Accelerator Simulation

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U.S. DEPARTMENT OF ENERGY

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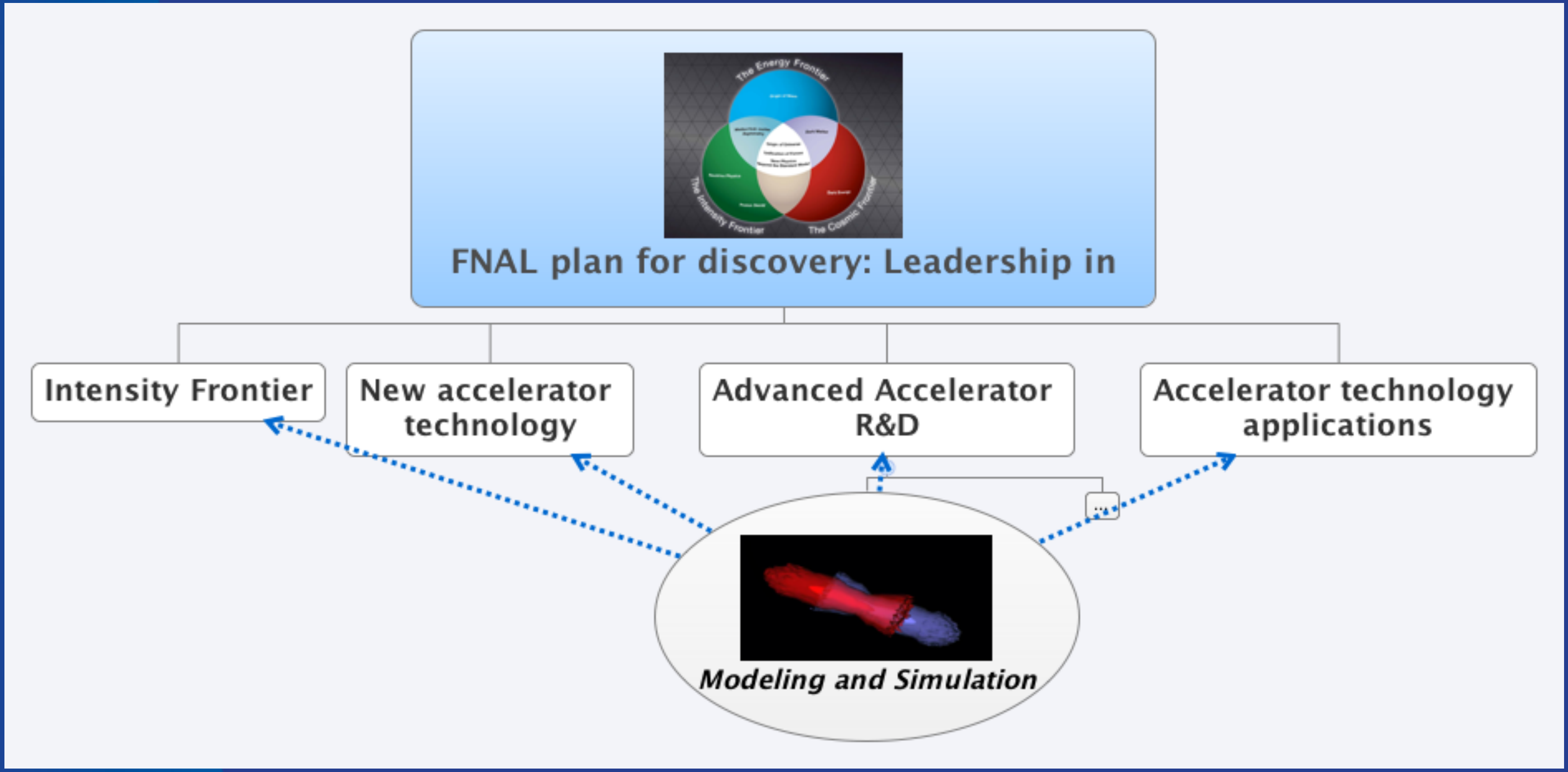
Accelerator Simulation and Modeling



- Computational physics is an essential component of accelerator science, complementing and adding to experiment and theory
  - Goals are driven by the other strategic area needs, and the need to develop the capability to utilize massive computational resources

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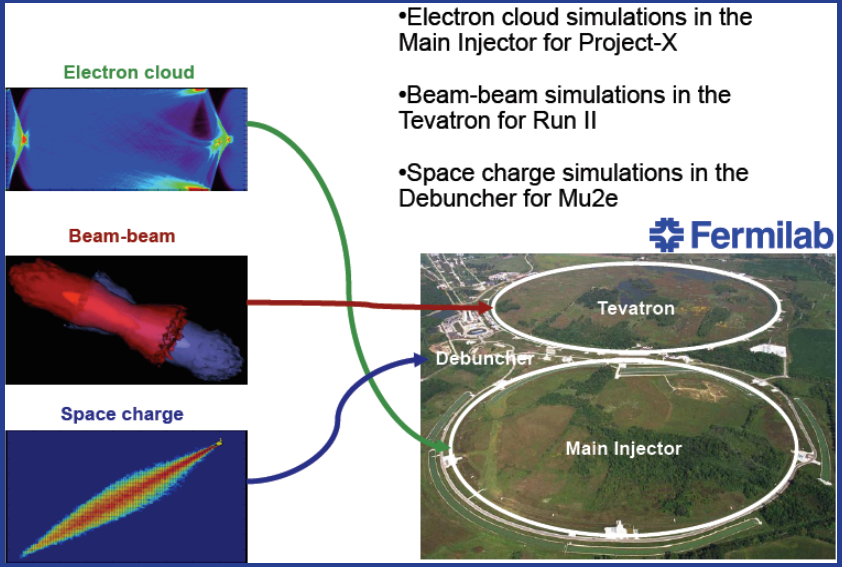
Accelerator Simulation in AA

- A mature activity (more than 10 year involvement)
  - '96-'02 ionization cooling (μ-collider/ν−factory)
  - '01-'11 multi-particle dynamics (Run-II)
  - '01-'07 single and multi-particle, electromagnetics (ILC)
  - '09-... Single-particle, multi-particle (Project-X, Mu2e, …)
- Emphasis on
  - Advanced computation development
  - Realistic applications (multi-scale, multi-physics)
- Shared service model required
  - Example: space-charge capabilities



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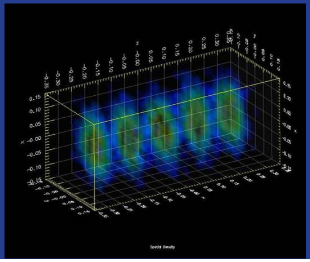
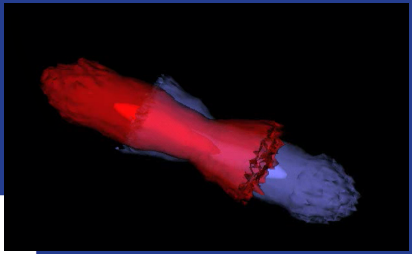
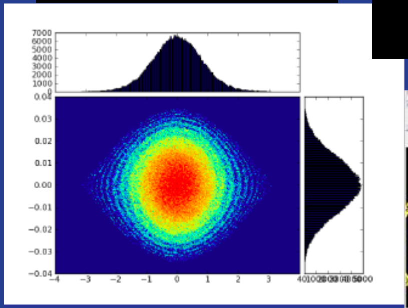
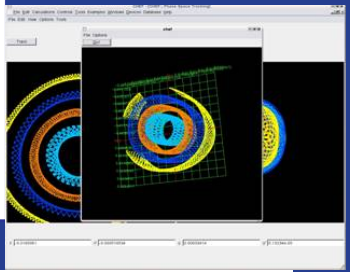
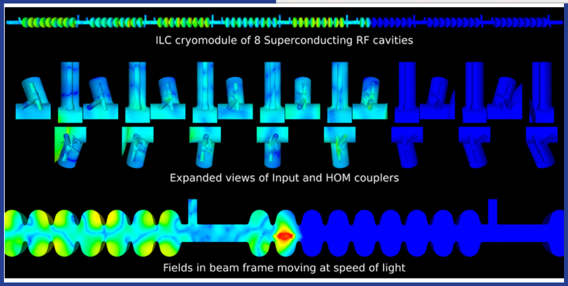
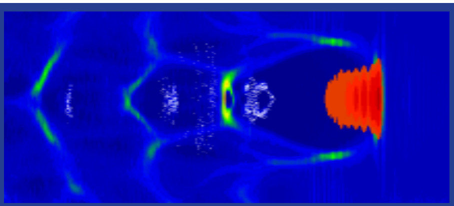
Major thrust areas of computationally challenging science

- Understand evolution of beams through optical systems, including self forces and the forces of interactions
  - Beam-beam, space-charge, electron cloud, …
  - Steering and phase-space manipulation systems (optics, cooling, …)
- Design of structures to maximize acceleration while minimizing deleterious effects of wakefields, heating, multipactoring, …
  - Electromagnetics, thermal, mechanical
- Advance accelerator science
  - Laser and plasma wakefields
  - Muon capture and acceleration
  - Two beam acceleration



BTW, all models are wrong, some models are useful

Ultimate goal is to maximize the usefulness of our models

In 10 years, we would like to be able to:

- Provide simulation support and guidance to future lepton collider design and R&D
  - Electron or muon, conventional or wakefield or ?
    - Develop expertise on required tools, develop and deploy required new capabilities
- Provide simulation support for parameter optimization of Project-X accelerators
  - in preparation for commissioning
  - design for possible interface with neutrino factory
- Deploy computational and physics algorithms that continue to take advantage of Leadership Computing Facility resources

Activity Strategy

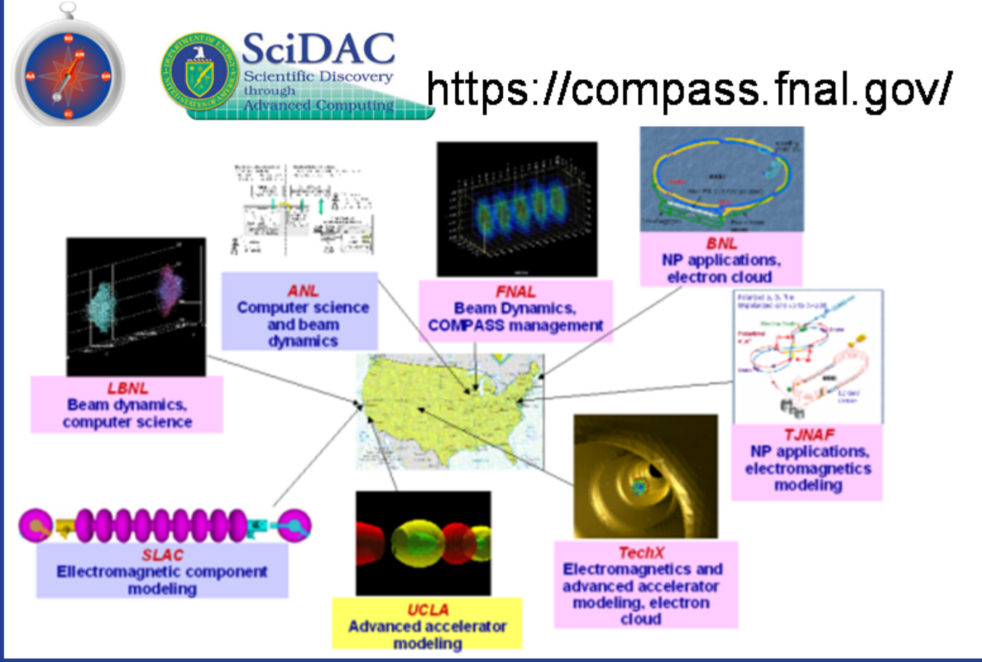
- Develop computational tools
  - Realistic physical system modeling (beam dynamics, accelerator components)
  - Emphasis on intense beams and their applications
    - High Performance Computing (HPC) requirements
- Provide expertise on deployment and utilization of computational tools
  - Both internally (FNAL) and externally developed
  - Emphasis on intense beam and AA applications
- Develop or contribute to the development of applications of such tools

