Vision for US Modeling and Design Tools for Long Term Accelerator R&D

P. Spentzouris, with input from J-L. Vay et al (LBNL), C. Ng et al (SLAC), W. Mori (UCLA), J. Cary (Univ. of Colorado & Tech-X)

Presentation guidance

- Goals for medium- and long-term U.S. program
- Scope of the current medium- and long-term program
- Execution plan and resources necessary for this program
- Impact of R&D (this area) on training
- Impact of potential funding increase in long-term R&D

Motivation

- Modeling and design tools are necessary for
  - optimizing the performance of existing accelerators
  - optimizing the design and cost of future accelerators
  - developing new, cost effective, accelerator techniques and technologies.
- **P5 report:**
  - Accelerator Research:
    - "The future of particle physics depends critically on transformational accelerator R&D to enable new capabilities and to advance existing technologies at lower cost. "
  - Computing:
    - "The use of high-performance computing, combined with new algorithms, is advancing full 3-D simulations at realistic beam intensities of nearly all types of accelerators."
    - "This will enable "virtual prototyping" of accelerator components on a larger scale than is currently possible."

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Vision

- Create a fully coordinated national program providing the community with a comprehensive, interoperable set of numerical tools for multi-scale, multi-physics accelerator design, to enable
  - "Virtual Prototyping" of accelerator components
  - "Virtual Accelerator Modeling" of beam dynamics
- Our strategy is to build a collaboration that will develop, maintain and support a common set of libraries and codes capable of utilizing high-performance computing
  - To enable long-term planning required for long-term applications across all accelerator R&D thrusts

Accelerator Modeling and Design Tools: Current Program

Development drivers for numerical tools

- Development of physics models is driven by accelerator science needs
- Code sophistication (multi-physics, …) is driven by design tolerances (beam loss, stability, …)
- High-performance-computing (HPC) needs are driven by the demand for sophisticated, higher fidelity simulations
- R&D on numerical algorithms is driven by the evolution of computing architectures and HPC
  - There is always tension between the need to “keep up” with computing technologies and “support” applications using current codes

Many codes “available” for research

- Covering different focus areas
  - beam dynamics, accelerating structures, plasmas
- Some specialized to a particular type of accelerator
- Some to particular physics, with different approximations
- Few are frameworks capable of incorporating multi-physics
- There is no overall coordination
  - Inefficient use of resources, difficult to support, thus difficult to use

~70 different codes , U.S. and international, not all actively developed and maintained

List of codes from the accelerator handbook (x3)

B

(Below, PIC refers to codes with particle-in-cell space-charge capability.)

Code	URL or Contact	Description/Comments
ASTRA	tesla.desy.de/~meykopff	3D parallel, general charged particle beams incl. space charge
AT	sourceforge.net/projects/atcollab/	Accelerator Toolbox
BETACOOL	betacool.jinr.ru	Long term beam dynamics: ECOOL, IBS, internal target
Bmad, Tao	www.lns.cornell.edu/~dcs/bmad/	General purpose toolbox library + driver program
COSY INFINITY	www.cosyinfinity.org	Arbitrary-order beam optics code
CSRTrack	www.desy.de/xfel-beam/csrtrack	3D parallel PIC; includes CSR; mainly for e^- dynamics
Elegant/SDDS suite	aps.anl.gov/elegant.html	parallel; track, optimize; errors; wakes; CSR
ESME	www-ap.fnal.gov/ESME	Longitudinal tracking in rings
HOMDYN	Massimo.Ferrario@LNF.INFN.IT	Envelope equations, analytic space charge and wake fields
IMPACT code suite	amac.lbl.gov	3D parallel multi-charge PIC for linacs and rings
LAACG code suite	laacg.lanl.gov	Includes PARMILA, PARMELA, PARMTEQ, TRACE2D/3D
LiTrack	www.slac.stanford.edu/~emma/	Longitudinal linac dynamics; wakes; GUI-based; error studies
LOCO	safranek@slac.stanford.edu	Analysis of optics of storage rings; runs under matlab
LUCRETIA	www.slac.stanford.edu/accel/ilc/codes	Matlab-based toolbox for simulation of single-pass e^- systems
MaryLie	www.physics.umd.edu/dsat	Lie algebraic code for maps, orbits, moments, fitting, analysis
MaryLie/IMPACT	amac.lbl.gov	3D parallel PIC; MaryLie optics + IMPACT space charge
MAD-X	mad.web.cern.ch/mad	General purpose beam optics
MERLIN	www.desy.de/~merlin	C++ class library for charged particle accelerator simulation
OPAL	amas.web.psi.ch	3D parallel PIC; cyclotrons, FFAGs, linacs; particle-matter int.
ORBIT	jzh@ornl.gov	Collective beam dynamics in rings and transport lines
PATH	Alessandra.Lombardi@cern.ch	3D PIC; linacs and transfer lines; matching and error studies
SAD	acc-physics.kek.jp/SAD/sad.html	Design, simulation, online modeling & control
SIMBAD	agsrhichome.bnl.gov/People/luccio	3D parallel PIC; mainly for hadron synchrotrons, storage rings
SIXTRACK	frs.home.cern.ch/frs/	Single particle optics; long term tracking in LHC
STRUCT	www-ap.fnal.gov/users/drozhdin	Long term tracking w/ emphasis on collimators
Synergia	https://compacc.fnal.gov/projects	3d parallel PIC: space charge, nonlinear tracking and wakes
TESLA	lyyang@bnl.gov	Parallel; tracking; analysis; optimization
TRACK	www.phy.anl.gov/atlas/TRACK	3D parallel PIC, mainly for ion or electron linacs
LIBTRACY	libtracy.sourceforge.net/	Library for beam dynamics simulation
TREDI	www.tredi.enea.it	3D parallel PIC; point-to-point Lienard-Wiechert
UAL	code.google.com/p/ual/	Unified Accelerator Libraries
WARP	DPGrote@lbl.gov	3D parallel ES and EM PIC with accelerator models
ZGOUBI	sourceforge.net/projects/zgoubi/	Magnetic optics; spin; sync radiation; in-flight decay

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Evolution of numerical tools timeline (a simplified view…)

"base" driven funding, individual efforts

Project driven (Grand Challenge, SciDAC), collaborative efforts

1970

Transport
MAD
Parmila
Parmela
….

Matrix codes
2D self-fields
Rms eqns

1980

MaryLie
mxyzptlk(CHEF)
COSY
SIMPSONS
….

Symp. Integration
Diff. Algebra
Normal Forms
Maps

1990

Impact
Omega
WARP
…

HPC era

3D self-fields
Freq. maps

2000

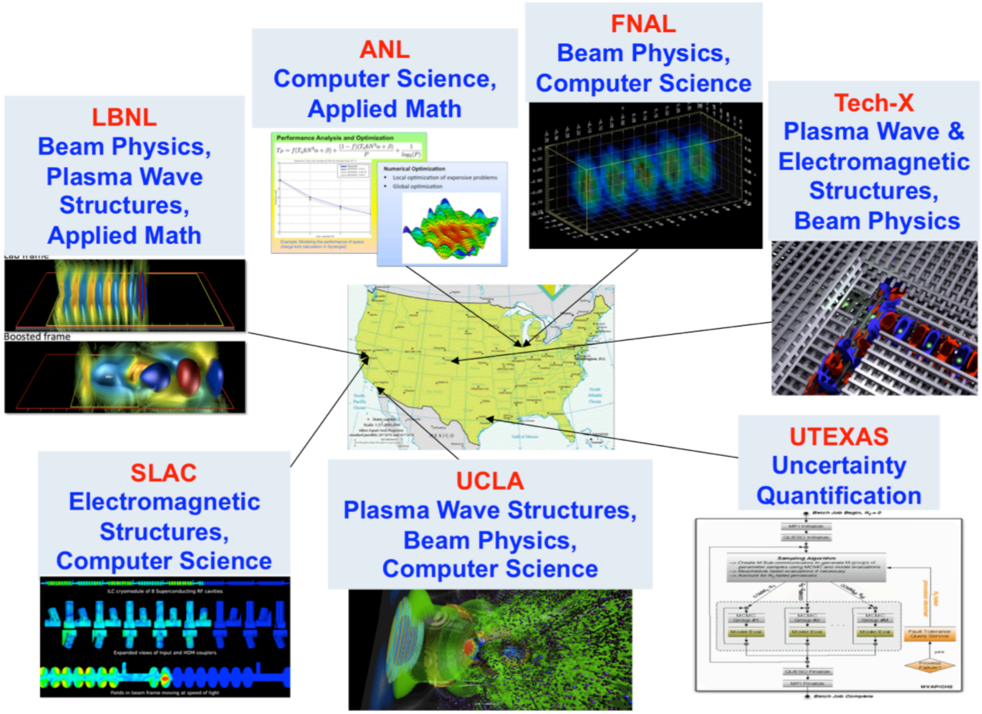
ACE3P
BeamBeam3D
MAD-X
MLI
Orbit
Synergia
Track
….

Multi-physics
Frameworks

Coordinated efforts for Modeling and Design in the last decade: ComPASS

- ComPASS, funded by SciDAC, develops modeling and design tools with emphasis on HPC
- GARD (or predecessor) and projects (in more recent years) support applications
- Code maintenance and user support not explicitly funded, thus not adequate

SciDAC: Scientific Discovery through Advanced Computing
ComPASS: Community Project for Accelerator Science and Simulation



ComPASS is the only current development activity organized as a national project

ComPASS under SciDAC

- ComPASS goals (2007 SciDAC2 proposal):
  - "*Our vision is to develop a comprehensive suite of interoperable accelerator modeling tools which will enable Virtual Prototyping of the design and optimization of accelerator components, and multi-physics Virtual Accelerator Modeling…*"
  - well matched to the 2014 P5 recommendations
- SciDAC is a partnership of ASCR with other DOE offices, now in its 3rd cycle (5 year cycles). ComPASS under
  - SciDAC2 a partnership of **ASCR**, **HEP**, **NP**, and **BES**, at ~$3M/year
  - SciDAC3 just **ASCR** and **HEP**, at $1.8M/year (50/50 split)
    - The HEP share comes from **Comp. HEP**, not **GARD**.
  - SciDAC enables collaboration and leveraging of non-HEP resources, but not truly programmatic for accelerator science
    - difficult to sustain a program with long term goals if many different funding sources with different funding cycles, etc
- To support long-term accelerator R&D we need a healthy GARD program for this activity area

