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SciDAC-3

ComPASS

Advanced Computation for HEP Accelerator Science and Technology

Panagiotis Spentzouris (Fermilab)
for the ComPASS collaboration

Argonne National Laboratory
Berkeley Lab
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Accelerators for America's Future

Particle accelerators enable discovery in basic research and applied sciences

- Probing fundamental laws of nature, discovering new particles
- Studying properties of nuclear matter
- Studying structure of crystals, amorphous materials, and organic matter
- Enhancing quality of life: medical treatment, nuclear waste transmutation, industrial applications

COURTESY OAK RIDGE NATIONAL LABORATORY.

Numerical modeling and simulation are essential for the development of new acceleration concepts and technologies and for machine design, optimization and successful operation

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Accelerators for High Energy Physics

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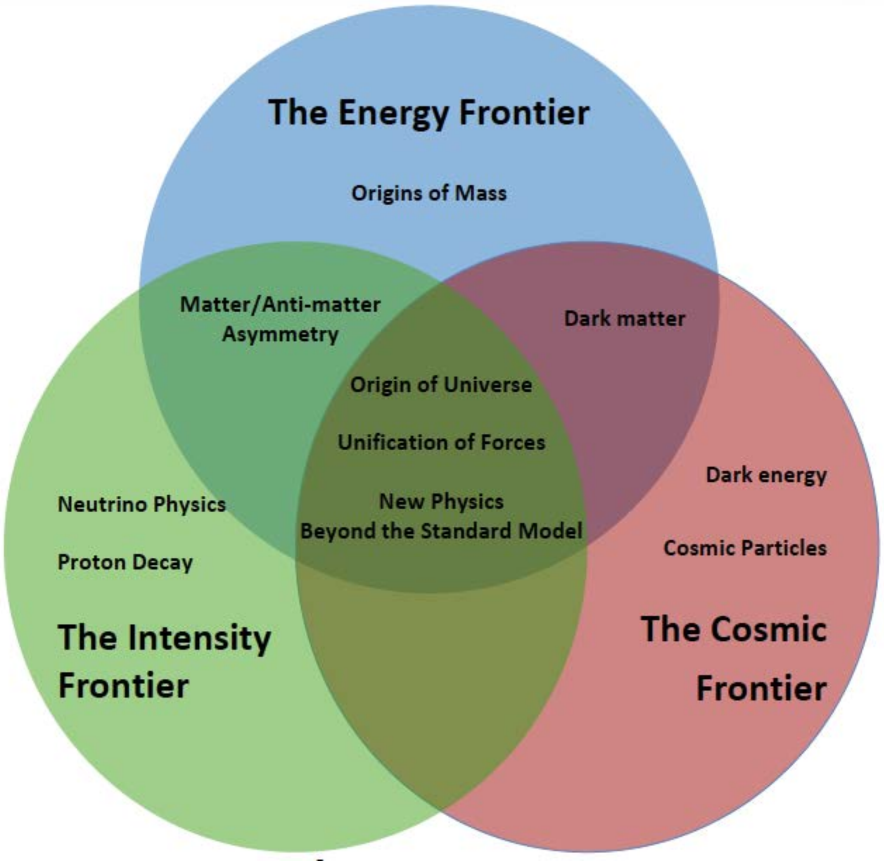
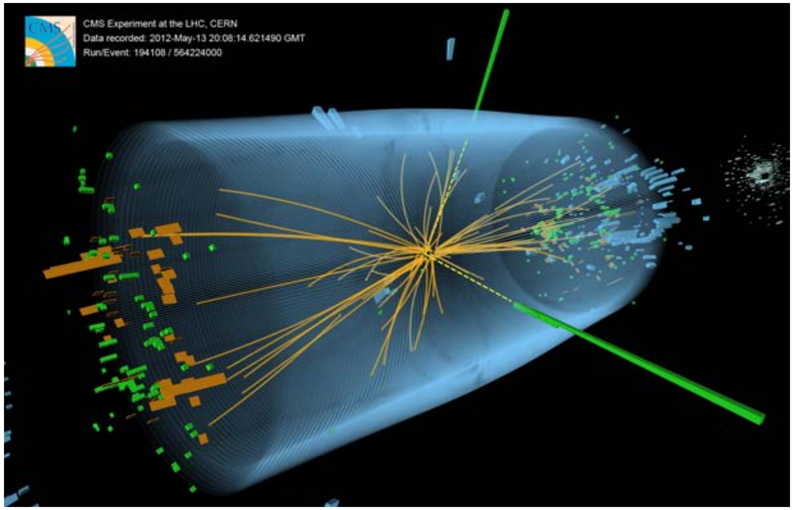
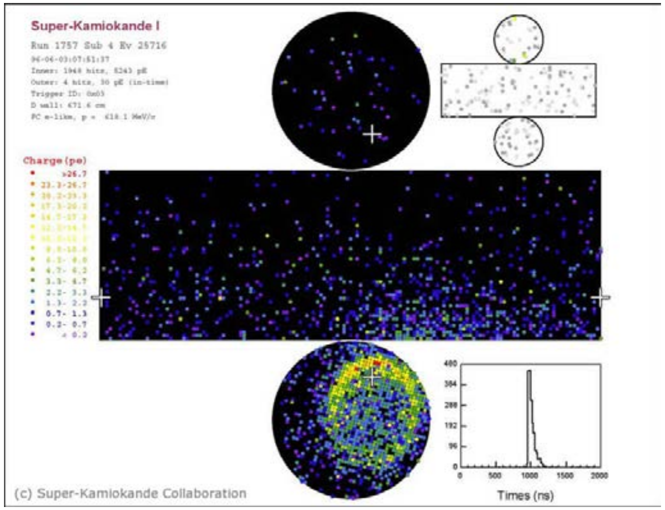
- At the Energy Frontier, high-energy particle beam collisions seek to uncover new phenomena
  - the origin of mass, the nature of dark matter, extra dimensions of space.
- At the Intensity Frontier, high-flux beams enable exploration of
  - neutrino interactions, to answer questions about the origins of the universe, matter-antimatter asymmetry, force unification.
  - rare processes, to open a doorway to realms to ultra-high energies, close to the unification scale
- Particle accelerators indirectly support the cosmic frontier by providing measurements of relevant physics processes