How do we reach these goals: plans and milestones

But first, where are we now

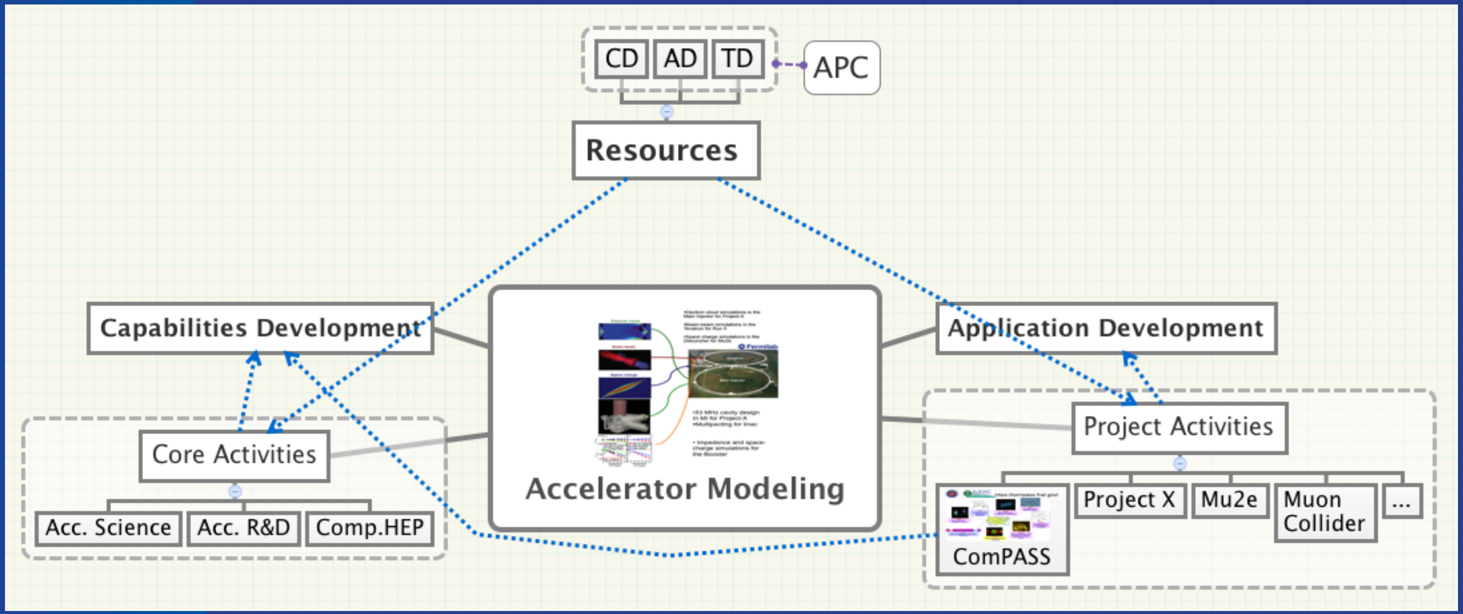
Accelerator Modeling Project: ComPASS*

- Fermilab leads the SciDAC2 ComPASS project, which aims to develop HPC accelerator modeling tools for
  - Beam dynamics: multi-physics, multi-scale
  - Component design: thermal, mechanical, electromagnetic
- Funded by the offices of HEP, ASCR, NP and BES at $3M/year
- The Fermilab team focuses on beam dynamics tools and application development



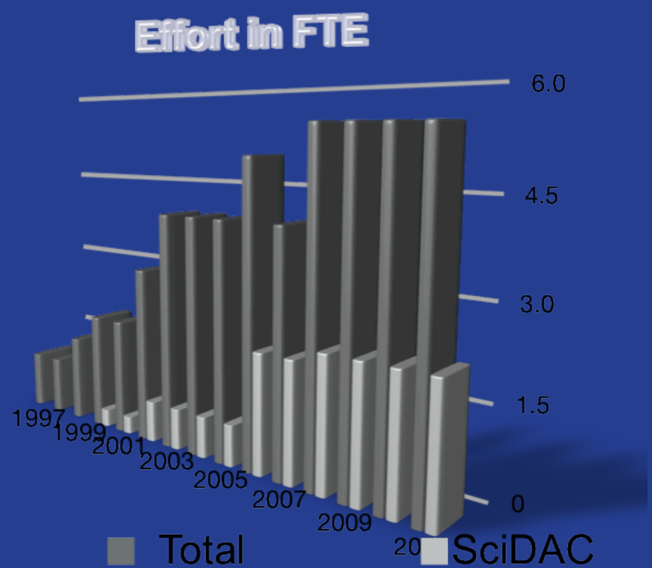
*Community Project for Accelerator Science and Simulations

Activities are highly leveraged



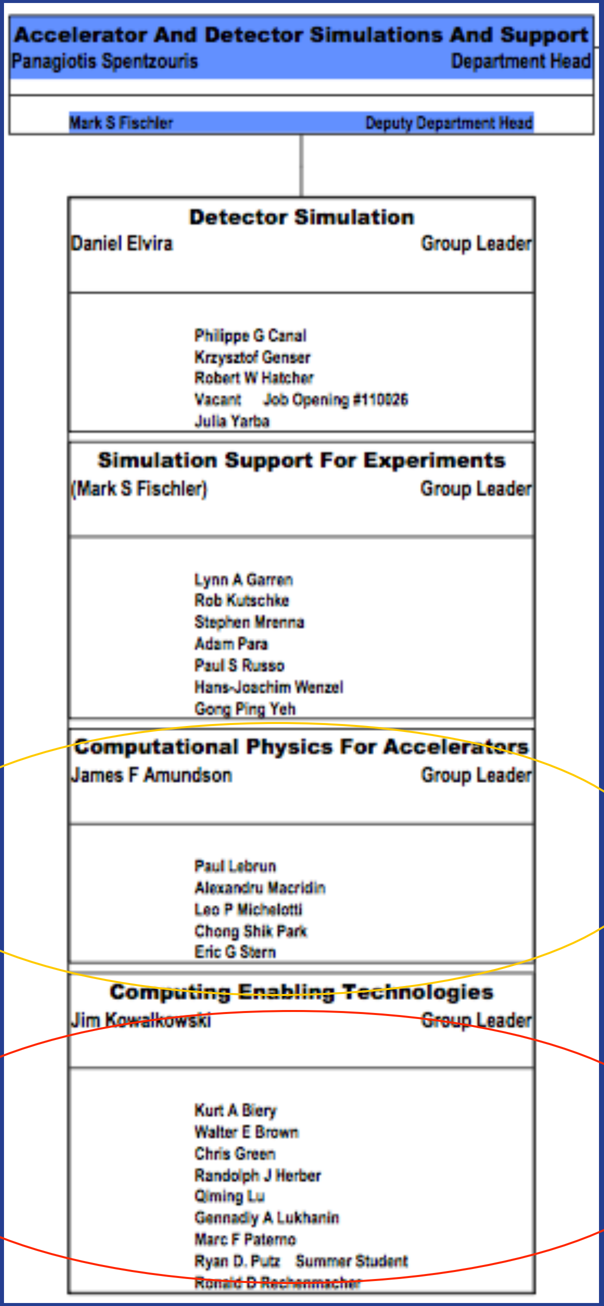
A well balanced but sensitive ecosystem!

- ComPASS & core supports computational capability development and provides access to
  - HPC resources
  - Math, computational and accelerator science expertise
- Projects support applications

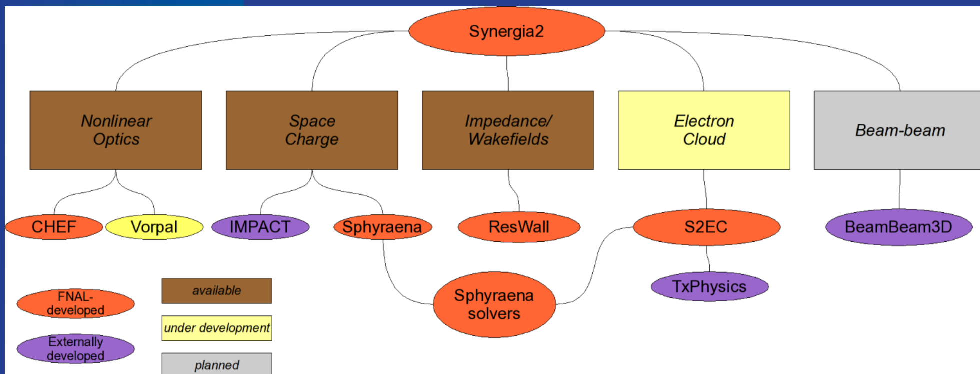


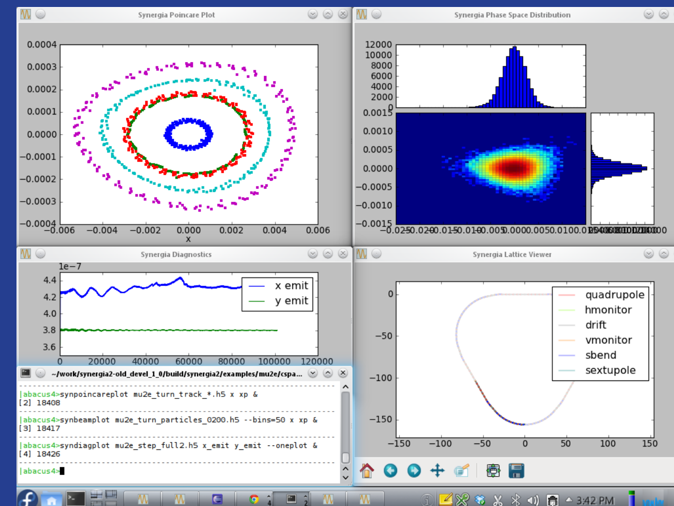
Resources

- Effort concentrated in CD/ADSS, but work closely with AD and APC, to develop and deploy accelerator science applications
  - 5 FTE in ADSS/CPA
    - Both “core” and project funds (~50/50 split): SciDAC, Project-X, Mu2e, ILC (in the past), proton research for RunII (past)
  - Services and generic infrastructure development support (tools, new technologies) from ADSS/CET
    - Computational HEP, proton research, project (indirectly; any new development is shared)