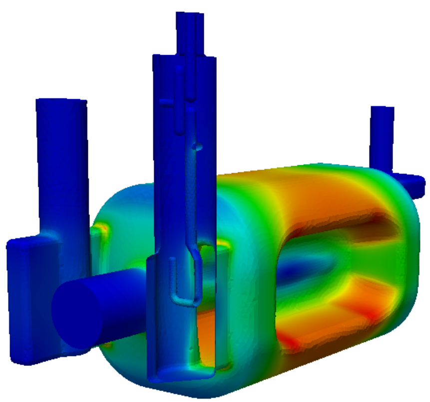
Codes currently (partially) supported under ComPASS

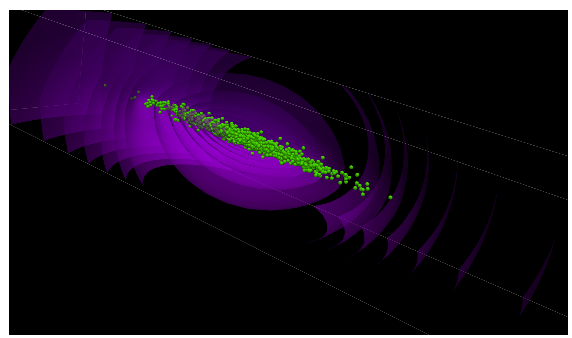
- **ComPASS toolkit: ACE3P (SLAC), Osiris & QuickPIC (UCLA), Synergia (FNAL), Vorpal (Tech-X), Warp (LBNL), in 3 focus areas**

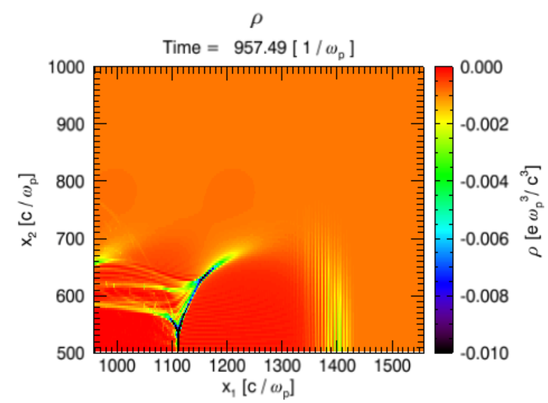
- Accelerator structure focus
  - Cavity modeling
    - Interaction of fields and particles with environment
  - Multi-physics analysis
    - Integrated EM, thermal and mechanical effects
  - **Applies to all GARD thrust areas**

- Beam Dynamics focus
  - Single and multi-particle dynamics and collective effects
  - Multi-physics, multi-scale modeling
  - **Applies to all GARD thrust areas**

- Plasma focus
  - Laser and beam-driven wakefields in plasmas
  - Multi-physics and scale
  - **Applies to the Advanced Accelerator Concept thrust**







Although they share low-level numerical algorithms, the physics, and numerical optimization have different requirements, thus require separate development effort

Many more codes with broad applicability are currently actively developed and used

- Codes that have HPC capabilities (partially developed under SCiDAC in the past), i.e.
  - IMPACT and BeamBeam3d (LBNL)
- Codes initially developed to target a particular need for one application, i.e.
  - Elegant (APS control room), Orbit (SNS design)
  - also codes developed for the Muon Accelerator Program
    - G4beamline, …
- University developed beam dynamics codes
  - COSY-INFINITY (MSU), MaryLie (Maryland)
- Specialized codes for activation and shielding calculations
  - MARS
- …

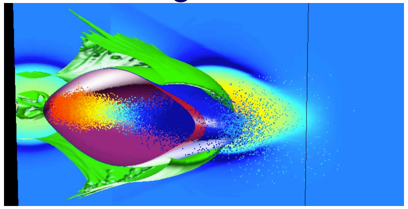
Capabilities

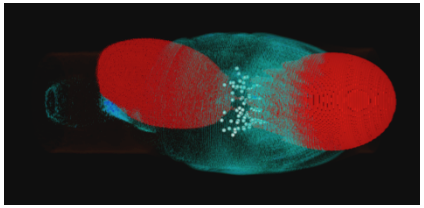
- State of-the-art codes, such as the ComPASS codes, are able to
  - simulate multi-particle and collective effects with millions of macro-particles, using higher-order optics
  - model complete accelerator structures with complicated shapes and millions of degrees of freedom
  - Model laser and beam propagation in plasmas and relevant physics
- ComPASS codes have been (and are) used for every HEP high-priority operations or design application, e.g.
  - PEP-II, ILC, LHC, FNAL Run II accelerators, FNAL PIP I and II, experiments at FACET and BELLA, MAP,… (and also non-HEP, such as CEBAF, RHIC, SNS, LCLS, …)
- This is an excellent demonstration of the effectiveness and reach of a coordinated program

Examples of Advanced Accelerator Concept applications

- Plasma-based acceleration:
  - support the BELLA (laser) and FACET (beam) experimental programs
  - improve staging for future lepton collider concepts.
- Dielectric laser acceleration:
  - design structures able to accelerate high quality beams

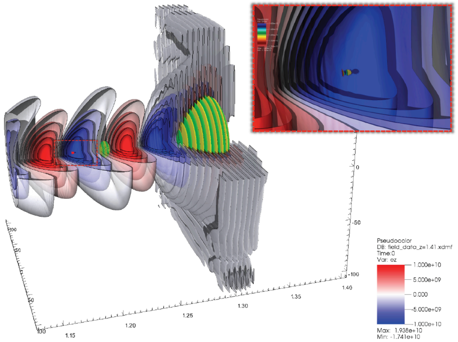
FACET stage, QuickPIC



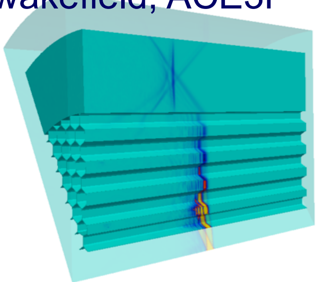


Colliding pulse injection, Vorpal

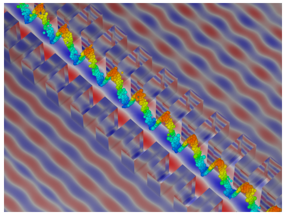
2-color injection, WARP



PBG wakefield, ACE3P



Dielectric grating structure, Vorpal



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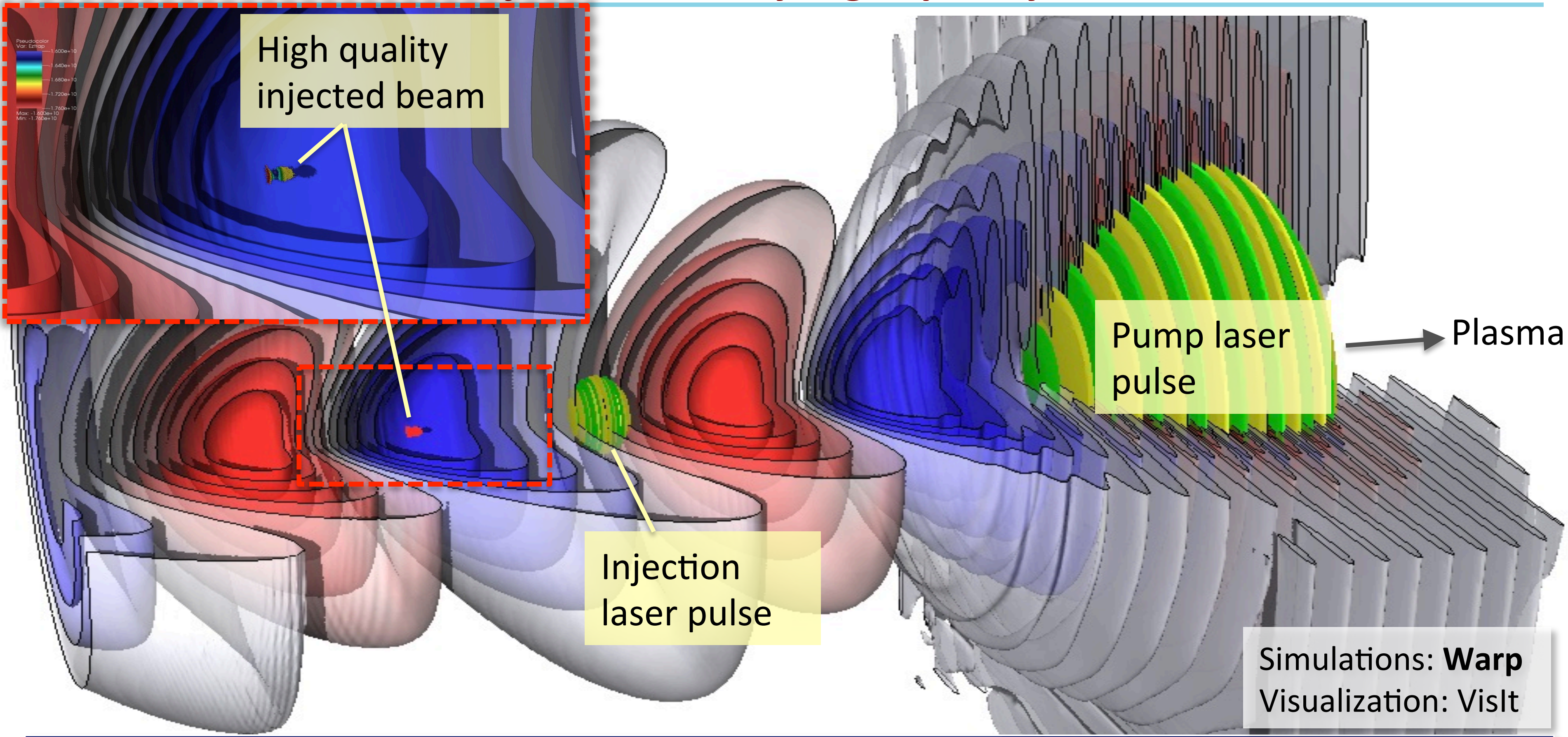
Multi-scale 3-D simulations validate a new concept for injection of very high-quality beams*