Where we are today

- Discovery of the Higgs particle, responsible for electroweak symmetry breaking and the mass of elementary particles
  - No physics beyond the “Standard Model” (SM) of HEP has been observed
- Neutrinos oscillate, thus have mass
  - No answers on mass hierarchy or symmetry properties





Where we would like to be (Energy Frontier)

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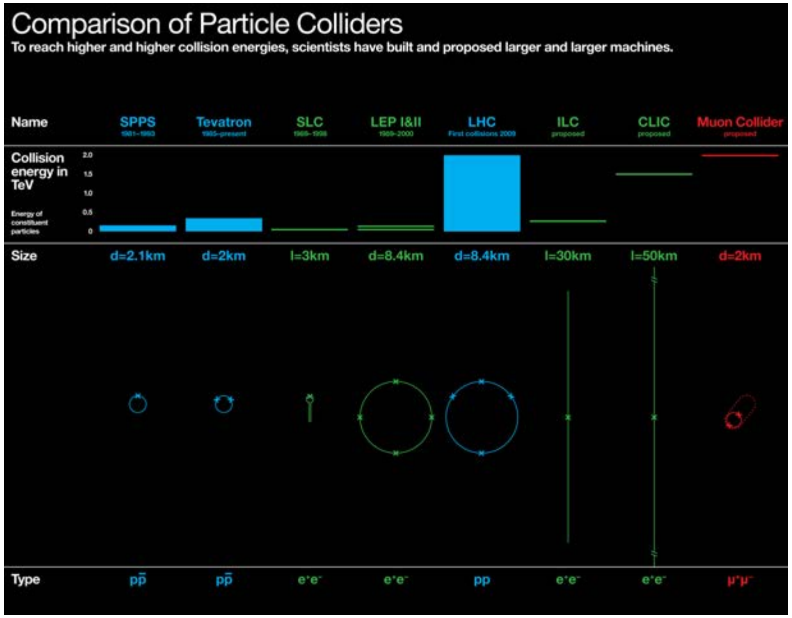
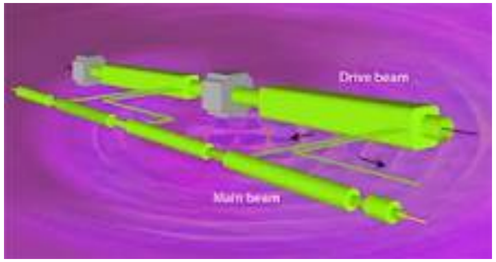
- A dedicated accelerator will be necessary to study Higgs properties
  - Is it a "Standard Model" Higgs?
- "Higgs Factory" candidate: lepton collider
- A great challenge for accelerator science!
  - Develop techniques, technologies and materials to achieve higher acceleration gradients
    - dielectric and plasma wave structures, beam cooling
  - Optimize existing technologies
    - Superconducting rf cavities
  - Optimize and test designs
    - CLIC, Muon Collider