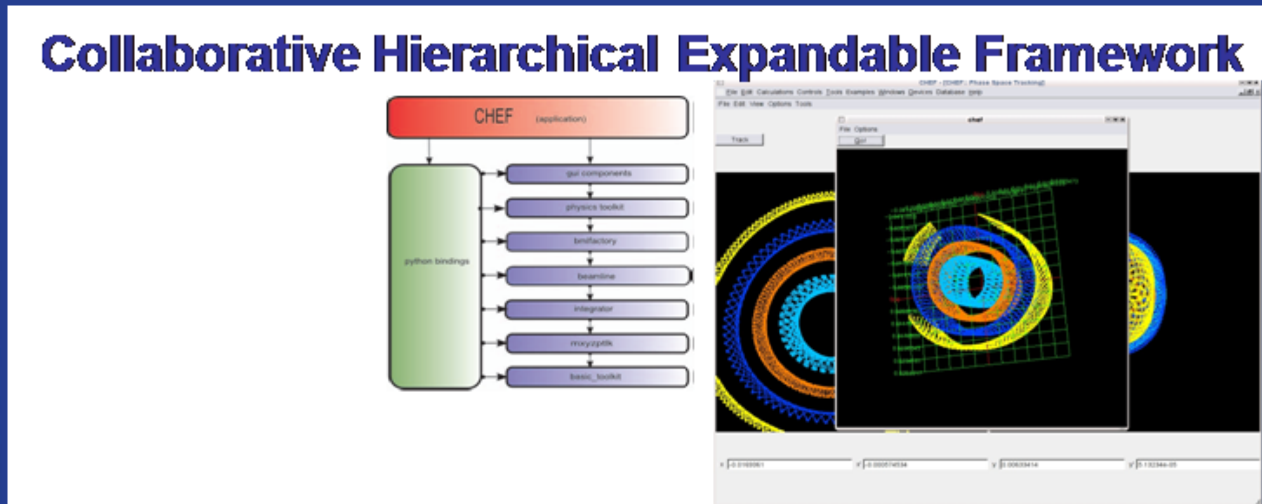
ComPASS tools development: Synergia





- Beam Dynamics framework with fully 3D PIC capabilities
  - Utilizes both native and external physics modules/algorithms
  - Includes space-charge & impedance (single and multi-bunch)
  - Single-particle physics from CHEF
- Runs on desktops, clusters and supercomputers
- Flexible framework allows for fully dynamic simulations including ramping, feedback, etc

Tools development, continued: CHEF

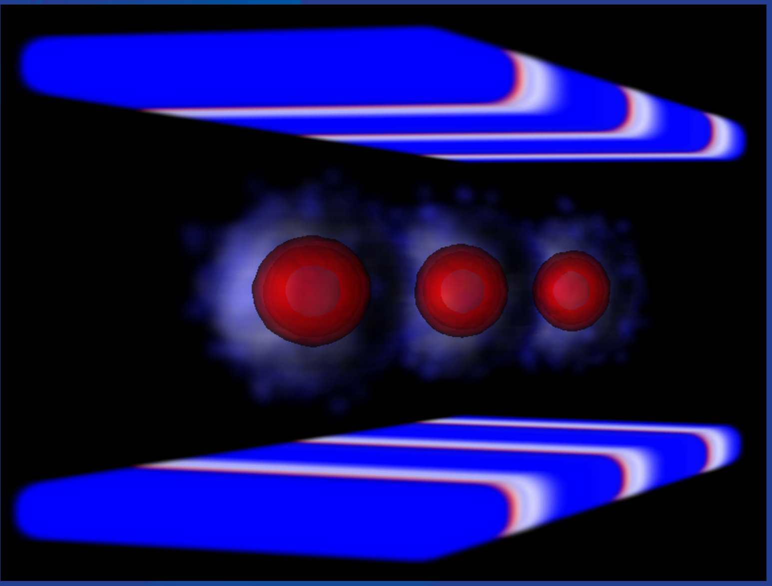


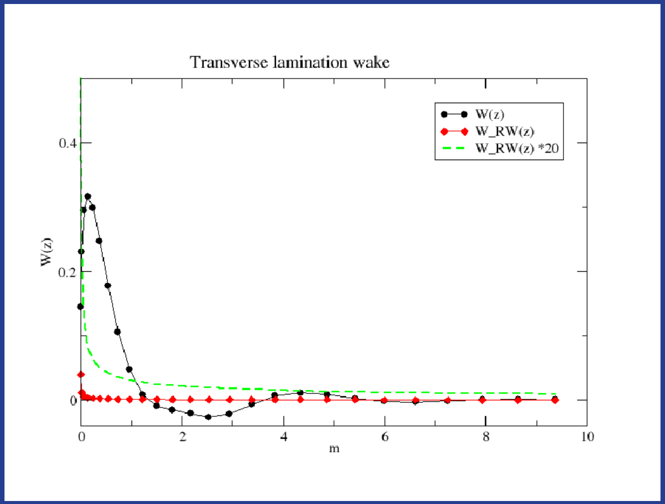
- CHEF originally developed at Fermilab starting in the early 90's
- Single-particle optics with full dynamics
- Can be reduced to arbitrary-order maps
  - We have done demonstration calculations in Synergia to 15th order
- Supports customizable propagators (fully extendable)
- MAD and XSIF parsers
  - Internal representation not limited by MAD parameters

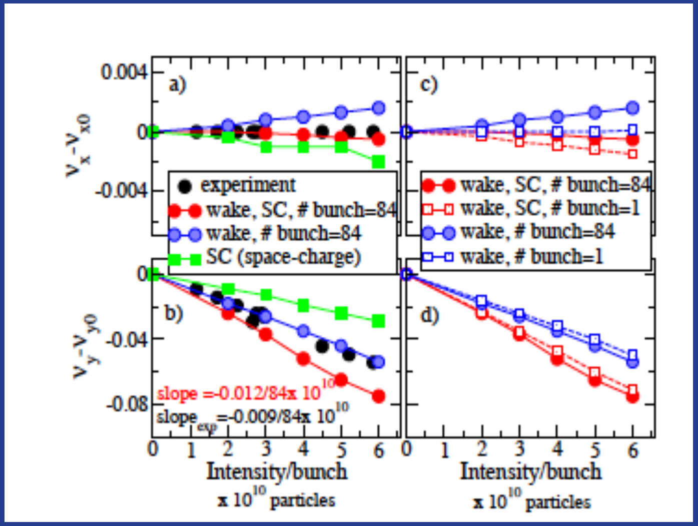
Recent Synergia applications: careful treatment of impedance of laminated structures

Literature calculations in frequency domain involving different regimes don't trivially translate to a "simulation ready" wake function.

➢Capability utilized for FNAL Booster modeling, Phys.Rev.ST Accel.Beams 14:061003,2011







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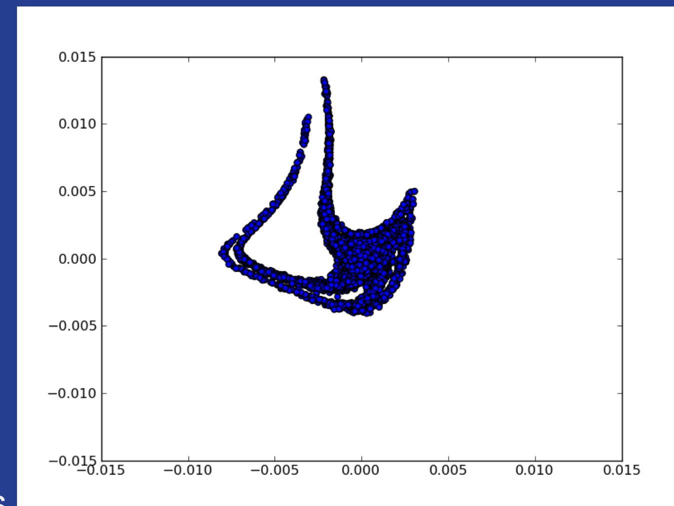
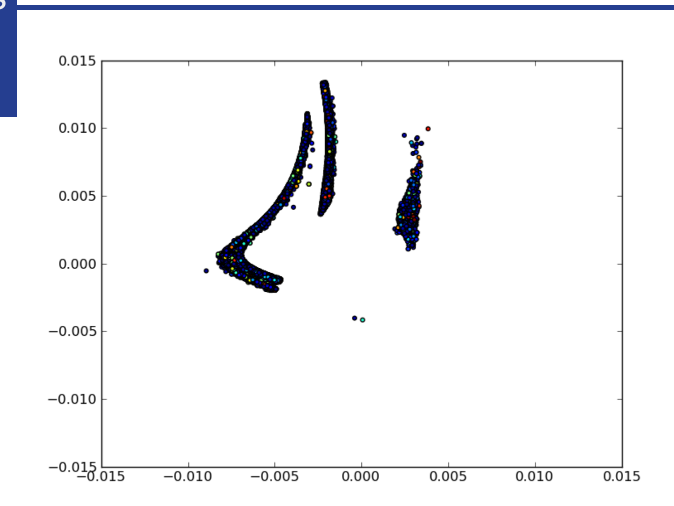
Recent application: Mu2e extraction design

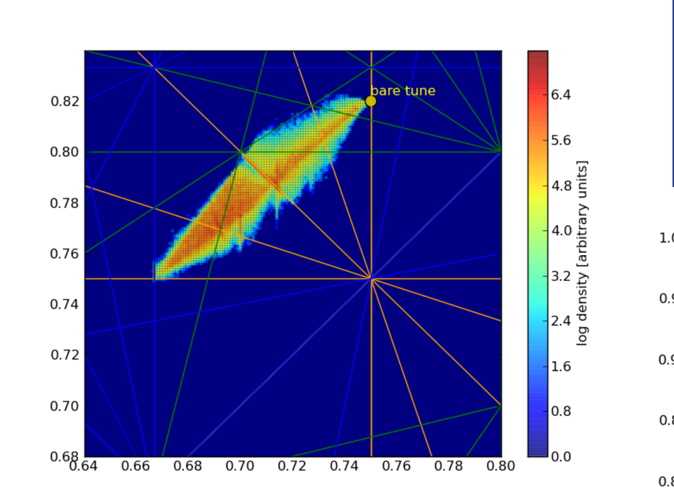
- Model resonant extraction including space-charge at the Debuncher :
  - Optimize tune and resonant extraction parameters to minimize losses