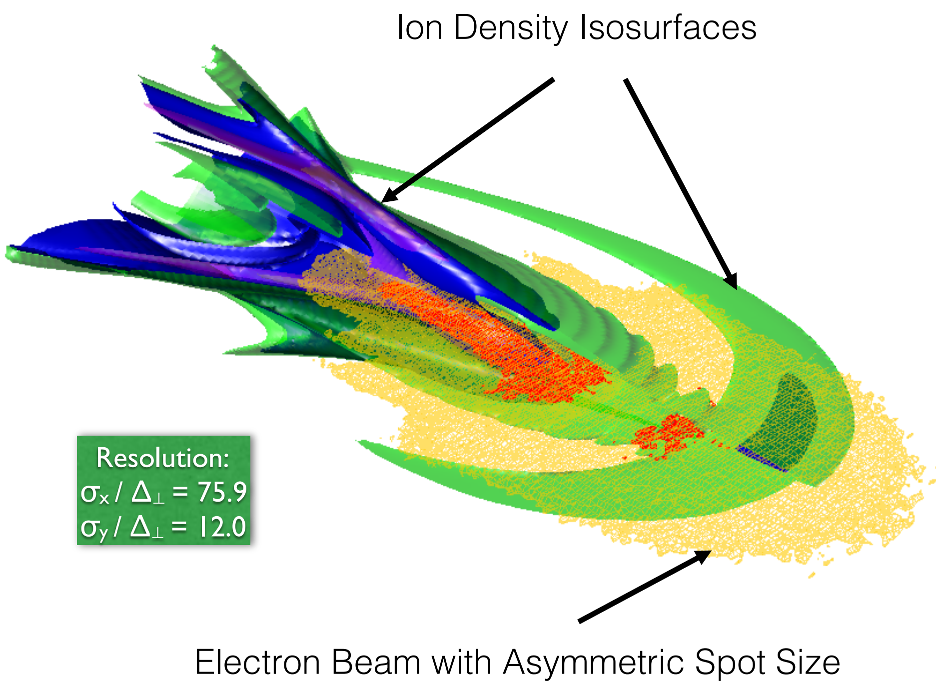
1 - Pump laser pulse creates accelerating wake in plasma.
2 - Injection laser ionizes pocket of Krypton gas, creating very high-quality electron beam.
3 - Electron beam is accelerated to high energy in short distance by wake.

Parametric runs necessitated over a million hours; typical 3-D run around 100k core-hours.

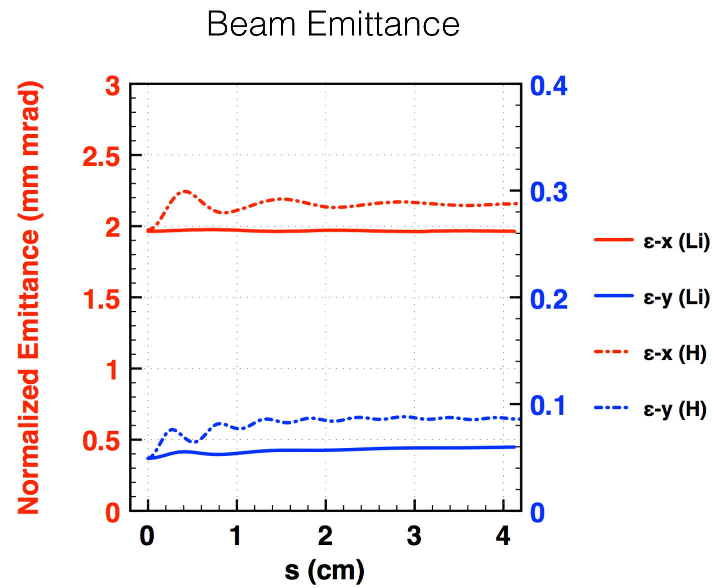
*L.-L. Yu, E. Esarey, C. B. Schroeder, J.-L. Vay, C. Benedetti, C. G. R. Geddes, M. Chen, and W. P. Leemans, *Phys. Rev. Lett.* **112**, 125001 (2014)

Large scale simulations show that emittance growth from ion motion is less severe than expected in PWFA blowout regime

Density Isosurfaces of the Ion Collapse in a Hydrogen Plasma



Trailing Beam: σ_z = 10.0 μm , N = 1.0 x 10^{10} ,
σ_x = 0.463 μm , ε_{Nx} = **2.0 mm·mrad** ,
σ_y = 0.0733 μm , ε_{Ny} = **0.05 mm·mrad**
γ = 48923.7 (25 GeV), Plasma Density : 1.0 x 10^{17} cm^{-3}



In Li, the emittance in x does not change, and in y direction it only increase by 20%.

In H, the emittance in x increase by 10%, and in y direction it increases by 70%.

This study required QuickPIC runs with 16384 x 16384 x 2048 cells on 32768 processors

W. An et al.

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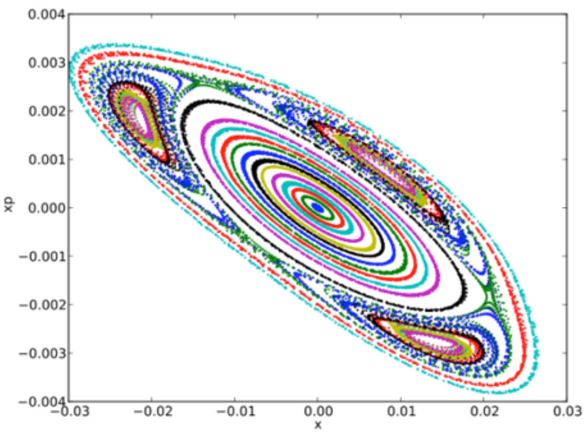
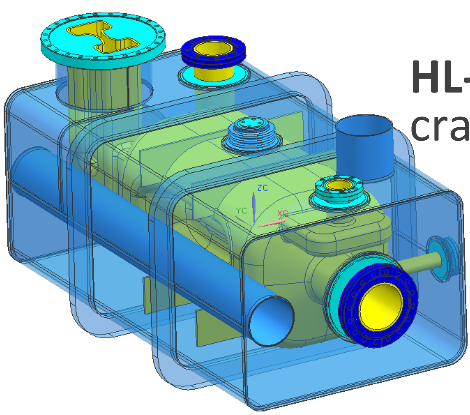
Advanced Modeling Benefits LHC and LHC Upgrades

LHC upgrades are a high priority for the US program

Collaboration with CERN scientists to utilize **Synergia** for the LHC Injector Upgrade (LIU). Massive simulations to validate using GSI SIS18 ring data

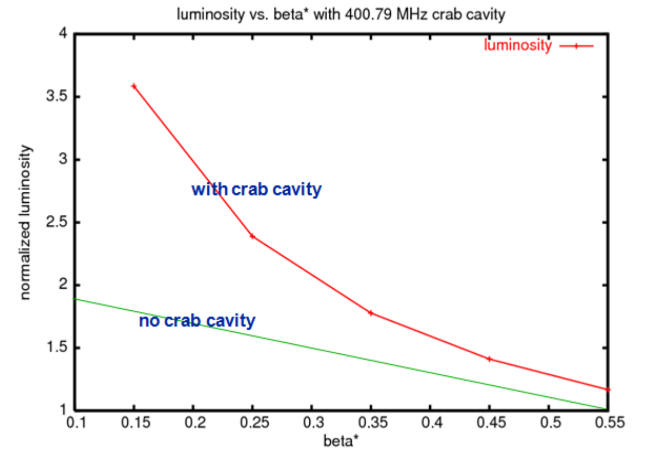


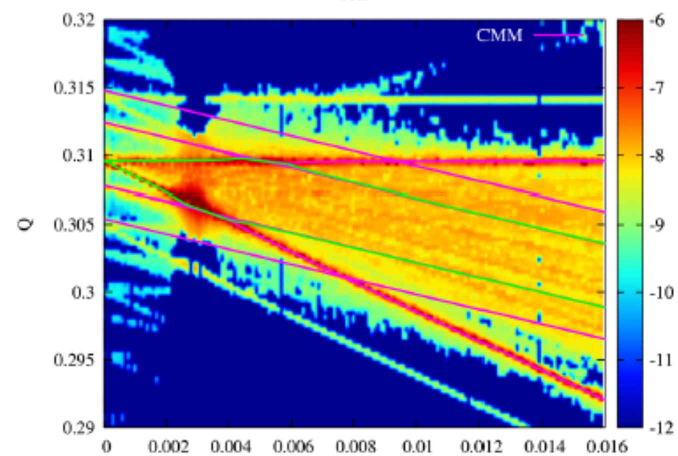
- *71 steps/turn*
- *100k turns*
- *7,100,000 steps*
- *4,194,304 particles*
- *29,779,558,400,000 particle-steps*
- *1,238,158,540,800,000 propagator calls*



HL-LHC – Prototyping of crab cavity using **ACE3P**

BeamBeam3D is used to support LHC and LHC upgrade with Crab Cavity





Synchro-betatron modes as a function of the beam-beam parameter at LHC.

S. White et al., PRST-AB 17, 041002, 2014.

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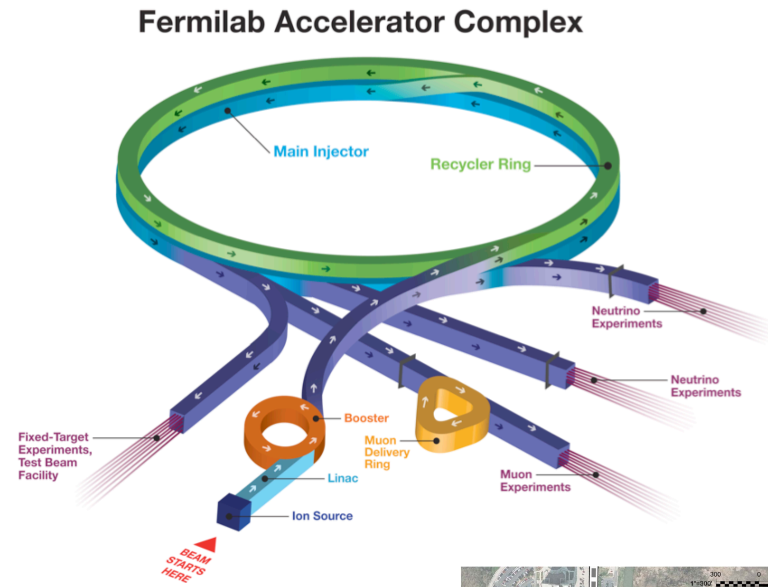
MARS: interaction region design for the LHC