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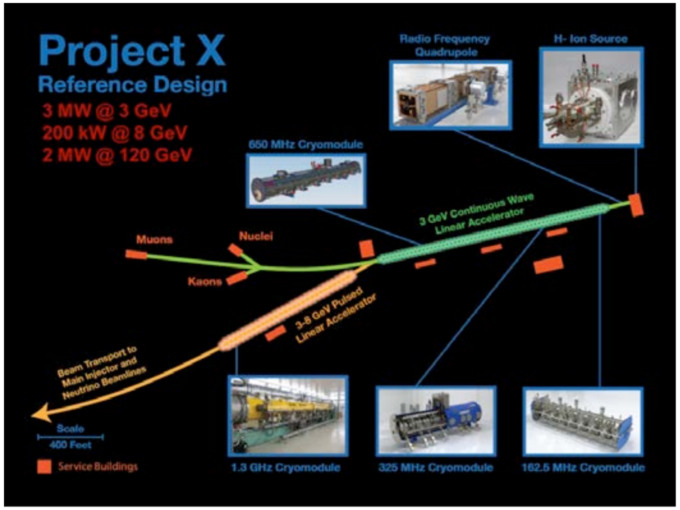
Where we would like to be (Intensity Frontier)

- A high-intensity proton accelerator to drive
  - long-baseline neutrino oscillation experiments
    - Mass hierarchy, matter-antimatter asymmetry, oscillation parameters
  - muon, kaon experiments
    - Physics beyond the SM
- Staged approach at Fermilab
  - Improvements of existing machines
  - New linear accelerator: Project-X
- A great challenge for accelerator science!
  - Controlling instabilities to minimize beam losses is essential
    - Self-fields, wakefields, interaction with materials, geometry and long term tracking accuracy



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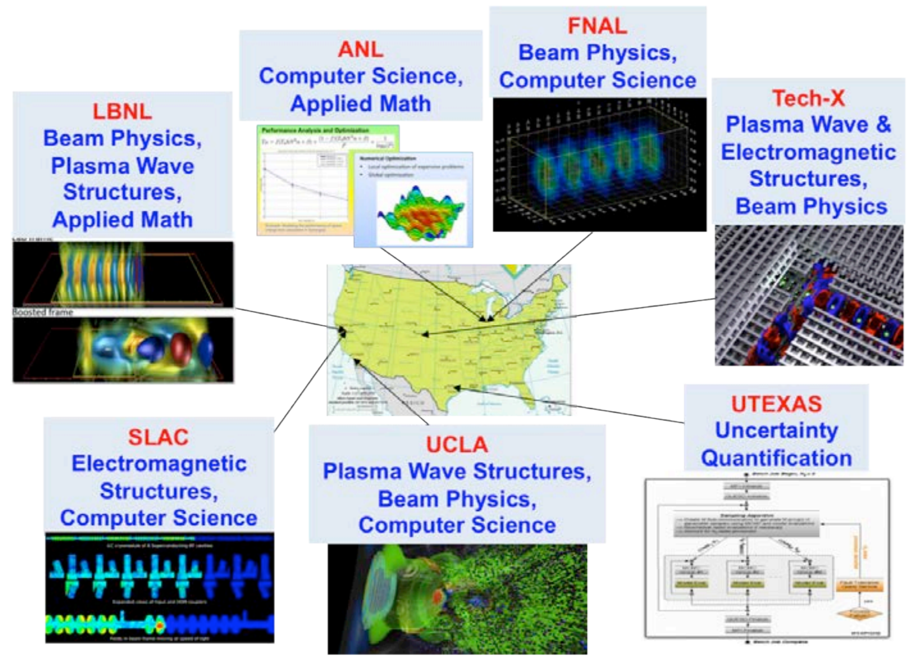
Advanced Computation for HEP Accelerator Science and Technology

- To enable scientific discovery in HEP, high-fidelity simulations are necessary to develop new designs, concepts and technologies for particle accelerators
- Under SciDAC3, ComPASS will develop and deploy state-of-the-art accelerator modeling tools that utilize
  - the most advanced algorithms on the latest most powerful supercomputers
  - cutting-edge non-linear parameter optimization and uncertainty quantification methods.

The ComPASS collaboration



Community Project for Accelerator Science and Simulation (ComPASS)

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ComPASS SciDAC3 applications

- Support the development and study of new technologies for smaller and possibly cheaper energy frontier accelerators:
  - accelerators based on standard technology are limited by the metallic electrical breakdown limit of 50-100 MV/m
  - dielectric laser accelerators: a laser propagating through a dielectric lattice can generate electric fields of few GV/m
  - plasma based acceleration: a driver beam (laser/particles) propagating through a plasma creates a wake with accelerating gradients exceeding 50 GV/m.
- Focus on plasma and dielectric R&D and optimization of conventional technology applications

- Support the design and optimization of high-intensity proton accelerators to minimize beam losses that cause radiation damage. Modeling of
  - many (all) beam bunches in circular machines and their coupling through impedance and wakefields
  - beam self-charge and instabilities caused by beam-matter interactions
  - field non-linearities and accelerator geometry
- Focus on Fermilab existing proton source improvements and Project-X