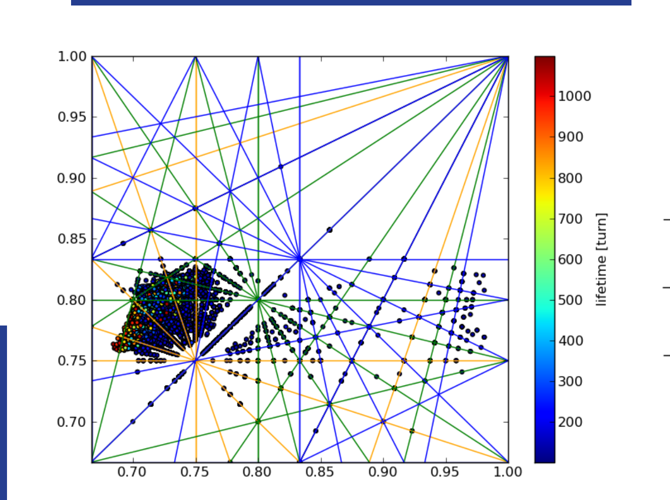
ν_x=9.75, ν_y=9.82

- phase space of entire beam
- phase space of lost particles
- tune footprint
- tunes of lost particles









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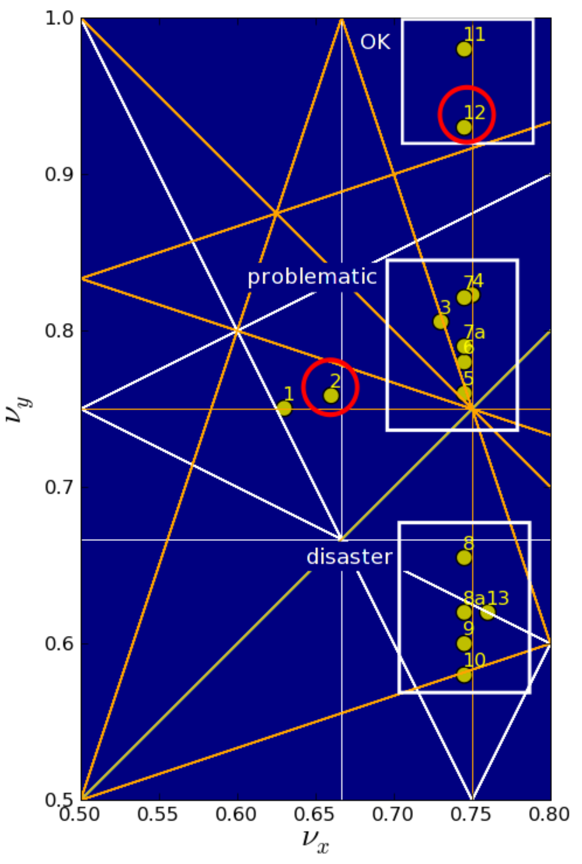
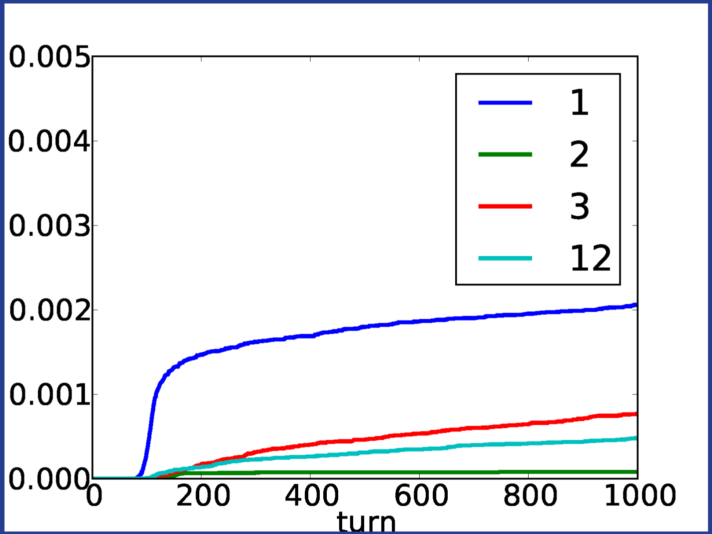
Original Mu2e design parameter scans



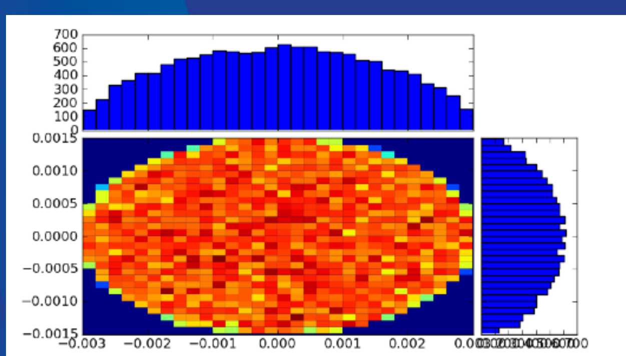


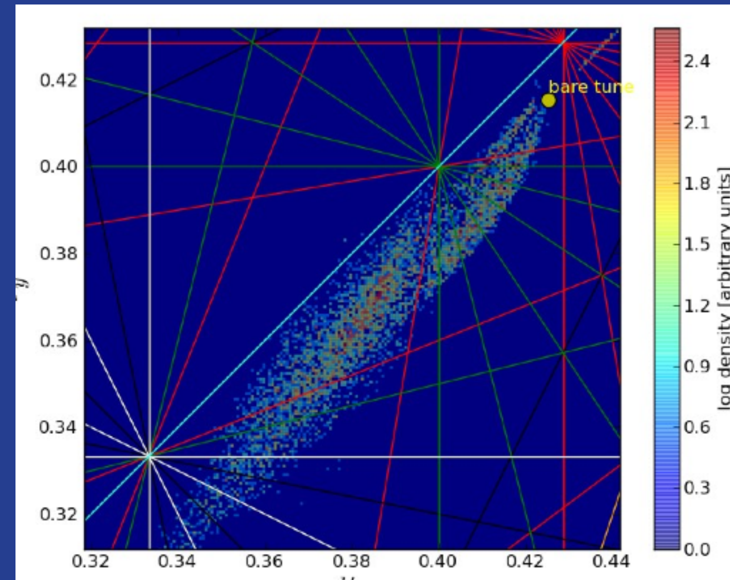
Each tune point required ~ 1day running on 2k cores

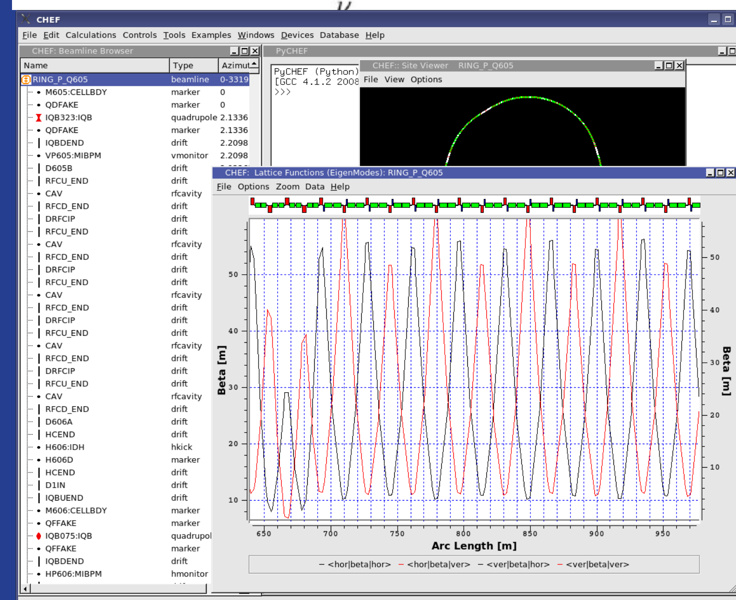
Even the most optimal case has unacceptable losses, so studies contributed in decision for different design parameters

Recent application : MI space-charge

- Begin modeling space charge effects and mitigation techniques for Main Injector with Project-X beam parameters
- Extend Synergia to include realistic apertures and fringe fields and study losses and mitigation, if necessary

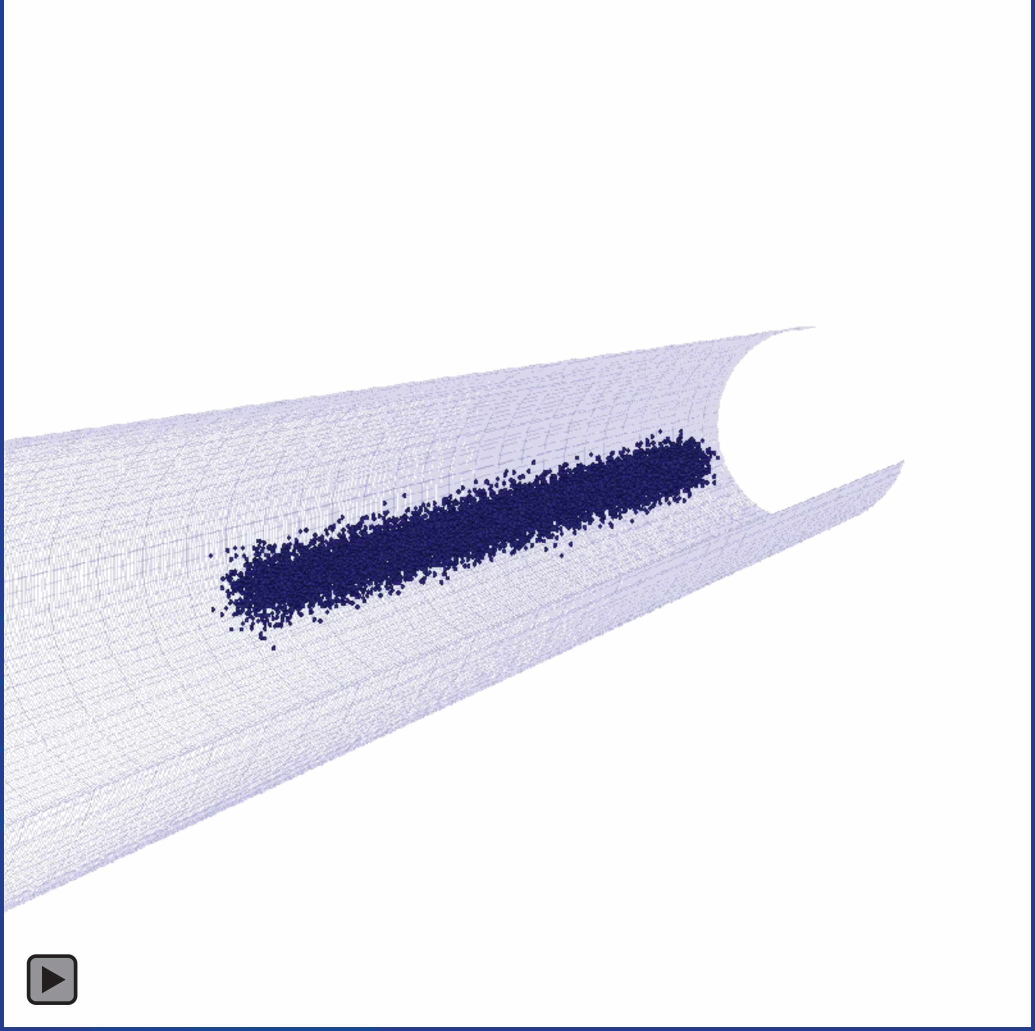




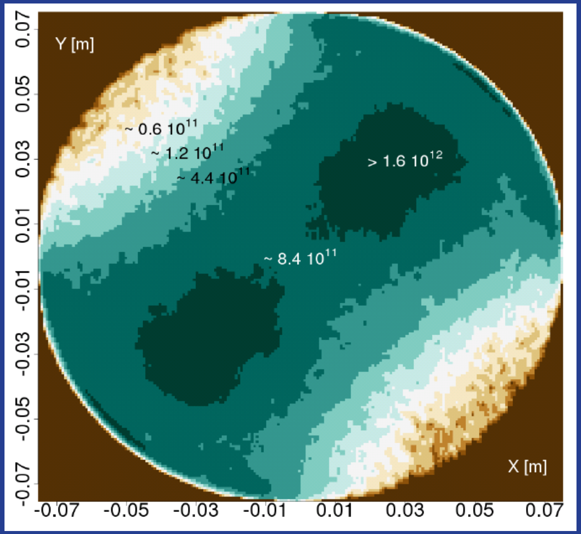


Utilization of ComPASS tools example

ComPASS VORPAL e-cloud simulation of MI experiments



Model microwave experiment (only possible with ComPASS tools), RFA response, code comparisons with “standard” tools such as POSINST