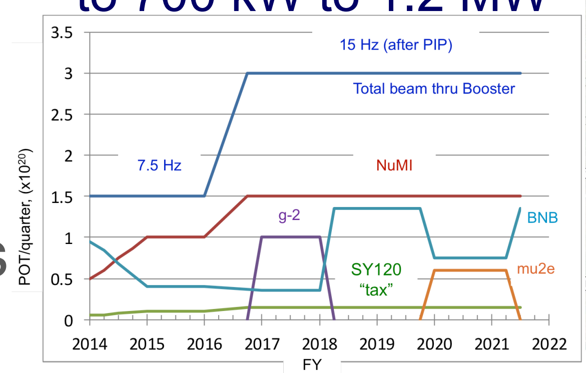
- MARS simulations in 1996 to 2003 helped design the optimal high-luminosity Interaction Regions IR1 and IR5 of LHC, including their absorbers, and predict superconducting magnet short-term (quench stability) and long-term (lifetime) performances.
- "MARS predictions of 16 years ago of energy deposition in the low-beta quads agree within 20% with recent measurements in the real LHC machine. No beam-induced quench has been observed at LHC". *Lucio Rossi*, talk at Fermilab, February 2014.
- One and a half decades ago there was no experimental data above 1 TeV to verify the code's physics models. Today – working on the HiLumi LHC upgrade – FLUKA and MARS codes are benchmarked in the TeV energy range.
- MARS provides another demonstration of the effectiveness and reach of a long development program (over 30 years development)

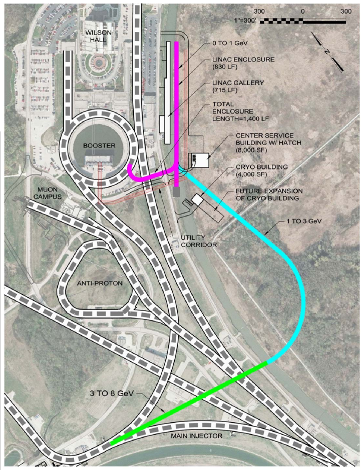
Examples of applications for high-intensity beams

- Fermilab Proton Improvement Plan (PIP)
  - Booster, Main Injector (MI), Recycler: instability control and mitigation, loss minimization
- Mu2e upgrades
  - Delivery Ring extraction design
- New srf Linac (PIP-II)
  - Linac design: wakefields



Power increase: 300 kW to 700 kW to 1.2 MW





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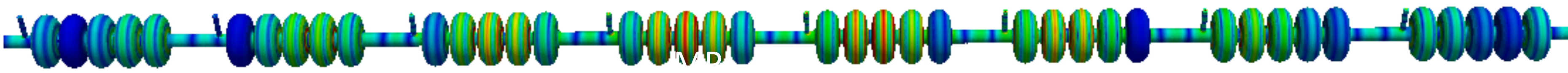
Full cryomodule model for PIP-II

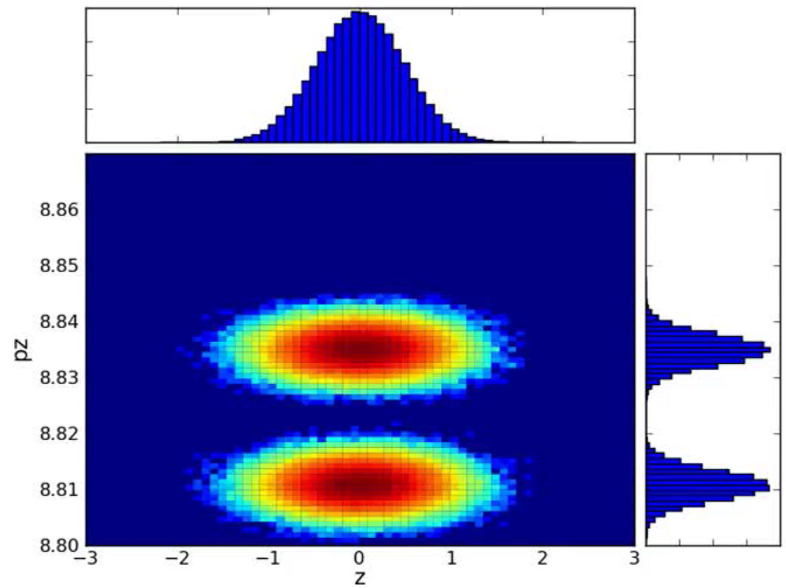
PIP-II – Trapped mode in PIP2 650 MHz cryomodule consisting of 8 SRF cavities



SciDAC collaboration in scalable solvers enables fast solution in such large problems using **ACE3P**. It took 3 min to calculate a mode frequency and its damping using 300 cores, 1.1 Tbytes of memory for a mesh with 14M degrees of freedom on the NERSC Edison supercomputer.

Recycler slip-stacking

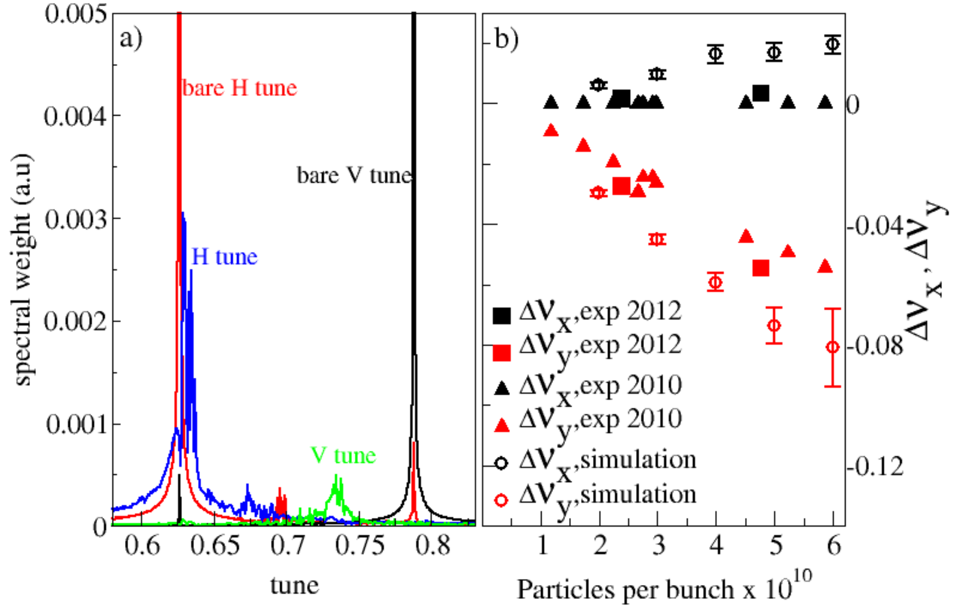
- Slip-stacking of Booster bunches increases intensity downstream
  - In the past, done in the MI
- Under PIP, slip-stacking moved to the Recycler to increase the MI ramp rate (thus beam power)
  - Must model the whole process to characterize localized losses and evaluate mitigation techniques
  - A very complex model, the simulation campaign underway
    - Include apertures, field measurements, impedance, …

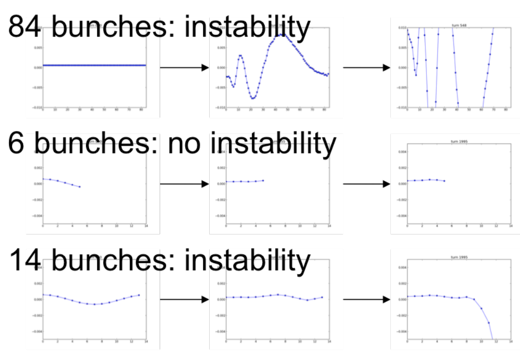


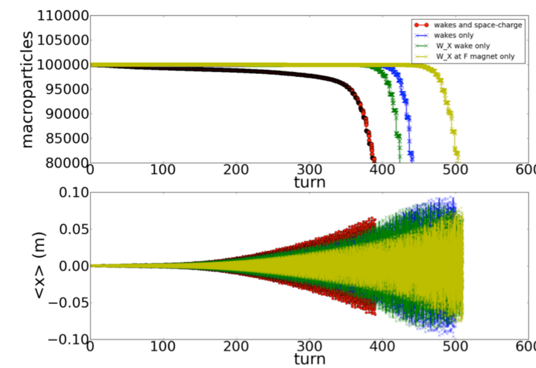
Synergia simulations

Booster PIP

- Horizontal plane coherent instability near injection
  - Mitigated by empirically changing chromaticity at a counterintuitive value
- **Synergia** multi-bunch simulations revealed the source of the wakefield-caused instability
  - Work closely with machine physicists to collect data for validation
  - Excellent example of the impact of long-term R&D on short term activities





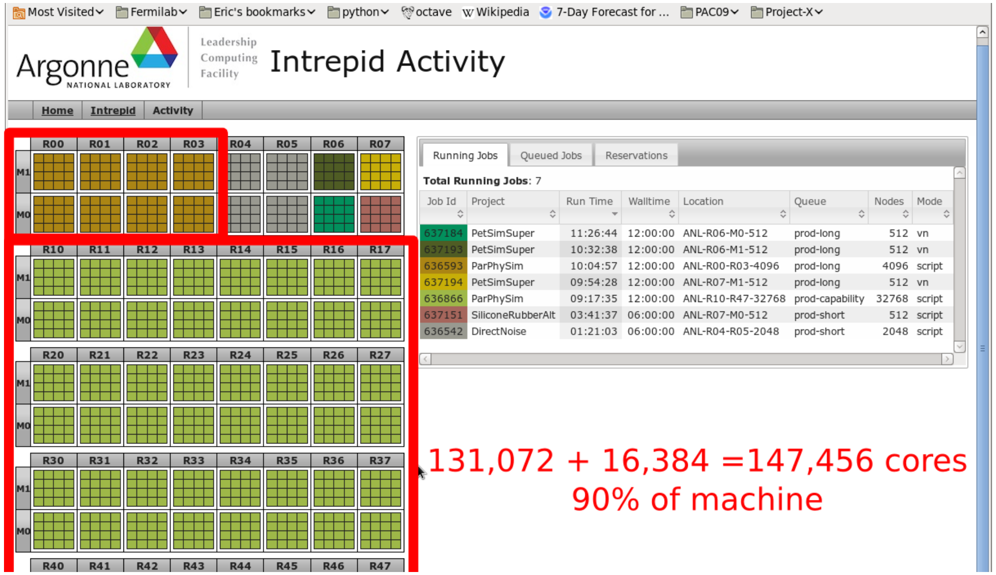


A. Macridin, et al., PRST-AB 16, 121001 (2013)

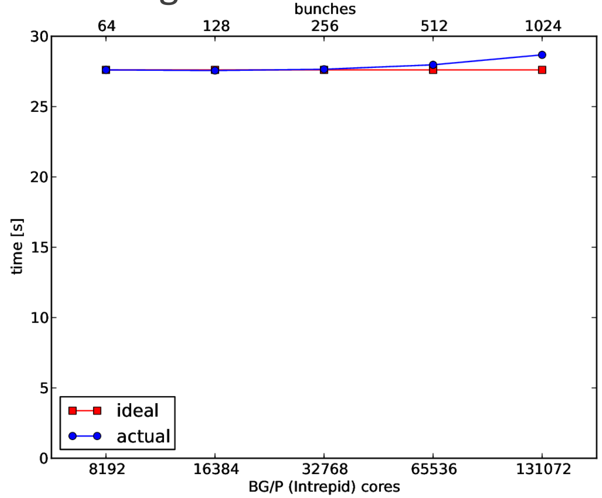
Very large computations: Synergia simulation campaign for PIP (I & II)

