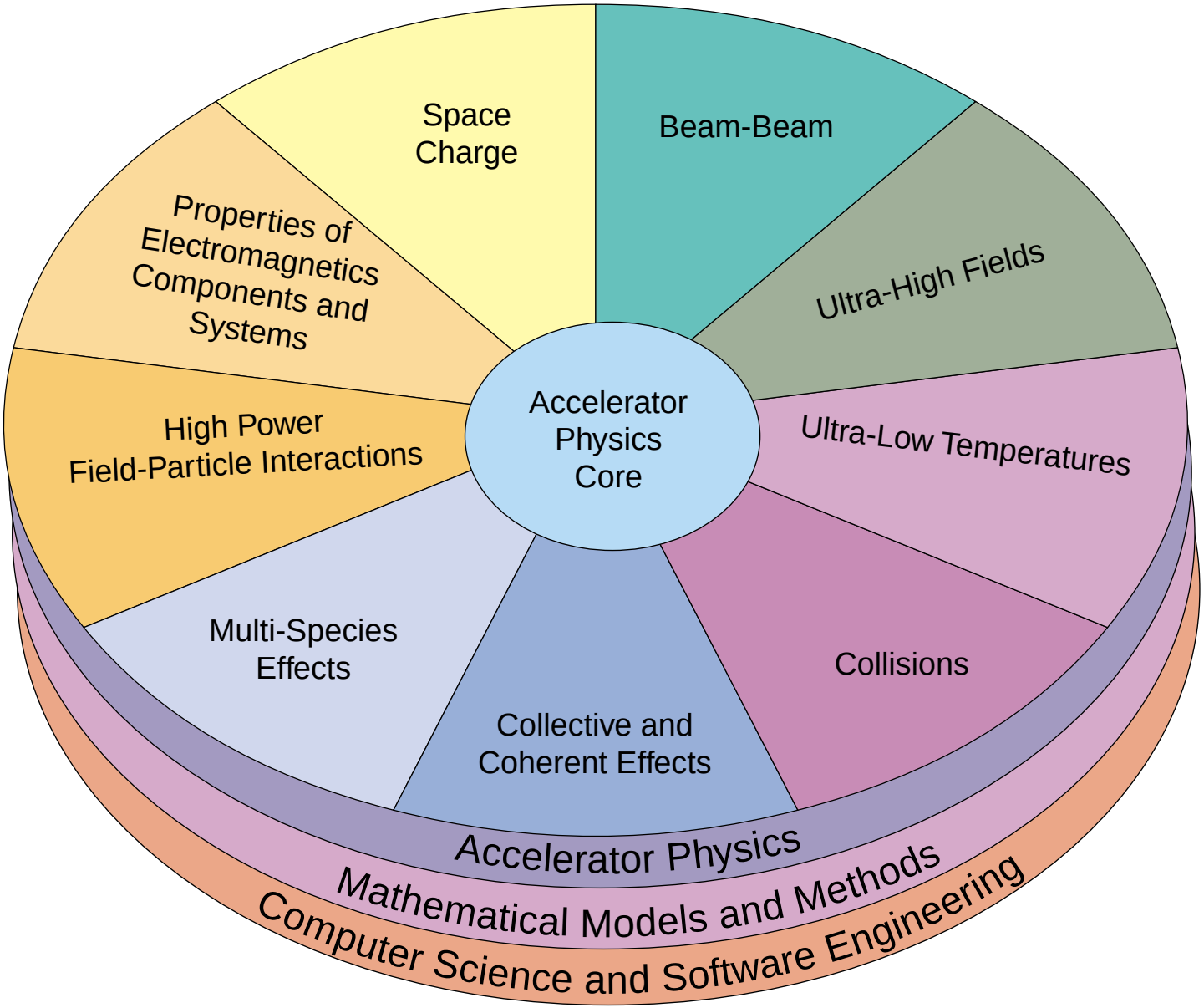
Where Do We Go From Here, as a Community?

- Pre-SSI activity initiated a multi-lab dialogue
- Identified 3 major focus areas:
  - Electromagnetics, Beam Systems, Extreme Conditions
- Recognized interdisciplinary nature
  - Accelerator Physics, Mathematical Models and Methods, Computer Science and Software Engineering
- Identified four 1st year topics
  - Damped Detuned Structure
  - Muon cooling system
  - Strong-strong beam-beam interaction
  - e-p instability in high-current rings
- Developed strong laboratory support
  - LANL/SLAC/LBNL/FNAL/BNL committee

Organization of Accelerator Physics Topics



Graphical depiction of proposed SSI effort, including Accelerator Physics topics



What is Needed to Meet the Challenges in HEP Accelerator Design over the Next 5 Years?

- Important HEP accelerator projects
  - **e^+e^- linear collider**
  - **muon collider/neutrino factory**
  - very large hadron collider
  - advanced accelerator research
- $3M/yr will support a healthy program in all these areas
- $1.5 M/yr would support a minimal effort aimed at
  - cost reduction in NLC
  - feasibility analysis in muon/neutrino systems
  - small simulation efforts for VLHC and adv. acc. research
- Note: Grand Challenge funding is ~ $1M/yr ($500K + leverage)

Summary

- Large-scale simulation is important to HEP accelerator projects
- The computational accelerator physics community
  - has a strong record of accomplishments in large-scale simulation
  - has a strong presence in the computational science community (major collaborators with NERSC and ACL)
- Large-scale accelerator simulation is already being supported jointly by HENP and MICS
  - The success of the Accelerator Grand Challenges makes a larger, multi-lab effort in Accelerator Simulation a strong candidate if DOE participates in IT^2 in the future.