FERMILAB-PUB-11-228-APC-CD, submitted to PRSTAB

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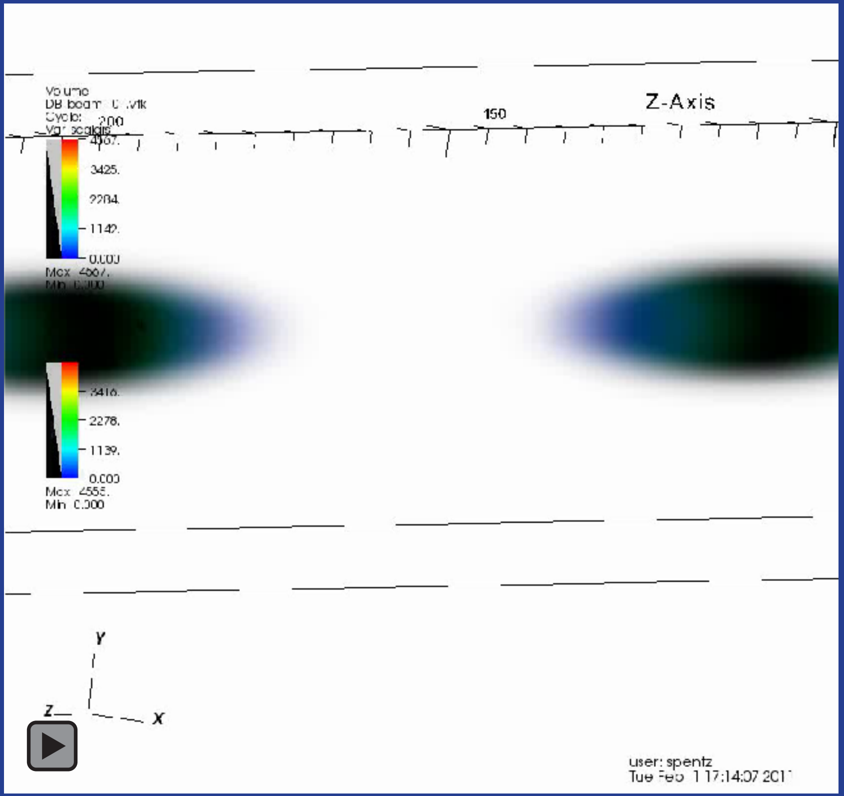
(A SciDAC Highlight) Tevatron example

- Improve Tevatron performance: understand beam-beam & impedance effects with 36 on 36 bunches
    - Simulations only possible with HPC resources: runs at NERSC and ALCF used 6M core-hours

➢ Success! Simulations result in improved operating parameters; reduce losses thus reducing radiation damage and increasing luminosity (physics reach)!

Phys. Rev. ST Accel. Beams 13, 024401 (2010)

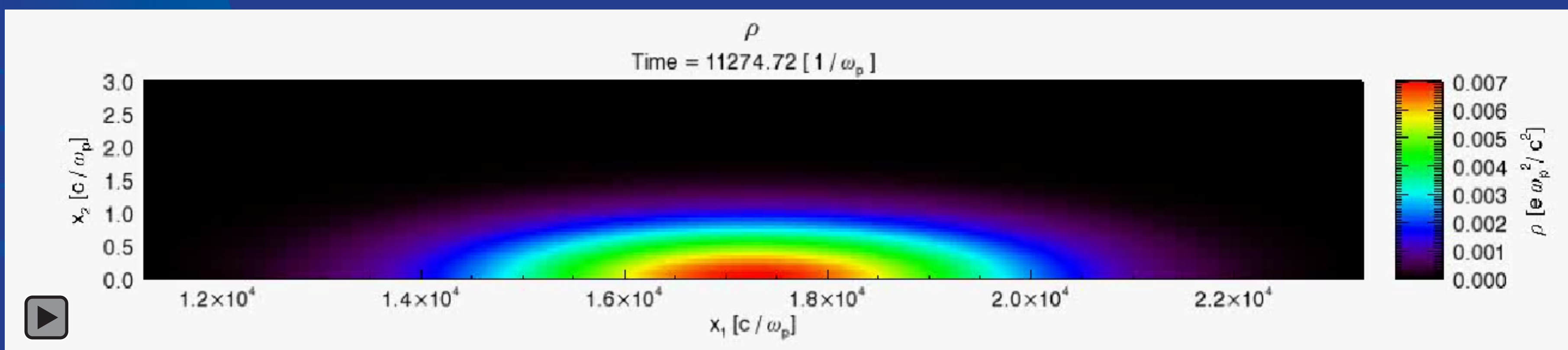


BeamBeam3D modeling of collective effects in Tevatron beam-beam collisions

Example of collaboration benefits: proton driven PWFA (protoplasma)

Work with UCLA to explore parameter space for the experiment

	n_p (10^{15} cm^{-3})	N (10^{11})	n_b/n_p (10^{-3})	ε_N (mm mrad)	γ	σ_r (μm)	σ_z (cm)	β^* (cm)	c (10^{-3})	L_{plasma} (cm)
FNAL1	10	1	7.05	3.33	128.89	30	10	3.52	552	~ 200
FNAL2	10	1	0.635	3.33	128.89	100	10	38.71	4.5	~ 200
FNAL3	10	1	7.05	0.33	128.89	30	10	35.15	5.5	~ 200
SPS CERN*	0.7	1.15	2.17	3.845	480.61	200	12	500	1.4	~ 1000



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Computing is evolving: new architectures

- **What will they look like?**
- **GPUs, SIMDs**
  - **How to move forward: porting code and developing new code**
    - **Parallel scalability**

SIMD units

VMX SSE/2/3/4

GPGPUs

CUDA STREAM

- SIMD
  - Vector co-processor
  - Available in most common CPUs
- GPGPU
  - Graphics Processing Units
  - Up to ~ 1 TFlop/s per board
  - "Add-on" co-processor
- Ultra-Massively Parallel
  - Scalability to over 10^5 cores

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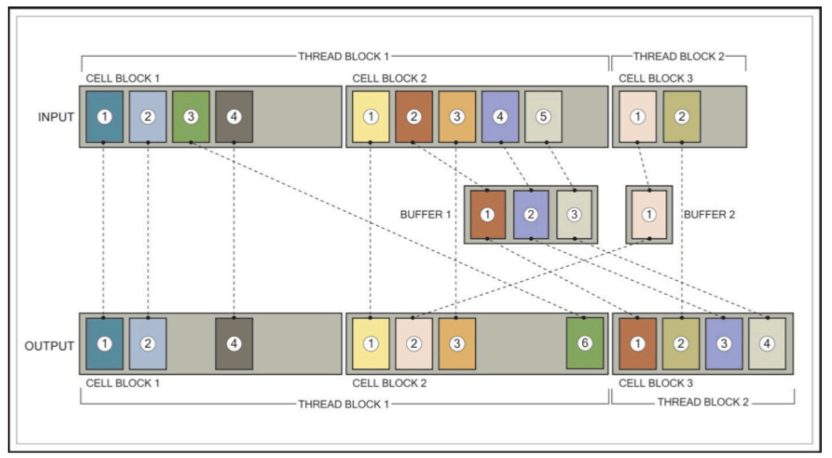
GPU acceleration for EM PIC

Solver Step	Intel Nehalem (ns)	Tesla C1060 (ns)	Fermi C2050 (ns)
Push	81.7	1.13	0.89
Deposit	40.7	1.06	0.78
Sort	0.5	1.13	0.57
Total	122.9	3.32	2.24

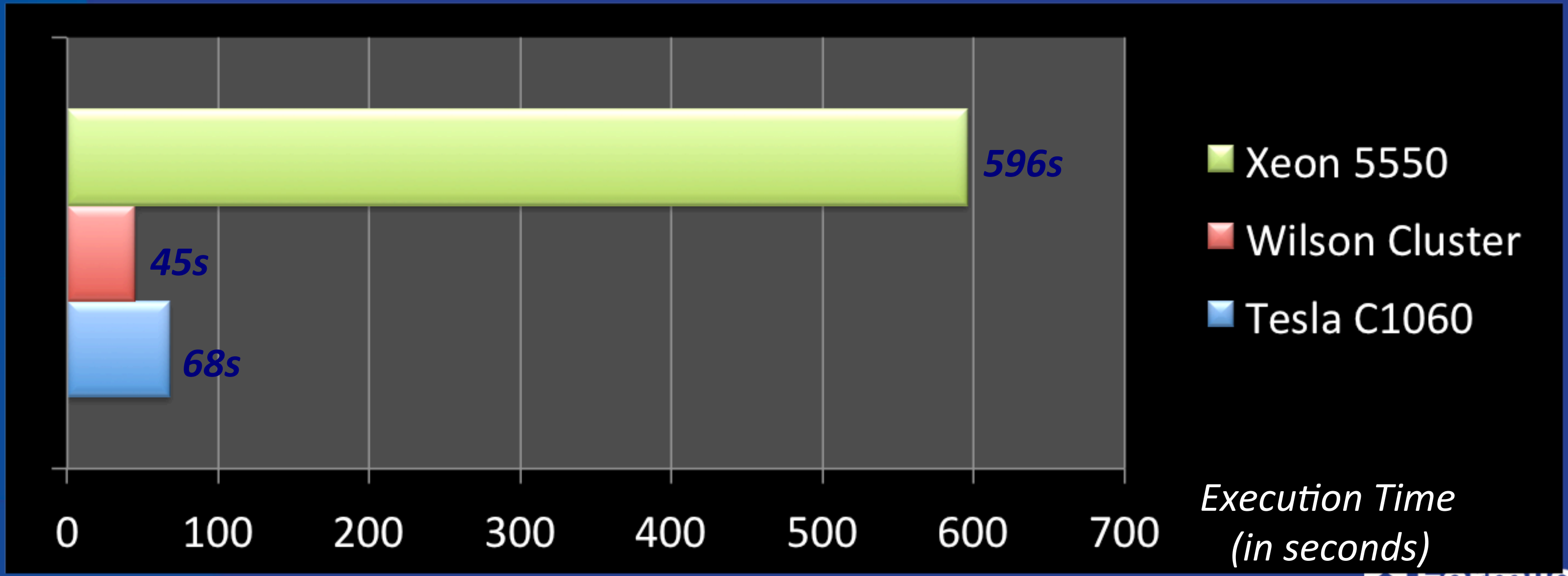


- Algorithms are hybrids of previously used techniques
  - Vector (from Cray), tiling (from cache-based), domain decomposition with particle re-ordering (from distributed memory)
- Overall speedup of about 55 for 2+1/2D EM PIC code