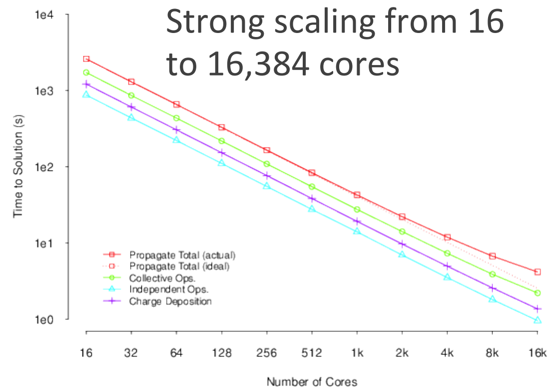
- Single job size for production
  - Booster 20k core
  - MI/Recycler 64 k core
  - Optimization scans 131k core

12 month simulation campaign used 80M core hours at the ANL Leadership Computing Facility (LCF)



Weak scaling from 8192 to 131072 cores

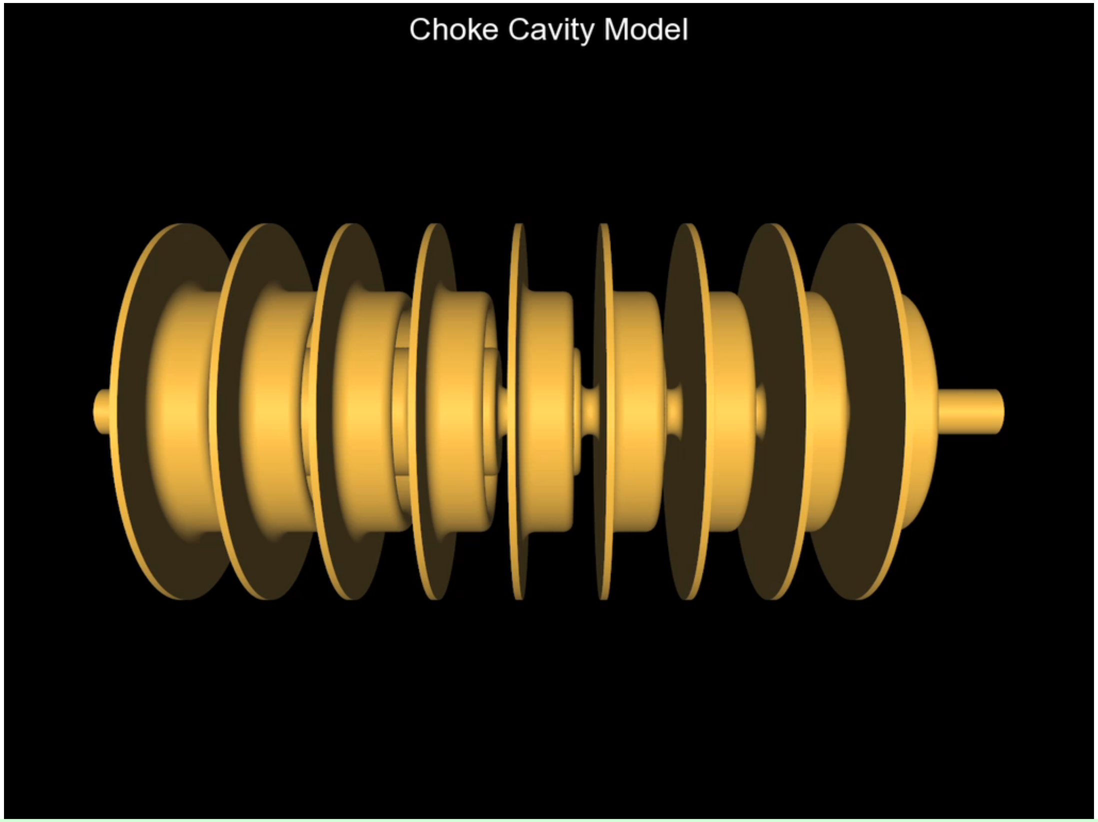




Note, time allocation to LCFs through competitive proposals; success depends on code scaling and performance

Virtual Prototyping using ACE3P

Optimize the performance of the choke mode cavity for high gradient acceleration by improving the damping of the higher-order dipole modes.



Parallel computation with advanced shape optimization techniques allows fast turnaround time to obtain the best design.

Community support, training and education

- Web based documentation and code downloads. Examples:
  - blast.lbl.gov (LBNL BLAST code set)
  - https://web.fnal.gov/sites/Synergia/SitePages/Synergia%20Home.aspx (FNAL Synergia framework)
  - https://confluence.slac.stanford.edu/display/AdvComp/Materials+for+cw11 (SLAC ACE3P framework, documentation and tutorials)
  - http://www-ap.fnal.gov/MARS/ (MARS code system)
- No rigorous user support process
- Codes used at USPAS, while developers serve as instructors
- Very rarely, code workshops and tutorials
  - SLAC group a notable exception, holds them regularly
- Few universities provide academic computational accelerator physics training (e.g. MSU), some train students on computation through participation in research programs (e.g. UCLA at FACET)

Accelerator Modeling and Design Tools: Moving Forward

R&D Drivers

- New accelerator designs and concepts have increasingly stringent performance requirements, calling for
  - Higher fidelity, faster codes
- New computing architectures require changes in computational paradigm
  - New numerical algorithms, workflows, infrastructure
- Need to provide better training and user support while maintaining development effort

Guided by the P5 recommendations

- **Recommendation 14 :** Upgrade the Fermilab proton accelerator complex… to provide proton beams of >1 MW…
- **Recommendation 23 :** Support… accelerator science… through advanced accelerator facilities … Strengthen national laboratory-university R&D partnerships…
- **Recommendation 26** : Align the present R&D program with the P5 priorities …outcomes and capabilities that will dramatically improve cost effectiveness for mid-term and far-term accelerators.
- **Recommendation 29:** Strengthen the global cooperation…to address computing and scientific software needs, and provide efficient training in next-generation hardware… Investigate models for the development and maintenance of major software….

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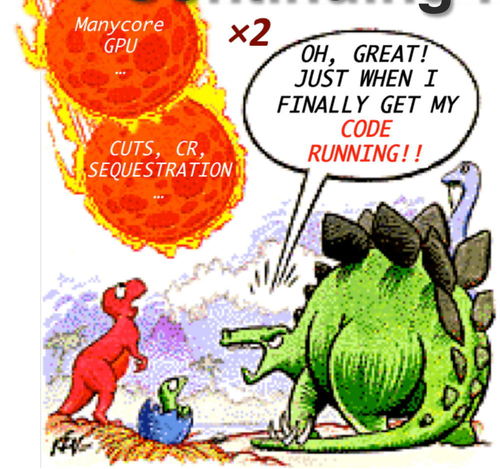
Snowmass 2013: capability requirements for future accelerators

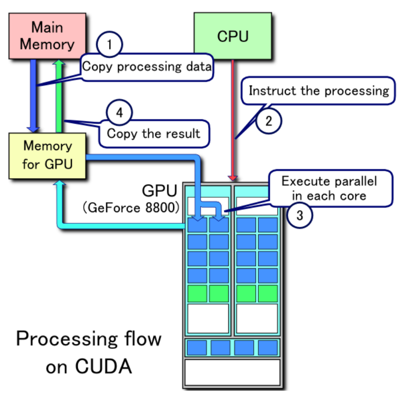
- High intensity accelerator needs
  - quantitative beam loss characterization and mitigation
  - ability to compare beam diagnostics data to simulated data
- High Energy accelerator needs
  - beam stability characterization
  - ability to produce end-to-end designs
  - new physics model capabilities (e.g., radiation, scattering)
- All applications
  - control room feedback: fast turnaround of simulations
  - integrated / multi physics modeling: improve algorithms to take advantage of massive computing resources
  - common interfaces, geometry and parameter description, workflow tools from tablet to supercomputer.
  - better numerical models (less numerical noise)

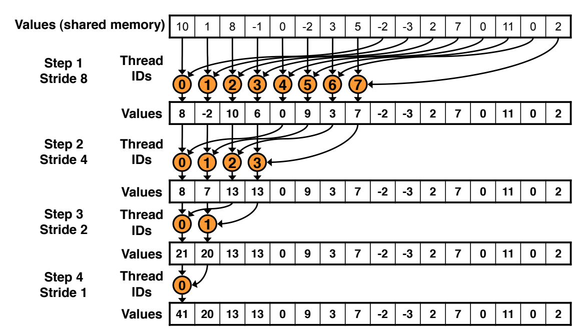
➢ **Requirements point to complex models in need of HPC**

Challenge: change of computing paradigm

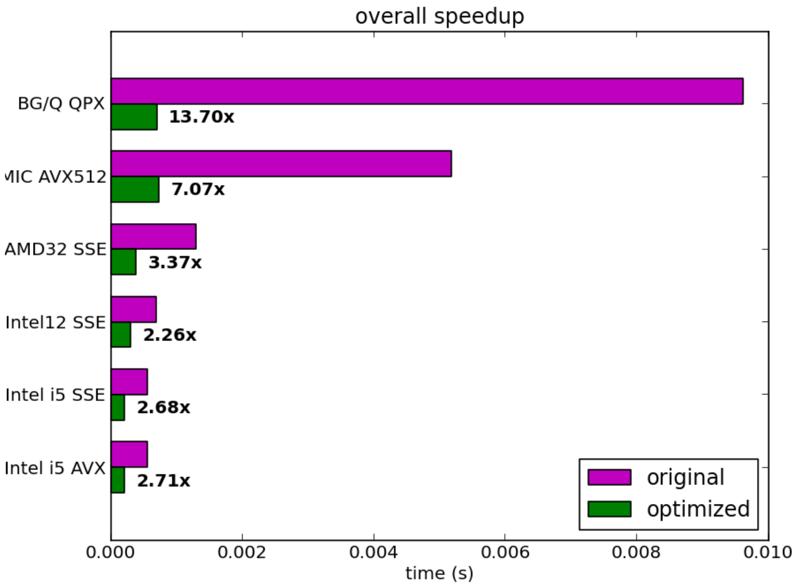
- We spent the last decade optimizing our codes on distributed memory systems. However, due to commercial pressure, computing architectures are moving to multi-core systems and accelerators (GPUs, …)
  - Shared memory, vectorization, multi-level parallelism
- Changes in programing paradigm needed
  - But, a great opportunity for multi-physics, multi-scale simulation leading to "Virtual accelerator" modeling
- **Continuing R&D on new architectures necessary**