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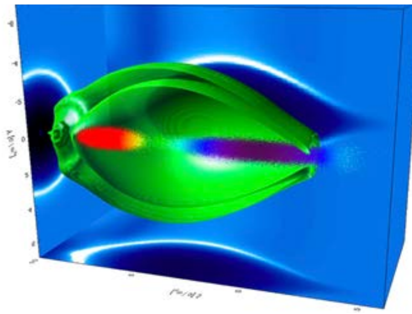
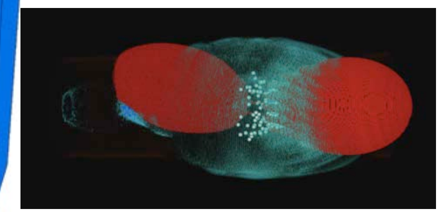
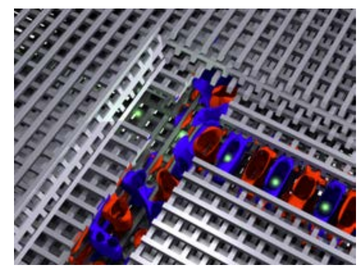
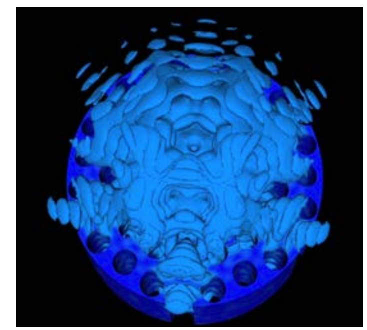
Energy Frontier Applications

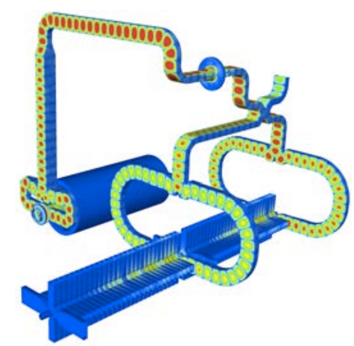
- Plasma-based acceleration:
  - support the BELLA (laser) and FACET (beam) experimental programs
  - develop techniques to improve beam quality
  - study controlled electron beam injection
  - improve staging for future lepton collider concepts.
- Dielectric laser acceleration:
  - design efficient power couplers between optical fiber and accelerator structure
  - explore wakefield effects and associated break-ups for different topologies
  - design structures able to accelerate high quality beams
- High Gradient acceleration:
  - understand wakefields in the Power Extraction and Transfer Structure (PETS) system of CLIC











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Intensity Frontier Applications

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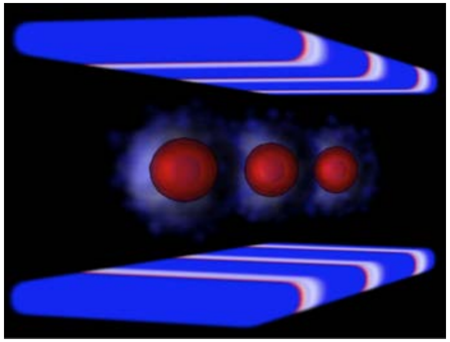
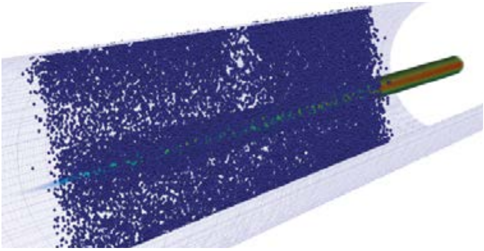
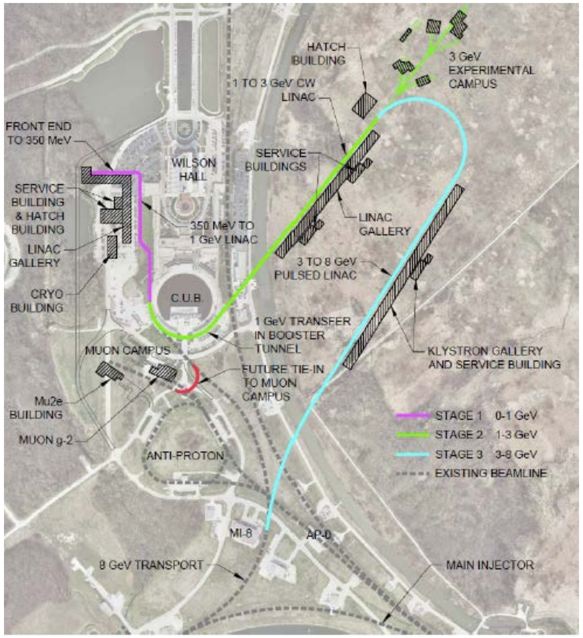
- Fermilab proton source upgrades for the Neutrino and Muon Programs
  - Booster synchrotron: instability control for beam quality and loss minimization (targeting 50% increase of beam flux)
  - Main Injector (MI) synchrotron: instability mitigation and loss minimization (targeting 100% increase of beam flux)
- Project-X: support staging
  - Study wakefields for the first stage of the linac
  - Model experiments of electron-cloud effects in the MI, currently underway
  - Study mitigation techniques to control losses in MI due to self-fields, wakefields, and electron-clouds