➢ **This is a new activity for ComPASS, in-house effort, we will need to formalize and define within SciDAC3 and co-design center era!**

GPU acceleration for electrostatic PIC

- Benchmark Problem:
  - Grid of 64x64x512 = 2,097,152 cells, with 20,971,520 particles (10 particles per cell)
- Comparison systems:
  - **1. Intel Xeon X5550, single process @ 2.67GHz;**
  - **2. Fermilab Wilson Cluster, dual Xeon X5650 2.67GHz nodes with 10Gbps Infiniband interfaces. 16 nodes / 128 cores used**
  - **3. NVidia Tesla C1060, 30 streaming multi-processors @ 1.30GHz in a single GPU**



Goals, risks, and milestones

ROADMAP TO OUR LONG TERM GOALS

FY12 Goals

From ADSS budget presentations, excuse the extreme detail…

- Application area: Project X, Main Injector
  1. Deliverable: model with multipole errors and simple apertures
     - Milestones: Technical note on losses. Q1
  2. Deliverable: Restart capability in Synergia 2.1.
     - Milestone: production with10,000 turn MI runs. Q2
  3. Deliverable: Advanced aperture capability in Synergia 2.1.
     - Milestone: Production with detailed tracking and loss recording. Q3.
  4. Deliverable: Simulations of transmission experiments.
     - Milestone: Technical note on comparisons between simulations and experiments. Q4
  - Risk: 1-3 project funding, (4) understanding experiment (systematics, setup)

FY12 Goals

- Application area Mu2e
  1. Deliverable: Synergia 2.1 simulation framework for new extraction plan.
     - Milestone: Presented to Mu2e Resonant Extraction Group. Q2.
  2. Deliverable: Simulations of RFKO
     - Participate in experimental studies of RFKO and analysis. Milestone: Data analysis results guide Synergia model, model used for design. Technical note. Q4
  - Risks: project funding, no experience with technique, experiment could not produce as expected.

FY12 Goals

- New Technologies:
  1. Deliverable: Optimization of GPU code.
     - Milestone: Technical note on profiling and optimization. Q1
     - Milestone: Full simulations using GPU. Q4.
  2. Deliverable: Development of hybrid OpenMP/MPI implementation. Q2.
     - Milestone: Hybrid code that passes unit tests. Q3
     - Milestone: Full simulations using hybrid OpenMP/MPI. Q4.
  3. Deliverable: Integration of hybrid OpenMP/MPI prototype in Synergia.
     - Milestone: hybrid code released. Q4
  - Risks: it is R&D in collaboration with UCLA and LBNL math & CS, utilizes SciDAC tools that we have no control of their development

FY12 Goals

- Booster (PIP): multi-bunch impedance simulations.
  - Milestone: Technical note on comparison with Booster experiments. Q3
  - Risk: experiment interpretation & parameter control impacts model accuracy
- SciDAC3 (ComPASS): prepare SciDAC3 proposal
  - Milestone: submit proposal to DOE. Q1.
  - Risk: smaller overall budgets prolong budget negotiations, weaken proposal

FY12 Goals

- Support e-cloud experimental effort.
  1. Deliverable: complete VORPAL/POSINST comparisons, improve models
     - Milestone: Technical note. Q2
     - Risk: depend on input from unfunded collaborators
  2. Deliverable: Detailed RFA simulations in VORPAL, begin model construction for experimental setup.
     - Milestone: Technical note. Q4

FY12

- Protoplasma support
  1. Deliverable: develop FNAL expertise on PWFA, utilizing ComPASS tools
     - Milestone: parameter optimization for self-modulation experiment
     - Risk: no available effort to develop application, need funding for post-docs
- Muon collider support for HPC needs
  1. Deliverable: understand needs, plan development
     - Milestone: Plans and requirements document
     - Risk: it takes two to dance (funding, resources)

FY13 activities

- SciDAC3 ComPASS
  - ComPASS proposal accepted mid of FY12
  - Risk: if not, reduced support for capability development, loss of access to non-FNAL HPC capable codes and expertise
- Parallel workflow Optimizer released (a ComPASS deliverable)
  - Begin developing applications for muon beams
    - Risk: clear plan for muon beam applications required
- Electron cloud experiment support and data driven model improvements
- Incorporate plasma code capabilities in beam-dynamics frameworks (a ComPASS goal for lepton collider design)
  - FNAL goal: Protoplasma design delivered
    - Risk: no manpower
- Continue Project-X, Mu2e applications, expand PIP support
- Continue algorithmic development for new technologies

FY14-16

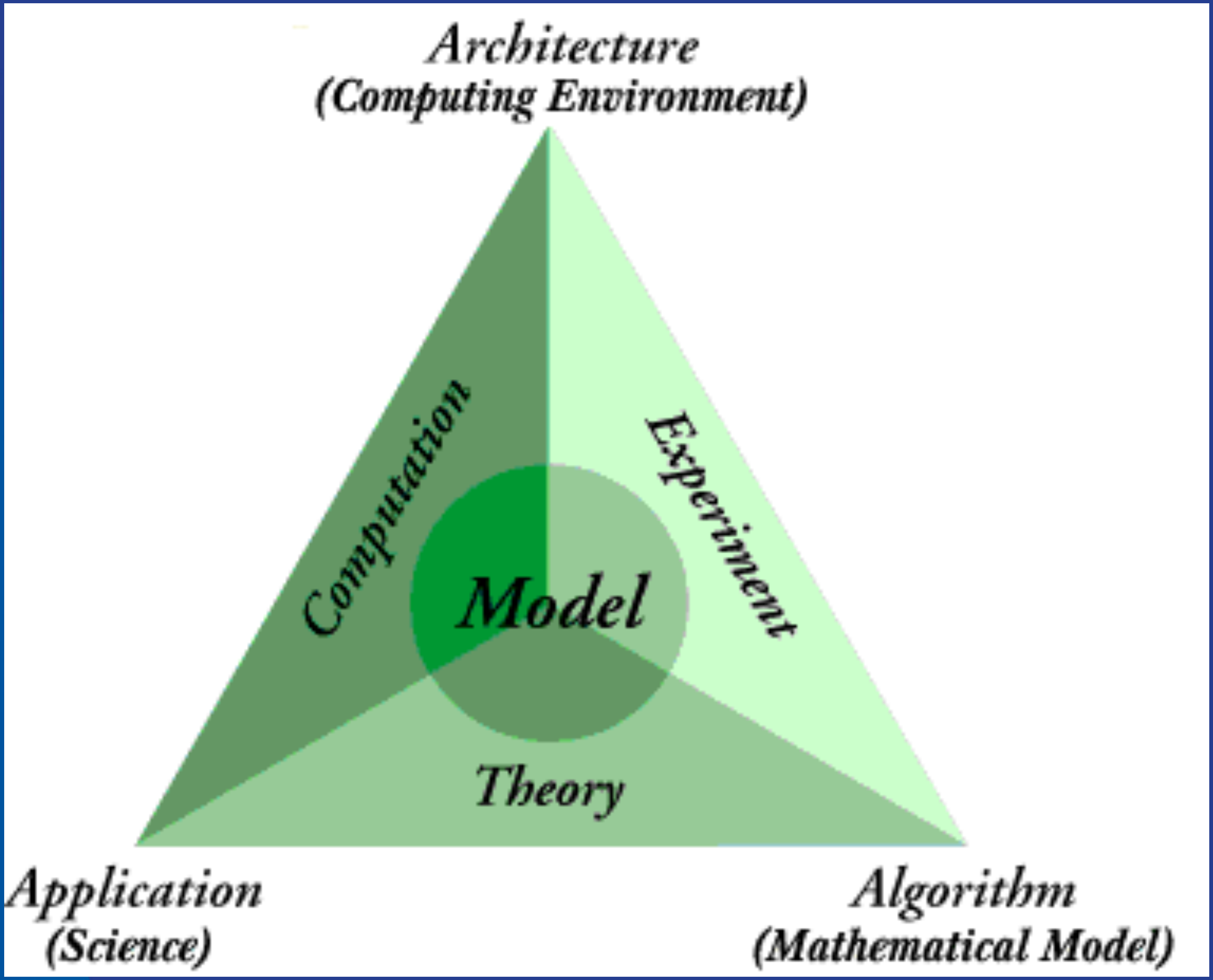
- Parallel optimization tools fully deployed
  - Utilization for Project-X and other FNAL design problems
- Improved scalability allows more multi-physics, multi-scale applications
- Production runs on “hybrid” computing environments
- ComPASS renewal
- Risk: HPC tools development is R&D, expect delays, especially if budgets continue to follow recent trends. Significant dependence on HPC technologies developed elsewhere. If ComPASS not renewed, see previous slide.

Out years

- ComPASS capabilities fully deployed on hybrid CPU+GPU(?) environments
- Performance optimization (of capabilities)
- Parameter optimization (of designs)
- Help guide development of new techniques and technologies.

Conclusions

- I hope it is clear that the above perception is false
- Computational accelerator physics has its own “cable mess” as it must balance capability development R&D with accelerator science R&D support
- Limited resources make planning and plan execution challenging, much like any hardware activity



And, BTW, I think that this is better than the Venn diagram

Mostly protoplasma design results

EXTRAS

UCLA

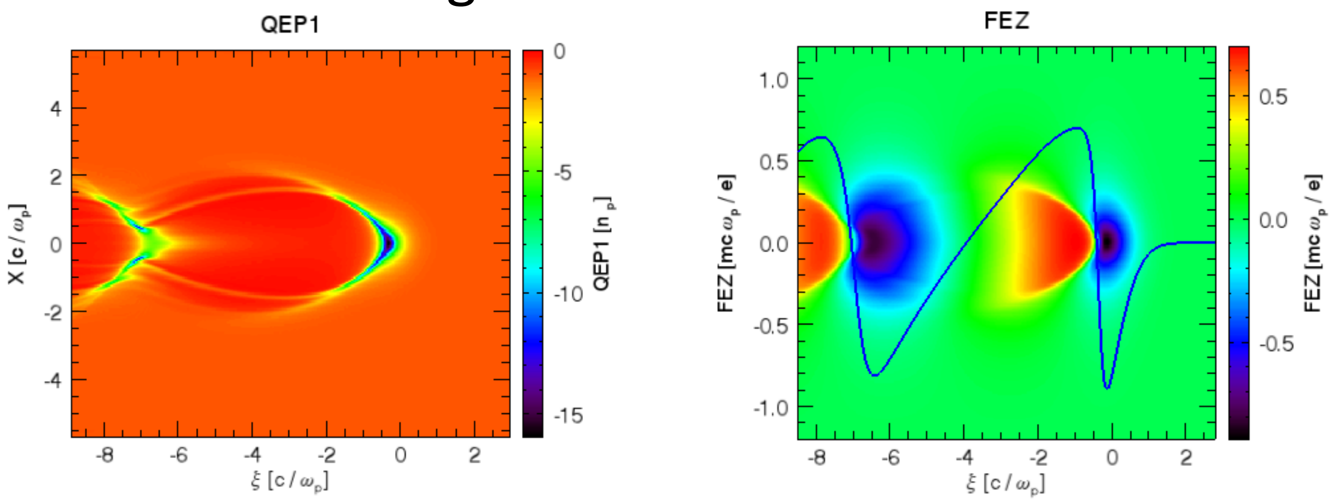
Proton Beam Driven Plasma Wake Field Accelerator At FNAL