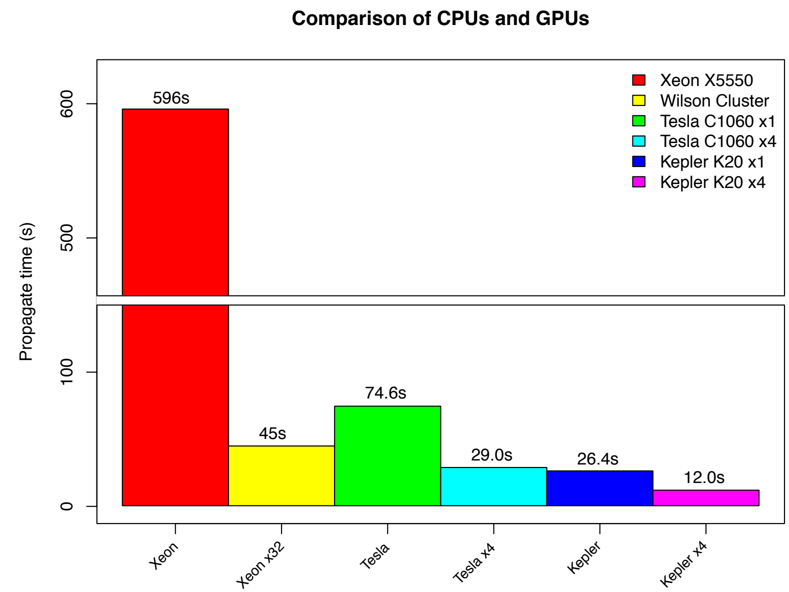
Already progress under SciDAC/ComPASS on GPU (CUDA) and MIC based systems



GPU-enhanced Synergia achieves better overall performance with 4 GPUs than an 128 node Linux cluster

First production Synergia runs on the GPU: Mu2e extraction

Explicit vectorization of Synergia leads to a large performance enhancement on each architecture, **but, requires a lot of effort!**



ASCR funded work at FNAL

Fermilab

CAMPA

- Running multi-physics codes on the next generation of supercomputers requires large investment
  - need for better integration of modeling efforts and planning
- No platform for sharing code or providing support
  - elements exist in projects such as ComPASS, but not globally
- New LBNL-SLAC-FNAL initiative: **Consortium for Advanced Modeling of Particle Accelerators (CAMPA)** aims to
  - develop, maintain & support an integrated suite of codes
  - train the next generation of computational physicists in accelerator modeling on the latest hardware
- Modest initial investment
  - First year activity \$250k in FY14 by LBNL-SLAC
  - Second year activity \$500k in FY15 by LBNL-SLAC-FNAL

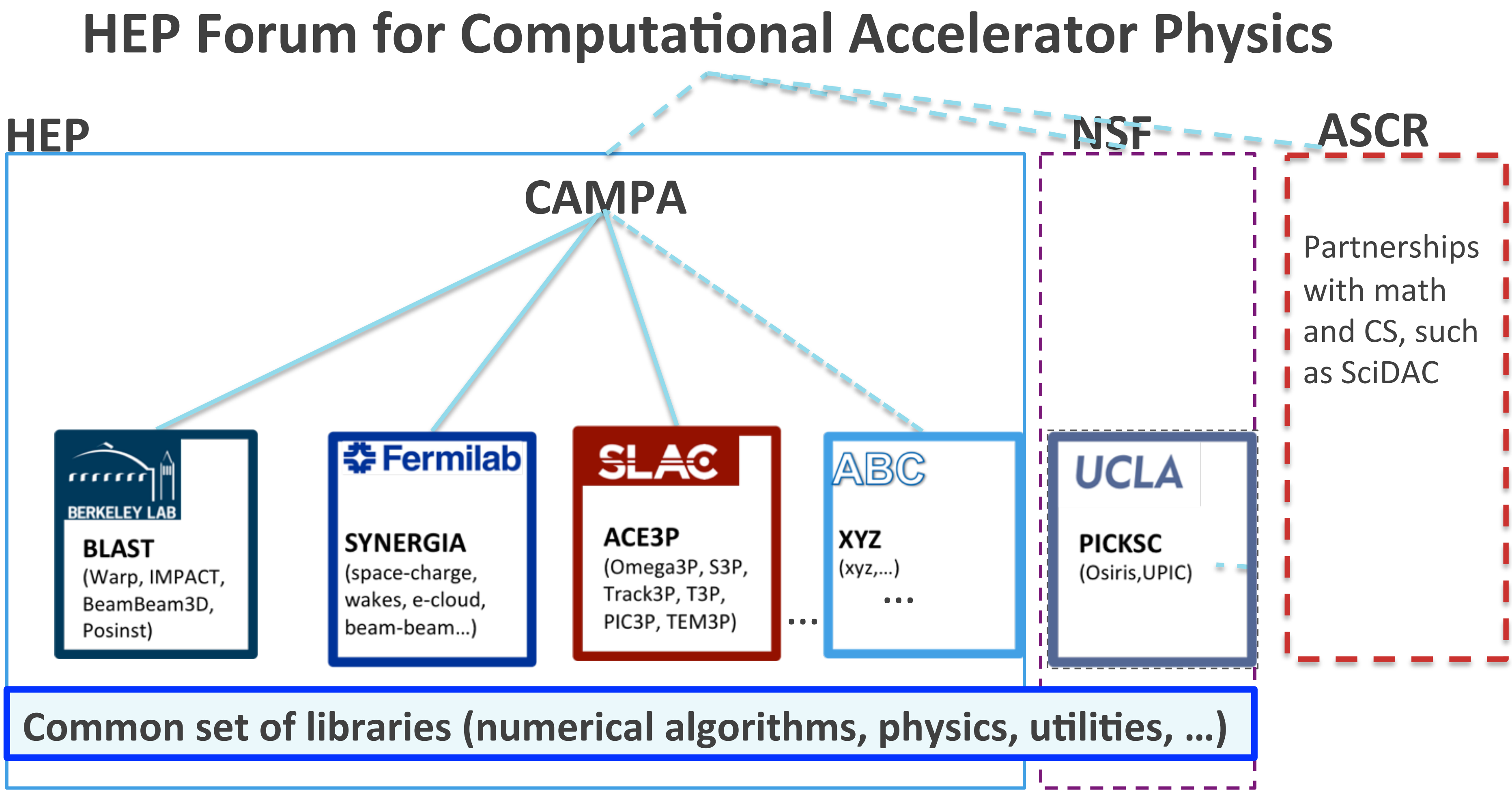
CAMPA strategy

- Building on the success of ComPASS, organize efforts from LBNL-SLAC-FNAL to work on
  - Interoperability of existing codes and capability consolidation
  - Common workflow, interface, data representation, analysis tools
- Coordinate with other national projects (SciDAC, SBIR,…) and University (NSF) efforts to develop
  - new physics and numerical models
  - porting to new hardware
- Develop infrastructure and user support process
  - Code distribution, release and documentation standards, repositories,…

University role

- University participation is essential for success, providing access to
  - students and post docs: the health of our field depends on training young scientists on all aspects of our activities
  - funding sources not available to labs (such as NSF)
- University computational physicists have well established connections to both lab and university experimental programs, increasing collaboration possibilities
- Universities provide access to multi-disciplinary research
  - Increasing program breadth and innovation possibilities
- For universities, a coherent program will provide
  - The means to support technical staff, not done traditionally in academia
  - The visibility necessary to attract the best students

CAMPA could help establish a broader forum



Could also expand - or link - to other DOE programs (BES, NP, FES) accelerator activities.

Forum for Computational Accelerator Physics *(scenario C)*

- With more resources available, consortium could expand to create a forum. Participating institutes would:
  - contribute to a common set of libraries of numerical tools
  - maintain and support these libraries and provide consultation.
  - sponsor student and computational researcher fellowships
- In order to create such an organization, we need
  - Incentives (funding, enhanced opportunities for research,…)
  - An inclusive governance model
- The forum should be funded for developing and deploying the common infrastructure
  - software libraries, repositories, code release and testing, user support and documentation, and fellowships
- This funding is in addition to development funding (at todays SciDAC levels) and CAMPA interoperability effort *[scenario B]*

Modeling and design tools applications

- Development driven by the needs of long-term program (P5)
  - Design of multi-MW facilities, 100 TeV scale pp and TeV scale lepton colliders
- Development also benefits mid-term activities, as more advanced tools become available
- For the success of modeling and design applications it is essential to work closely with machine physicists
  - FNAL team experience with RUN II and PIP, LBNL with BELLA, SLAC with MI, UCLA with FACET,… supports this.
- Applications should be driven by individual partnerships of computational teams with accelerator projects and facilities, according to accelerator R&D priorities and individual group research interests

Accelerator Modeling and Design Tools: Application focus and resource needs

FNAL vision, assets, and strategy

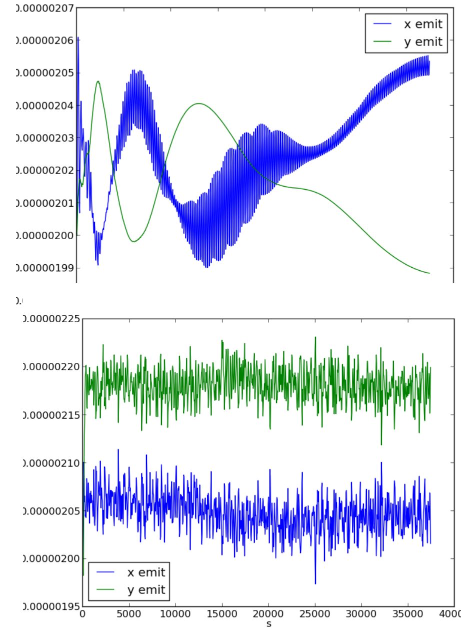
- FNAL vision, within the national program, is to
  - become *a "center of excellence"* for numerical simulations of high-intensity beams and beam-material interactions (energy deposition and radiological effects) to support multi-MW driver design, while enhancing capabilities of the mid-term program
- Main emphasis on numerical tools for R&D studies for a ring multi-MW driver option
  - Quantitative beam loss prediction
  - Passive and active mitigation techniques
  - New design concepts
- Utilize the multi-physics Synergia framework, MARS (and other codes -through CAMPA- where appropriate)

FNAL development focus

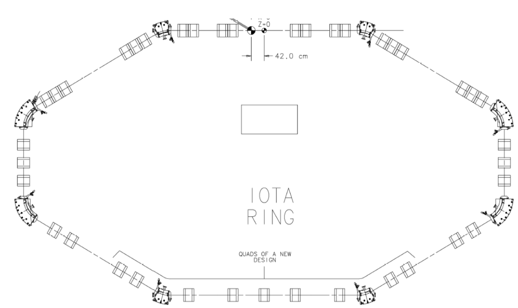
- Co-processor algorithms, capable of multi-million step simulations for accurate beam loss modeling in Synergia. Data driven model validation at FNAL accelerator complex
- Improved MARS models for highly-accurate large scale simulation of beam interactions with accelerator and target components.
- Interface Synergia with MARS for accurate characterization of activation and for design of shielding, collimators, …
- Common interfaces and data representations for interoperability between Synergia and other codes (CAMPA)
- Numerical models for non-linear elements in Synergia. Data driven model validation from the IOTA facility
- Detailed RF models in Synergia for linac simulations
- User and application deployment support and consortium infrastructure support

FNAL application focus

a. Booster, Recycler, and MI applications at 700KW operation (guidance for loss modeling studies).
b. PIP-II accelerator chain for performance optimization, leading to 1.2MW.
c. Support of the IOTA R&D program (see A. Valishev's talk)
d. Support of instability and halo control experimental program (see B. Zwaska's talk)
e. Design concept development for the next-generation booster for a post-PIP-II multi-MW accelerator complex upgrade.
f. Support upgrades of existing and design of next-generation proton-proton colliders.