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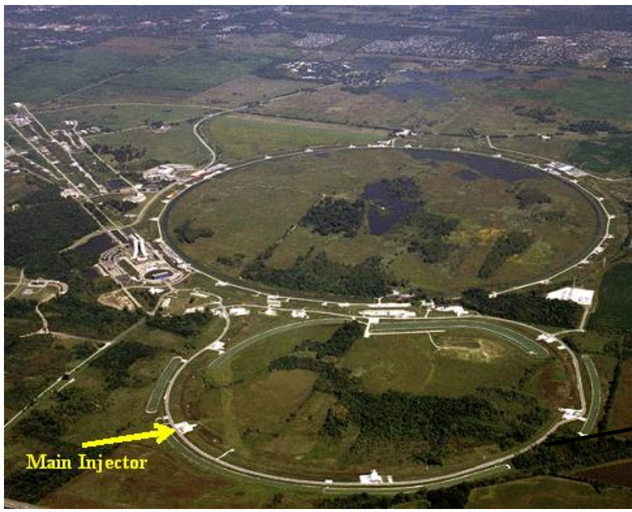
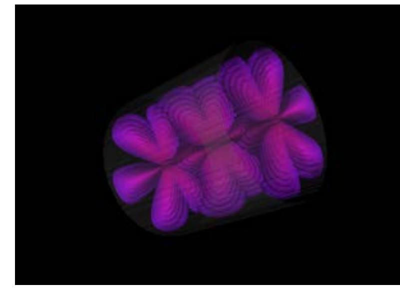
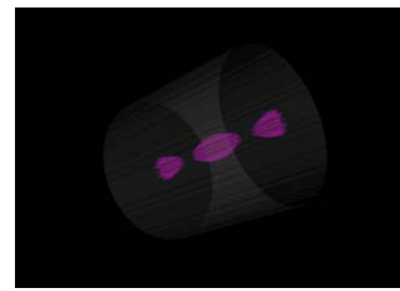
Accelerator applications span a wide range of physics and scales







- Wide range of scales:
  - accelerator complex (10^3m) → EM wavelength (10^2-10 m) → component (10-1 m) → particle bunch (10^{-3} m) → beam in plasma wakefields (10^{-8})
- Advancing accelerator science requires development of a wide range of mathematical models and numerical algorithms!

ComPASS Methods and Tools

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- We are developing a comprehensive set of codes that incorporate state-of-the-art field solvers
  - Electrostatic: multigrid (*Synergia*, *Warp*-FastMATH); AMR multigrid (*Warp*-FastMATH)
  - Electrostatic: spectral (*Synergia*)
  - Electromagnetic: finite element direct and hybrid (*ACE3P*-FastMATH)
  - Electromagnetic: extended stencil finite-difference (*Osiris*, *Vorpal, Warp*-FastTMATH); AMR finite-difference (*Warp*-FastMATH)
  - Quasi-static: spectral (*QuickPIC*)
- Collaboration with SciDAC Institutes
  - FastMATH: Particle in Cell techniques, field solvers (Chombo); linear algebra solvers (SuperLU) and eigensolvers
  - QUEST: statistical calibrations and quantitative ranking of models for plasma applications (QUESO)
  - SDAV: visualization (ParaView, VisIt), indexing (FastBit); domain customized applications*
  - SUPER: performance analysis & optimization, non-linear parameter optimization.