Weiming An, Warren Mori, Chan Joshi

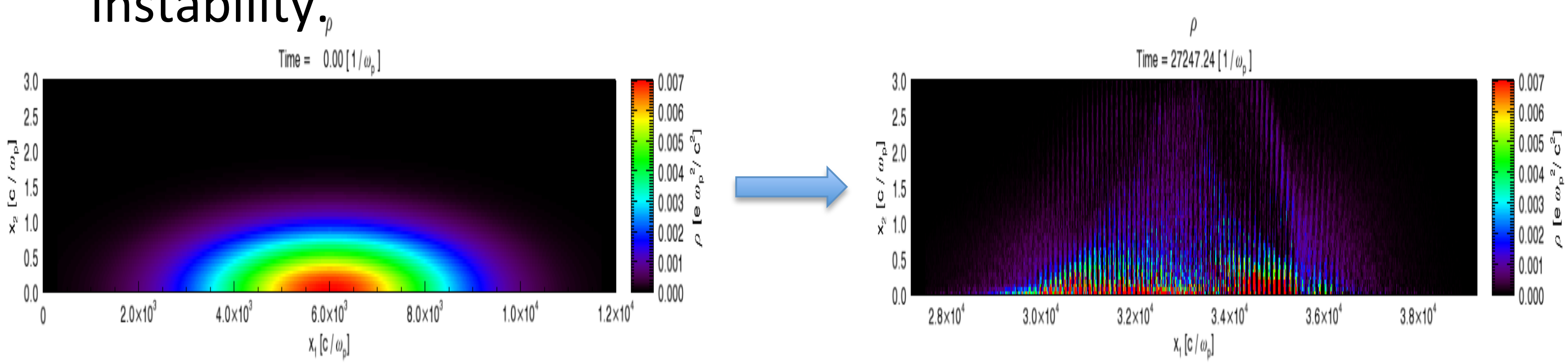
UCLA

Introduction: Two Options

- A compressed proton beam makes a bubble-like plasma wake: Ideal for accelerating an electron beam.

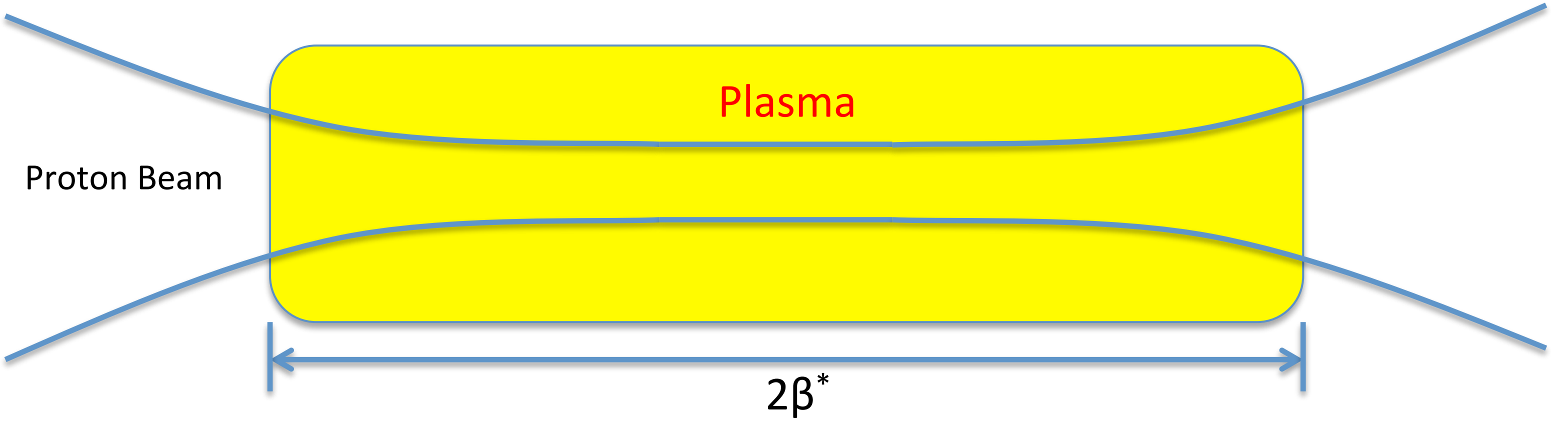


- If a short bunch is not available, we can allow a long beam to self-modulate into a sequence of short bunches: Relies on an instability.

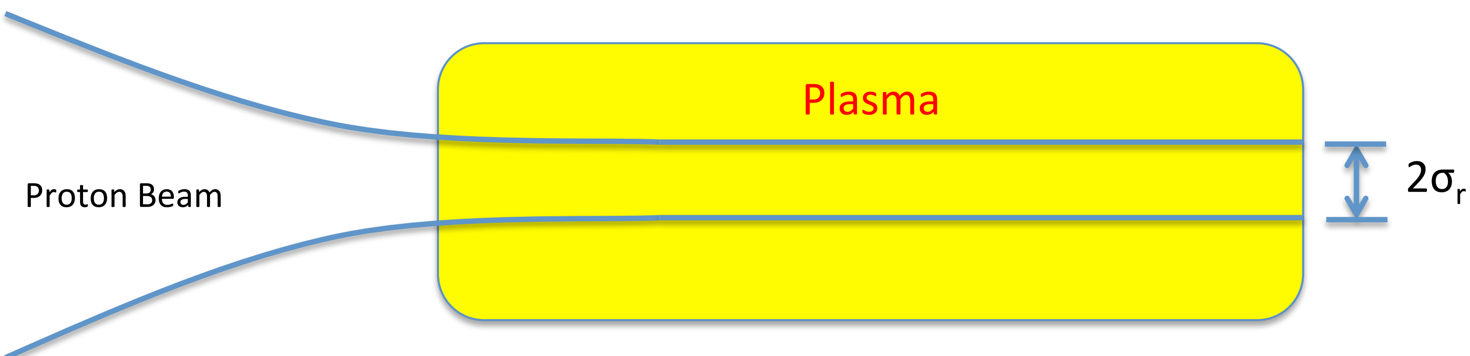


Conditions For SM-PDPWA

- **Instability must grow within $2\beta^*$ or the beam must be self guided.**



1. $L_{plasma} > 2\beta^* > L_{instability}$



2. Self Guiding Condition : $c = \frac{\sigma_{rM}^4}{2\sigma_r^4} < \frac{\delta n_p}{n_p} \sim \frac{n_b}{n_p}$, where σ_{rM} is the matched spot size of the beam propagating in an ion column.

UCLA

FNAL Beam Parameters For SM-PDPWA

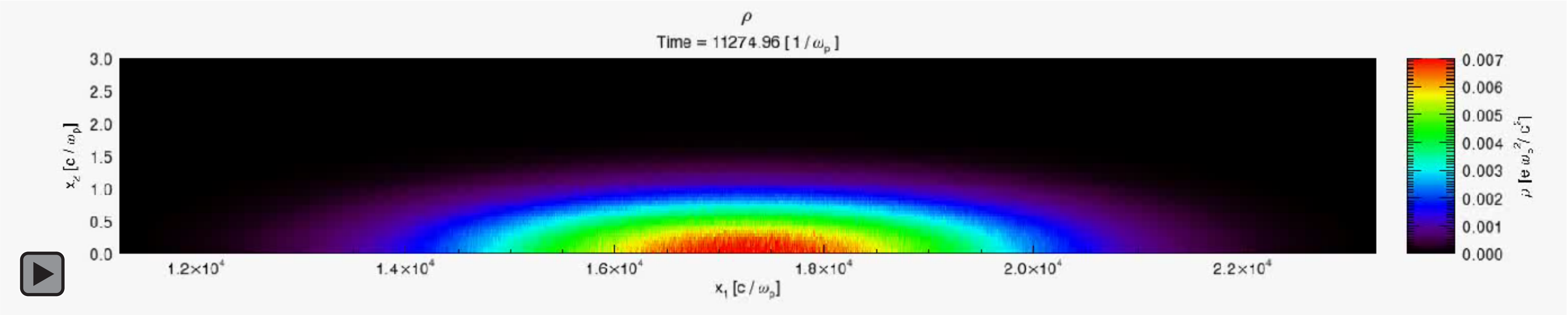
	n_p (10^{15} cm^{-3})	N (10^{11})	n_b/n_p (10^{-3})	ε_N (mm mrad)	γ	σ_r (μm)	σ_z (cm)	β^* (cm)	c (10^{-3})	L_{plasma} (cm)
Set 1	10	1	7.05	3.33	128.89	30	10	3.52	552	~ 200
Set 2	10	1	0.635	3.33	128.89	100	10	38.71	4.5	~ 200
Set 3	10	1	7.05	0.33	128.89	30	10	35.15	5.5	~ 200
SPS CERN*	0.7	1.15	2.17	3.845	480.61	200	12	500	1.4	~ 1000

[+] **Beam parameters are r.m.s. values.**

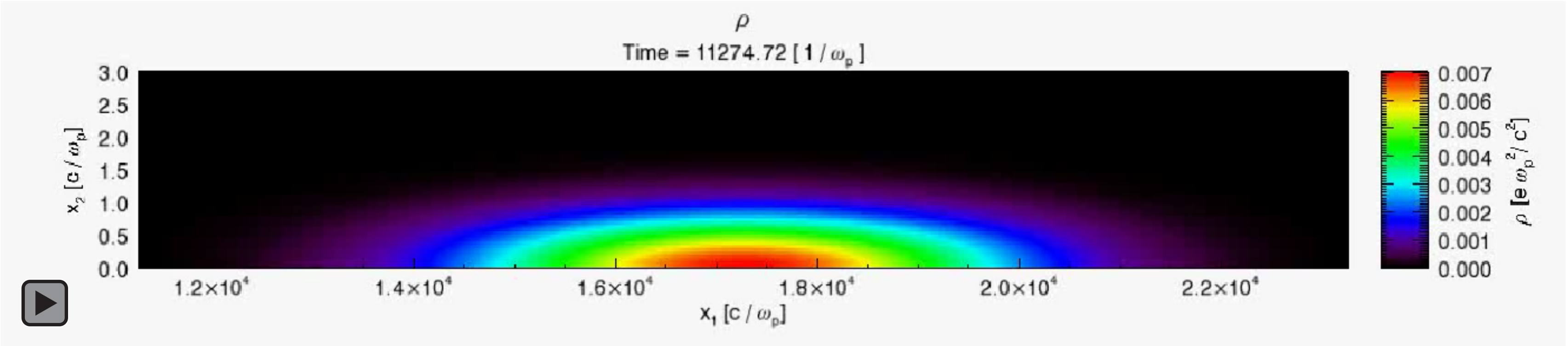
- With ε_N = 0.33 mm mrad and σ_r = 30 μm (Set 3), the parameter $c < n_b/n_p$ and the beam can self-modulate within 1 meter.
- For parameters Set 1 and Set 2, $c > n_b/n_p$ and the beam cannot self-modulate.
- We need to explore the self-modulation parameter space.