Synergia simulations of IOTA, D. Bruhwiler



LBNL vision, assets and strategy for accelerator modeling

- **LBNL Center of excellence in accelerator/plasma modeling & hub for computational accelerator physics**
  - Berkeley Lab Accelerator Simulation Toolkit spans breadth of DOE/SC
    - Intense multiphysics beam dynamics (space charge, beam-beam, ecloud), Advanced light sources, Plasma based accelerators
  - Breakthrough algorithms – e.g. boosted frame, spectral Maxwell solver
  - Worldwide users: > 40 institutes use BeamBeam3D, IMPACT, Posinst, Warp (blast.lbl.gov)
    - current HEP: BELLA, LHC, ILC, Tevatron, MI, NML injector, SPS, PS, CESR-TA, MAP
      - e.g.: beam-beam for increased Tevatron luminosity, SPS/LHC e-cloud modeling/mitigation
    - current NP: FRIB, RHIC, eRHIC, ELIC, BES: LAS, APS, SNS, LCLS, NSLS-II, LCLS-II, FES: NDCX-II

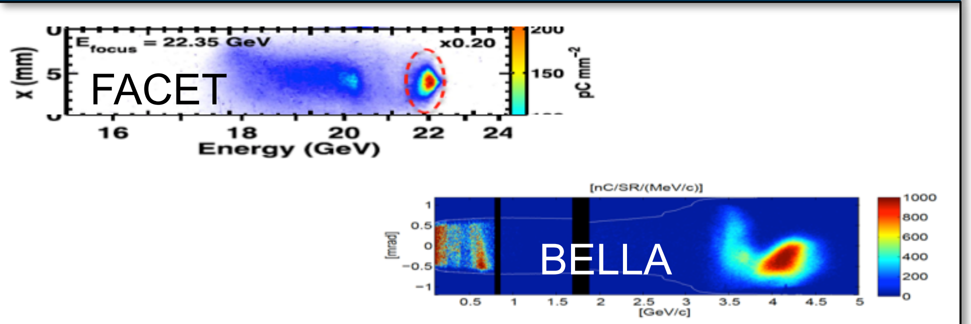
- **Team work for integration of multi-physics packages & algorithmic advances**
  - Established CAMPA collaboration (LBNL+SLAC+FNAL) for integrated accelerator modeling
    - White paper of CAMPA, input to P5 & to Snowmass: http://hifweb.lbl.gov/public/CAMPA/white_papers/
  - Strong computational collabations: e.g. NERSC, LBNL Computer Science Division, U. Md…

- **Implementation requires core programmatic support of several FTE (+ postdocs):**
  - new algorithms/physics/architectures, modularization, validation and maintenance
  - documentation, distribution (incl. website), user support, training and management
  - Funding-dependent additional efforts: integration of additional codes, consolidation, innovative accelerator concepts & technologies (not covered by existing projects), improved human interface

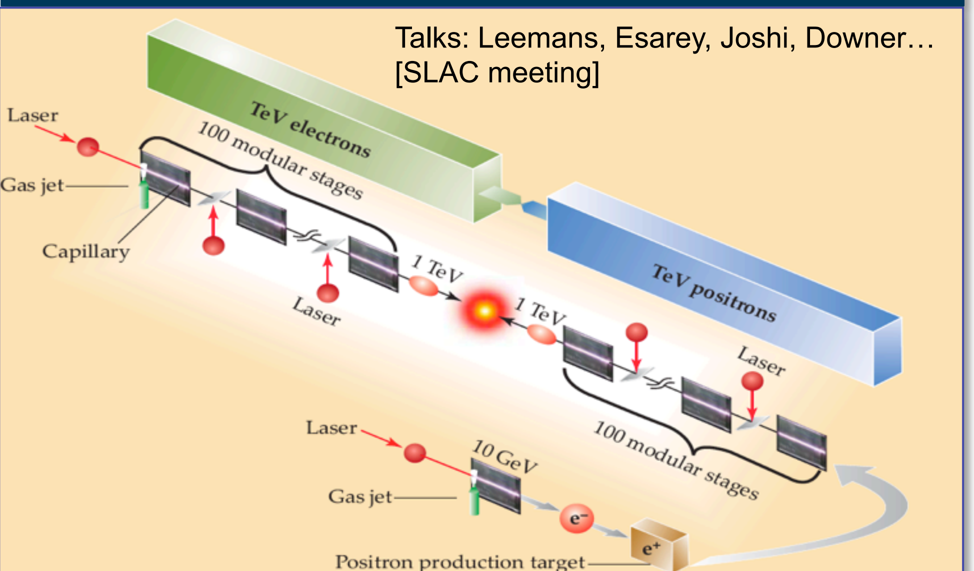
Future-generation accelerators at dramatically lower cost
advances in modeling will offer new opportunities

BERKELEY LAB

Multi-GeV beam/laser plasma accelerators



Laser-plasma (LPA) collider concept:
100x 10 GeV stages (1m ea.), injector, focus, e+



Beam driven-plasma collider concept:
40x25 GeV stages (1m ea.), injector, focus, e+

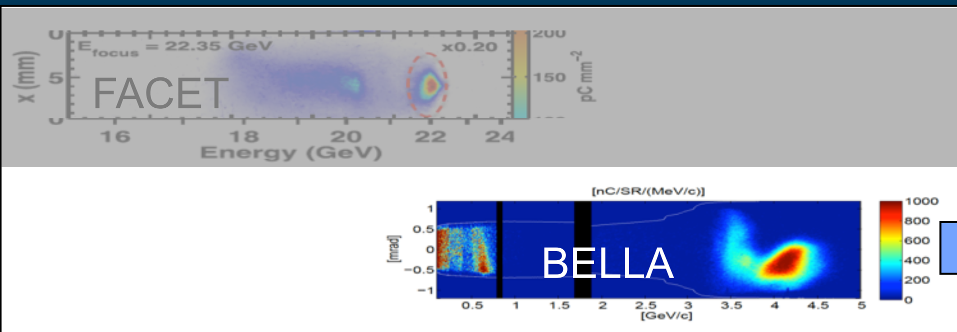
- Accelerator: EM + plasma + beam
  - Current: PIC-MPI: meter scale, 10 GeV, ε~0.1μm
  - Goal: 100 m scale, 1 TeV, ε~0.01μm
    - Radiation, scattering, e+ production
- Target plasma + guide: hydrodynamics
  - Current: 1D MHD plasmas, commercial gas flow
  - Goal: 3D shaped plasmas + kHz operation + heat
- Beam transport + focusing
  - Goal: fs, kA beams, focusing and intera
- High average power lasers
  - Goal: materials, dammage, optical propagation

Advances in computers & algorithms:
- real-time of single stages on clusters,
- design of colliders on supercomputers.

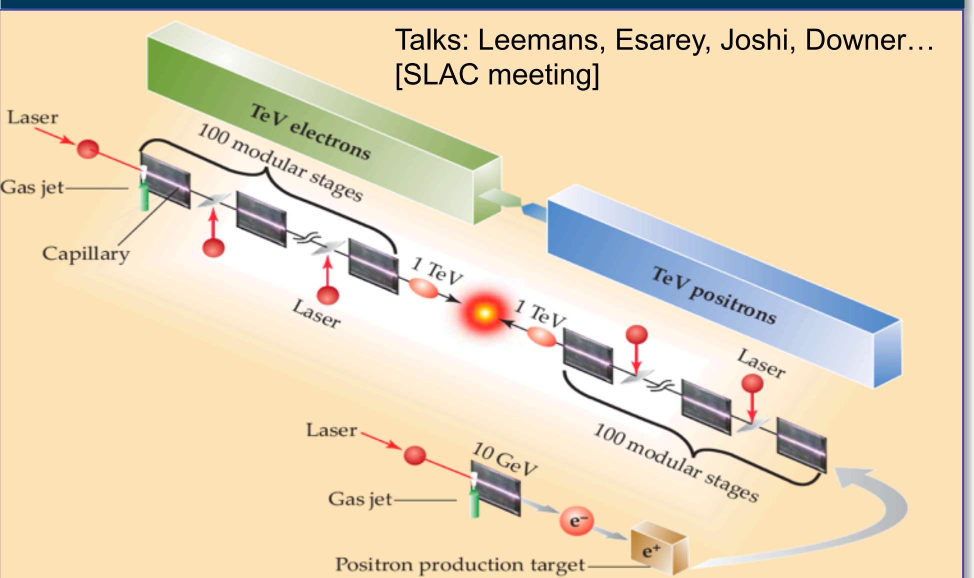
LPA example

Future-generation accelerators at dramatically lower cost
advances in modeling will offer new opportunities

Multi-GeV laser plasma accelerators



Laser-plasma (LPA) collider concept:
100x 10 GeV stages (1m ea.), injector, focus, e+



– Accelerator: EM + plasma + beam

3-D full PIC	K-BELLA	Collider
	$\sigma_{x,beam}$~1μm L_{acc}~1m	$\sigma_{x,beam}$~0.1μm L_{acc}~100m
Now Lab frame	~ 1year	~ 10^4 year
Now Boosted frame	~ 1hour	~ 1 year
Goal 2024 Boosted frame	<1min	~ 3-4 days
Goal 2024 Boosted frame + AMR + env. 10^6 cores	<10ms real-time on clusters	~ 1 hour parametric studies on supercomputers

Advances in computers & algorithms:

- real-time of single stages on clusters,
- design of colliders on supercomputers.