ComPASS toolkit: ACE3P, Osiris, QuickPIC, Synergia, Vorpal, Warp

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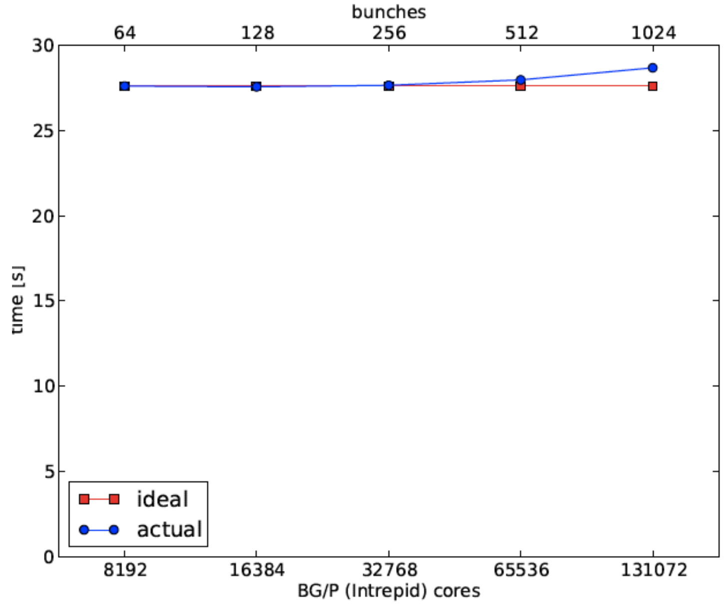
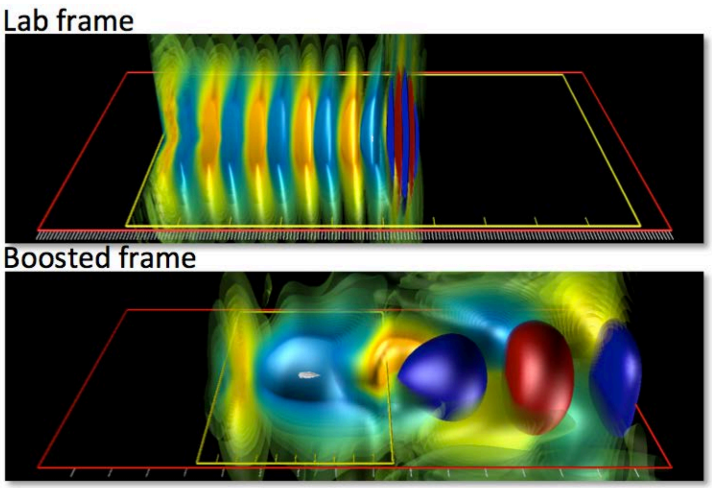
ComPASS collaboration building on tools, expertise and partnerships developed under SciDAC2

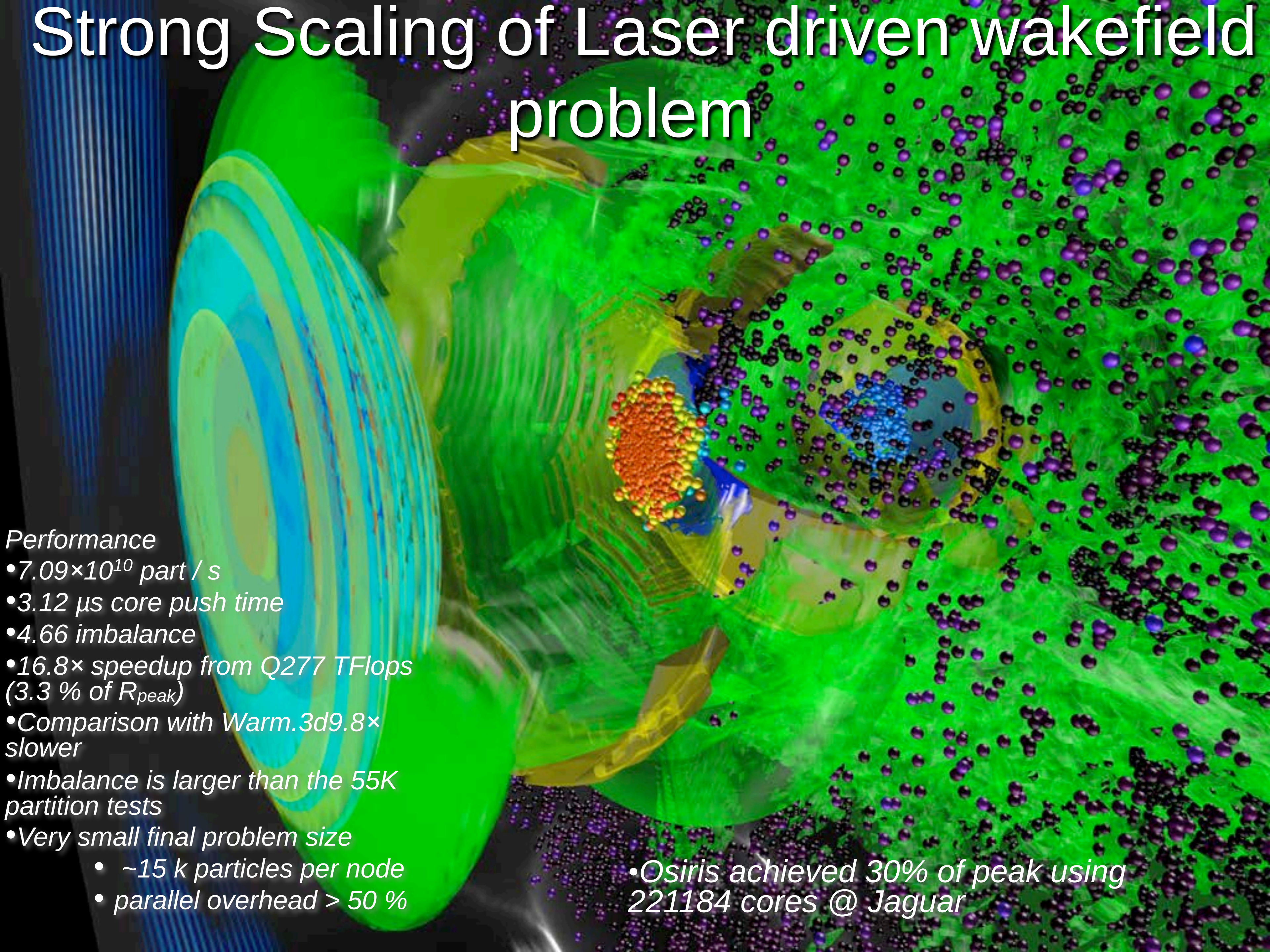
- Enabled by our partnerships with computer scientists and applied mathematicians, ComPASS codes have
  - improved parallelism both at the MPI and node level, better data partitioning
    - allowing realistic multi-physics, multi-scale simulations
  - new techniques and algorithms
    - allowing modeling of previously computationally prohibitive problems
  - prototypes of algorithms and computational framework infrastructure on modern architectures (CUDA-GPU)



Synegia MI full machine simulations



Strong Scaling of Laser driven wakefield problem



Performance

- *7.09×10^{10} part / s*
- *3.12 μs core push time*
- *4.66 imbalance*
- *16.8× speedup from Q277 TFlops (3.3 % of R_{peak})*
- *Comparison with Warm.3d9.8× slower*
- *Imbalance is larger than the 55K partition tests*
- *Very small final problem size*
  - *~15 k particles per node*
  - *parallel overhead > 50 %*

- *Osiris achieved 30% of peak using 221184 cores @ Jaguar*

Plasma-based acceleration is rich in science:

- *Compass codes have been essential to the progress of this field*

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Beam Breakup in RF cavity

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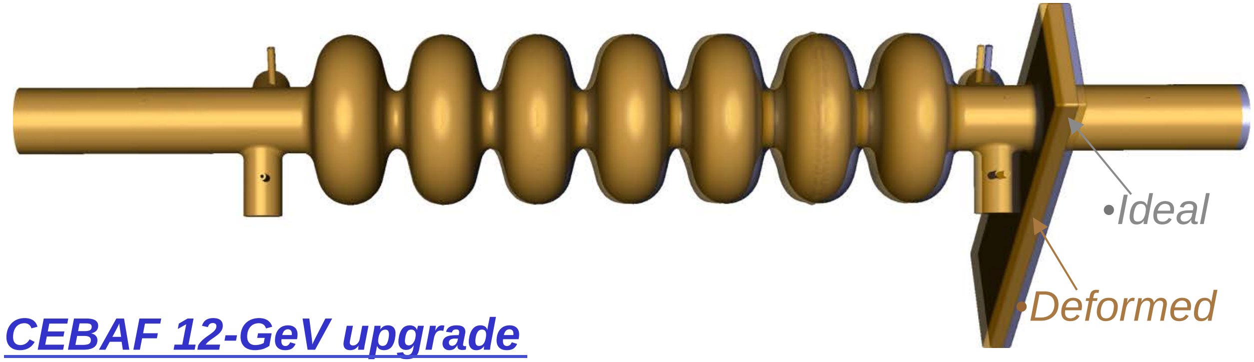
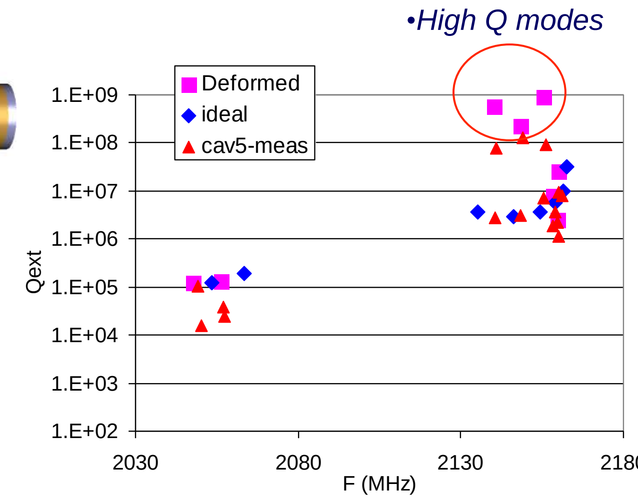
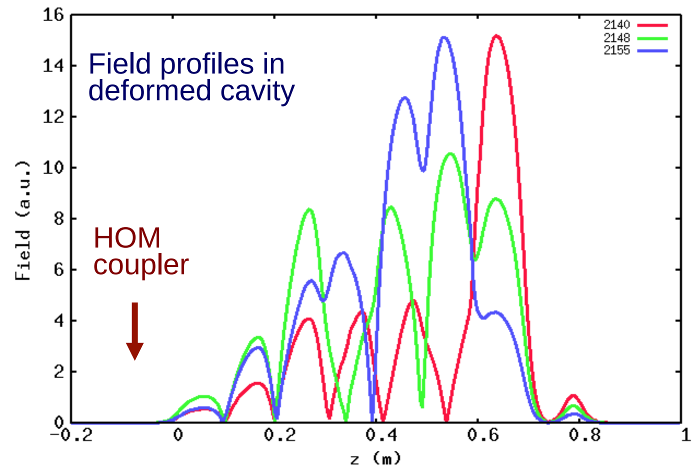