SLAC R&D Plans

Key thrusts of advanced accelerator computation at SLAC

- Maintain **ACE3P** as the premier parallel EM software for accelerator modeling through development of novel numerical algorithms in coordination with SciDAC.
- Collaborate under the CAMPA initiative on code integration in EM and beam dynamics for enhancing accelerator system simulation.

Medium-term Plan

- Develop a multi-physics modeling toolset including integrated EM, thermal and mechanical effects for SRF cavities.
- Integrate **ACE3P** with IMPACT for system-scale accelerator simulation.
- Implement new algorithms in **ACE3P** for efficient and accurate modeling of space-charge dominated devices such as klystrons.
- Collaborate with CS/AM scientists in nonlinear eigensolver and parallel adaptive mesh refinement for virtual prototyping of accelerators.
- Code support for **ACE3P** user community (~50 users & growing).

Long-term Plan

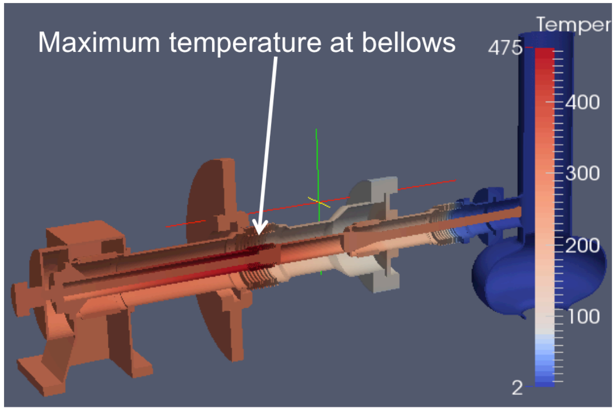
- Develop parallel optimization for multi-physics modeling of accelerators.
- Perform simulations for accelerator projects such as PIP2 and ILC to ensure operation reliability for specified machine design goals.

Multi-Physics Analysis for SRF Cavities

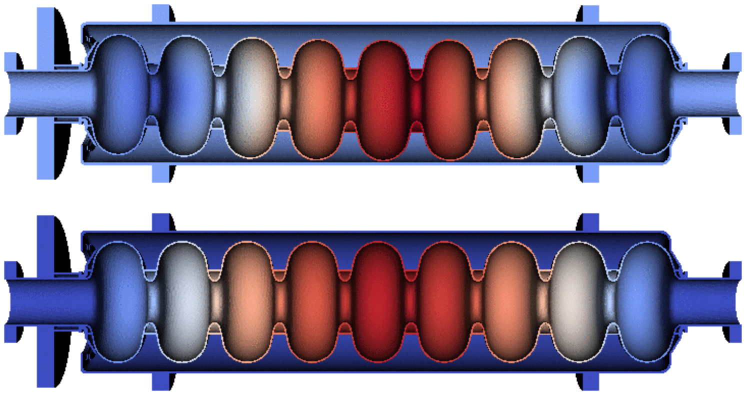
Develop an ***integrated modeling toolset*** including EM, thermal and mechanical effects for SRF cavities with emphasis on enhancing the following simulation capabilities.

- Study effects of *cavity imperfection* on higher-order-modes.
- Simulate *dark current* in cryomodule and evaluate its radiation effects through the cavity wall.
- Determine *Lorentz force detuning* and study *microphonics* of SRF cavities for pulsed and CW operations.

Temperature distribution in TTF coupler



Mechanical modes of dressed TTF cavity



ACE3P multi-physics modeling

Aim at providing a transformative modeling capability that can facilitate a full, realistic design for optimal machine performance and operation reliability.

Resource needs (US wide)

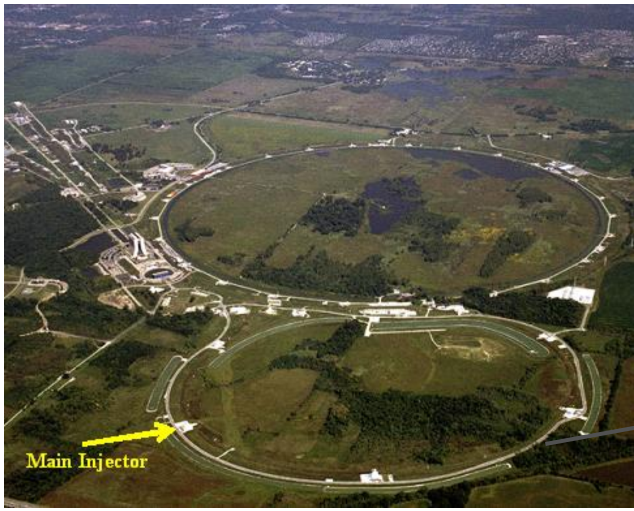
	Scenario B (FTE)	Scenario C (FTE)
Development for AA	3	4
Development for multi-MW	3	4
Development for structures	3	4
Development for energy deposition	1	2
Common Interfaces	1.5	2
Common Libraries	0	2
User Support	0	1
Students	4	10
Comp. Accel. Fellows	0	4
postdocs	4	8

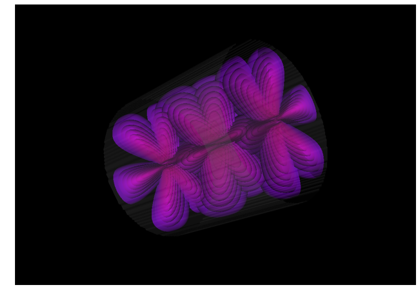
Summary of resource requests assuming effort in accelerator R&D thrusts remains the same as today. If will be adjusted if the overall program changes.

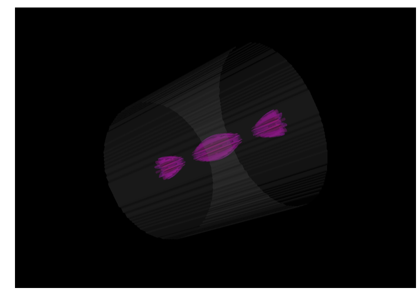
Summary

- Machines planned under the P5 advised program have increased complexity and stringent design requirements
  - need for multi-physics models and HPC capabilities
- Evolution of computing architectures requires continuing R&D on numerical algorithms
- To move forward we need a coherent, coordinated program
  - Start with a consortium of developers (building on ComPASS success)
  - Funded at the same level as the current individual efforts and projects, with modest increase for interoperability/coordination
  - If additional funding, establish a forum to develop and maintain common numerical and physics libraries
    - With increased training and education reach, through fellowships and additional opportunities for students, through enhanced University participation

Why HPC: accelerator numerical models 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!

Readiness for exascale computing on new architectures essential for Virtual Accelerator Modeling and Prototyping

- Impact (LBNL), Synergia (FNAL), and WARP (LBNL) selected for the NERSC Exascale Science Applications Program (NESAP)
  - early access to new architecture with help from NERSC, Cray & Intel staff
- Synergia and OSIRIS (UCLA) already ported on GPU and MIC
- CAMPA could provide the means to
  - Propagate know-how to other codes and, eventually,
  - development of common infrastructure optimized for new architectures

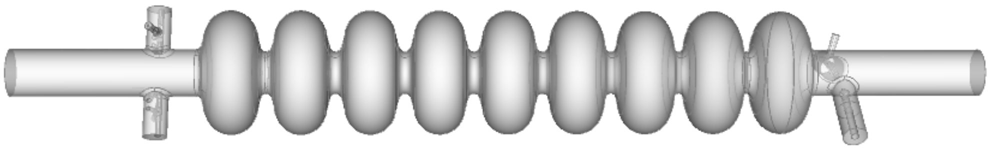
MARS

- MARS15 is a general purpose Monte-Carlo code for simulation of hadronic and electromagnetic cascades that is used worldwide for shielding, accelerator and detector applications.
  - Originated in 1974 at IHEP (Russia) and is developed since early 80's at Fermilab
  - Used in design of numerous accelerator systems and machine-detector interfaces in USA (Tevatron, Main Injector, Muon Collider, ILC etc.), Japan (J-PARC) and Europe (LHC, GSI, PSI, ESS etc).
  - Success proven by performance of the above systems and by overwhelming performance in international benchmarking over last two decades.
- Current State
  - It is unique in quality of description of physics processes from multi-TeV energies down to a fraction of electron-volt, with user-controlled possibilities to enhance certain phase-space regions.
  - It is unique in modeling of the 3D magnetic systems ranging in size from many kilometers to microns in the same setup, e.g. the entire 27-km LHC collider with tiny machine and detector components of interest.
  - 40 MARS installations worldwide with 300 users at ~33 Labs/Universities.

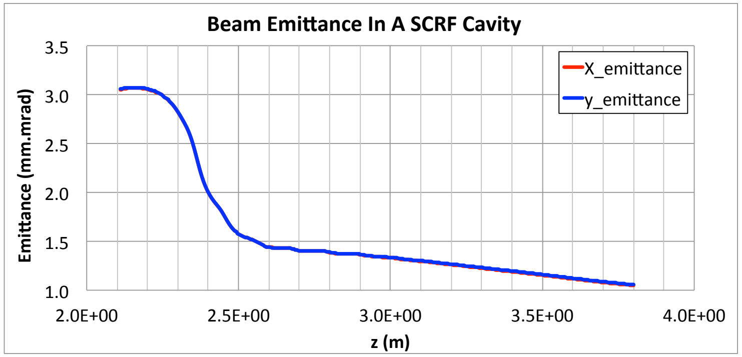
First-Year Accomplishments under CAMPA

LBNL and SLAC have started integrating **ACE3P** EM and **BLAST** beam dynamics codes' simulation capabilities.

- **ACE3P** and **IMPACT** for beam dynamics simulations with realistic models of electromagnetic elements - Impacts our ability to confidently predict performance including nonlinear effects.



Cavity geometry modeled with ACE3P to produce a 3D field map, followed by IMPACT tracking of a low energy beam using the field map



- **BLAST** codes integration for electron cloud simulation
  - Modularization of IMPACT mapping routines for future inclusion in multibunch Warp-Posinst ecloud effects simulations
- **ACE3P** and **Posinst** for secondary electron emission
  - Enables *high fidelity modeling* of realistic secondary electron emission provided by Posinst on accurate representation of cavity surface in ACE3P simulation.
- User support including email & phone exchanges, documentation and workshops