CEBAF 12-GeV upgrade

- Beam breakup (BBU) observed at beam currents well below design threshold
- Used measured RF parameters as input
- Solutions to the inverse problem identified the main cause of the BBU instability: **cavity is 8 mm short – *confirmed later from measurements***
- Combination of **experimental data and ComPASS tools** enabled solution of a real accelerator problem

ACE3P



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Intensity Frontier: Mu2e extraction design

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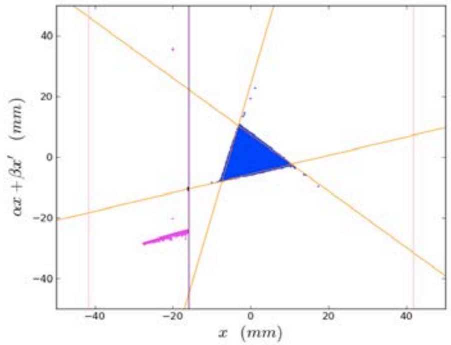
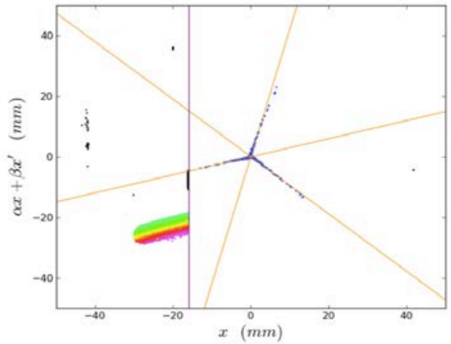
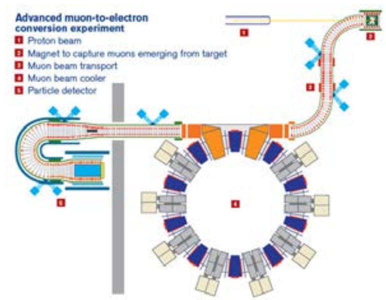
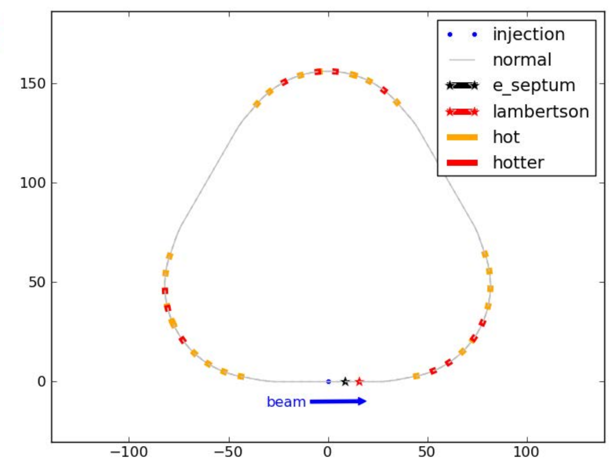
- Synergia full extraction simulation for the Muon to Electron (Mu2e) Fermilab proposed experiment
  - 26k turns, 240 3D solves/turn, 1M macroparticles; include apertures and non-linear fields
  - Quantitative loss predictions
- Results contributed to CD1 approval for the experiment
- Only possible because of performance improvement obtained under SciDAC2!
- Activity is continuing but supported by the experiment
  - SciDAC supported development moves to "mainstream" production!









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Summary

- Particle Accelerators are the most important instruments of discovery in HEP
  - in addition, they have many quality-of-life-enhancing applied science and industrial applications outside HEP
- Numerical modeling and simulation are essential for the development of new concepts and technologies and design and operation optimization
  - because of the complexity and many scales involved HPC is required for model fidelity
- ComPASS under SciDAC3 will develop and deploy state-of-the-art HPC accelerator modeling tools
  - major collaboration (and opportunity for) with SciDAC institutes
  - already mature tools and presence both in SciDAC and the community due to successful SciDAC2 ComPASS campaign