* A. Caldwell, K. V. Lotov, Phys. Plasmas 18, 103101 (2011).

OSIRIS Simulation Results Of SM-PDPWA



Set 1 (ε_N = 3.33 mm mrad, σ_r = 30 μm): Not guided and not Self-Modulated



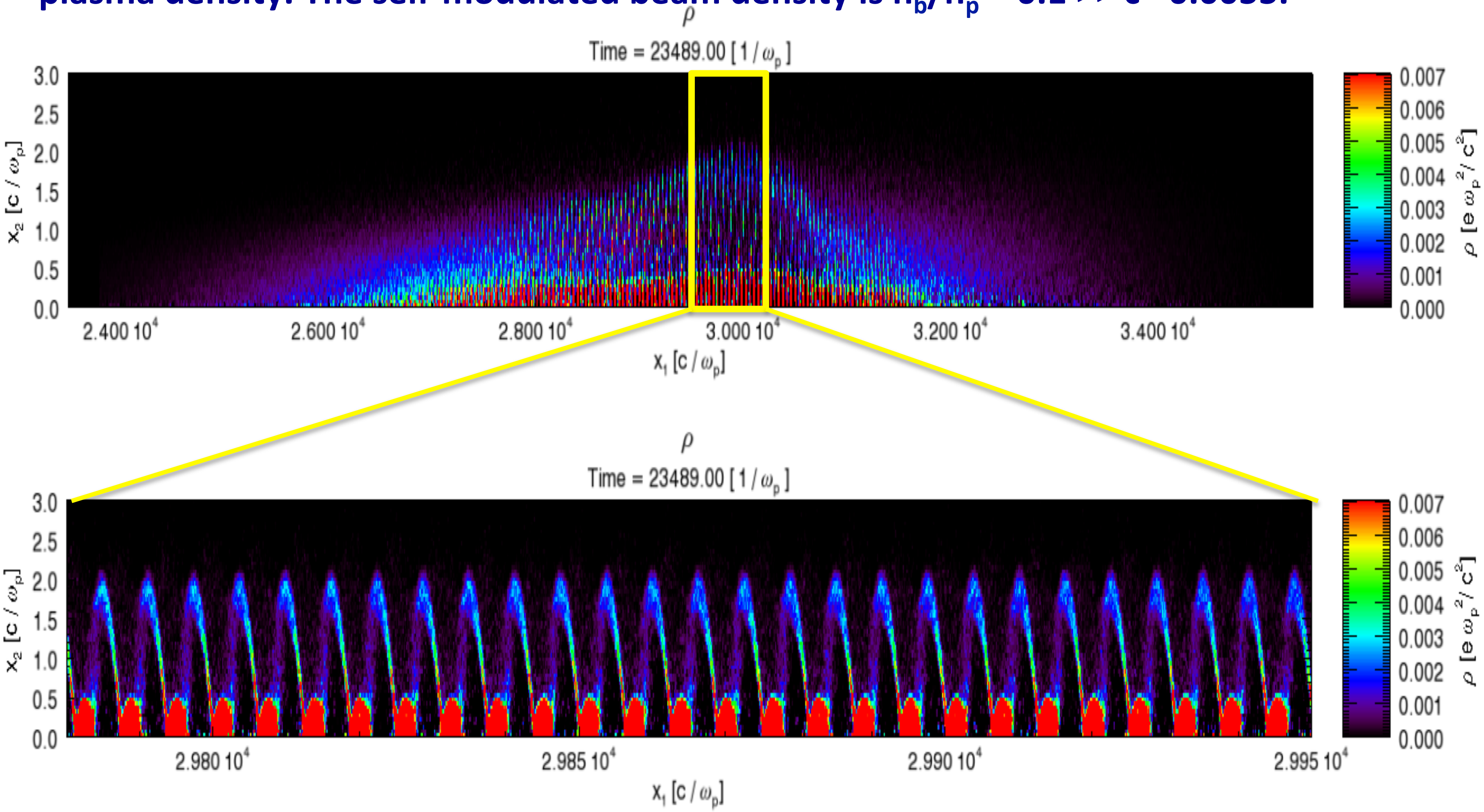
Set 3 (ε_N = 0.33 mm mrad, σ_r = 30 μm): Guided and Self-Modulated

- We need to explore on intermediate values of ε_N and σ_r.

+ The simulation is using 2D cylindrical coordinates.

OSIRIS Simulation Results Of SM-PDPWA

Snapshot of the beam charge density at the time when the beam center propagating in the plasma for 30 cm. The beam density is normalized to the plasma density. The self-modulated beam density is n_b/n_p = 0.1 >> c =0.0055.

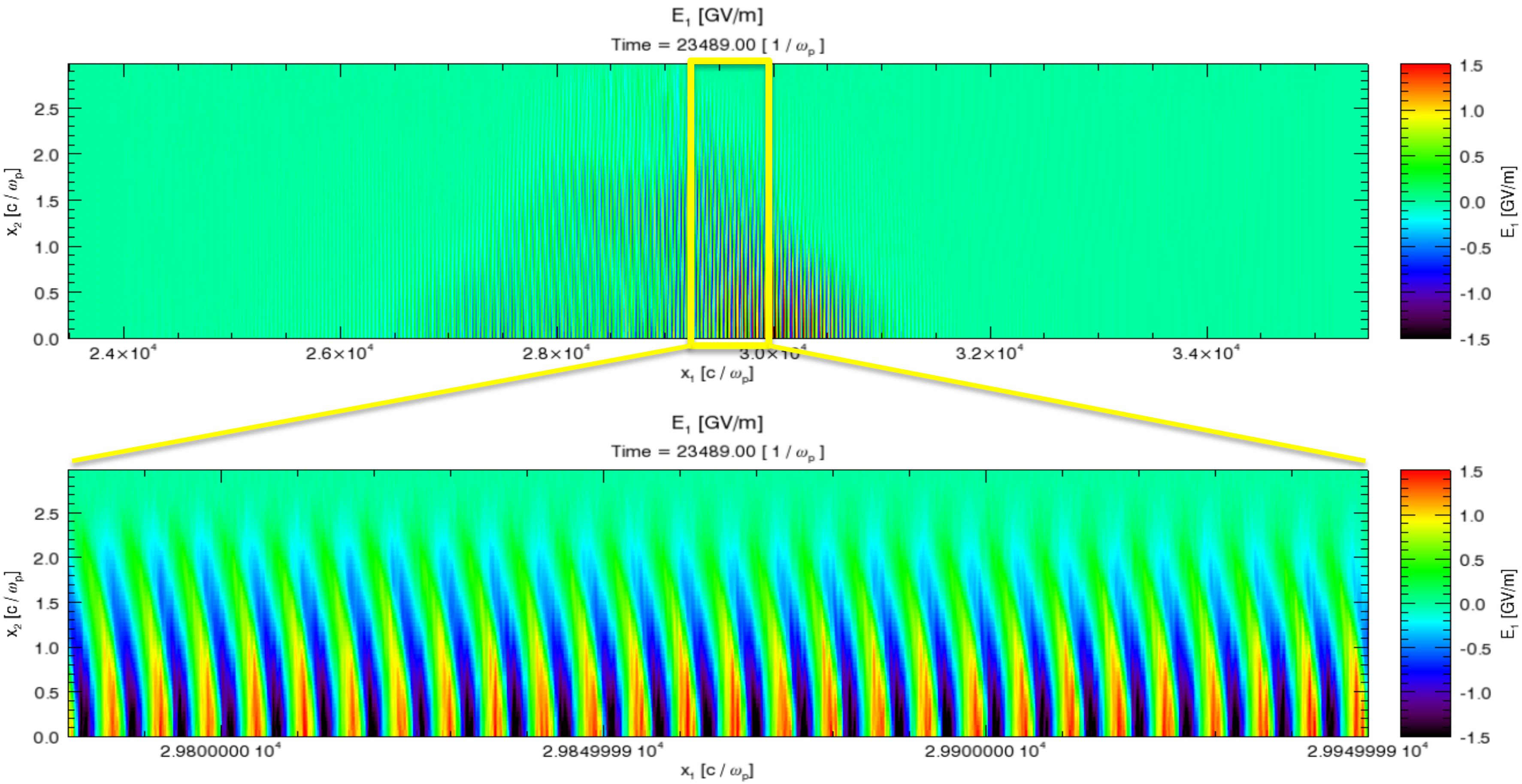


Beam Parameters (Set3): N = 1 x 10^{11}, σ_r = 30 µm, σ_z = 10 cm, ε_N = 0.33 mm mrad
Plasma Denstiy: n_p = 1 x 10^{16} cm^{-3}

UCLA

OSIRIS Simulation Results Of SM-PDPWA

Snapshot of the E_z at the time when the beam center propagating in the plasma for 30 cm. The maximum E_z reaches 1.5 GV/m at this time.



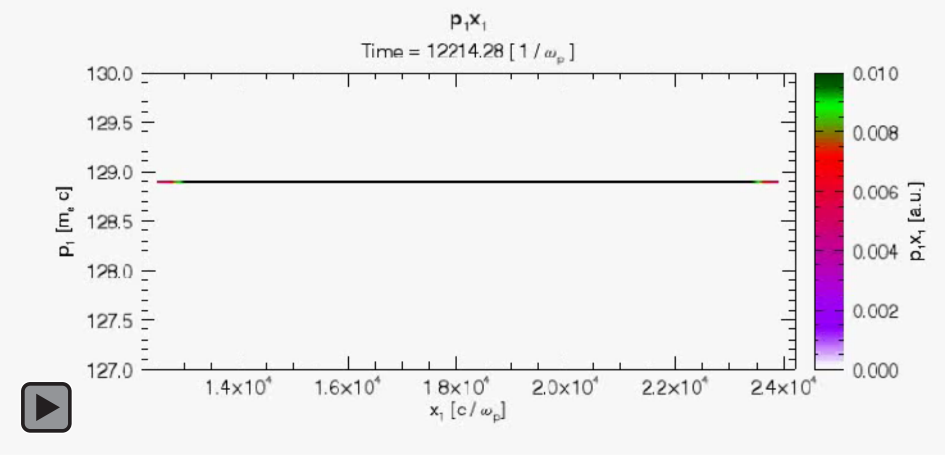
Beam Parameters (Set3): $N = 1 \times 10^{11}$, $\sigma_r = 30$ µm, $\sigma_z = 10$ cm, $\varepsilon_N = 0.33$ mm mrad

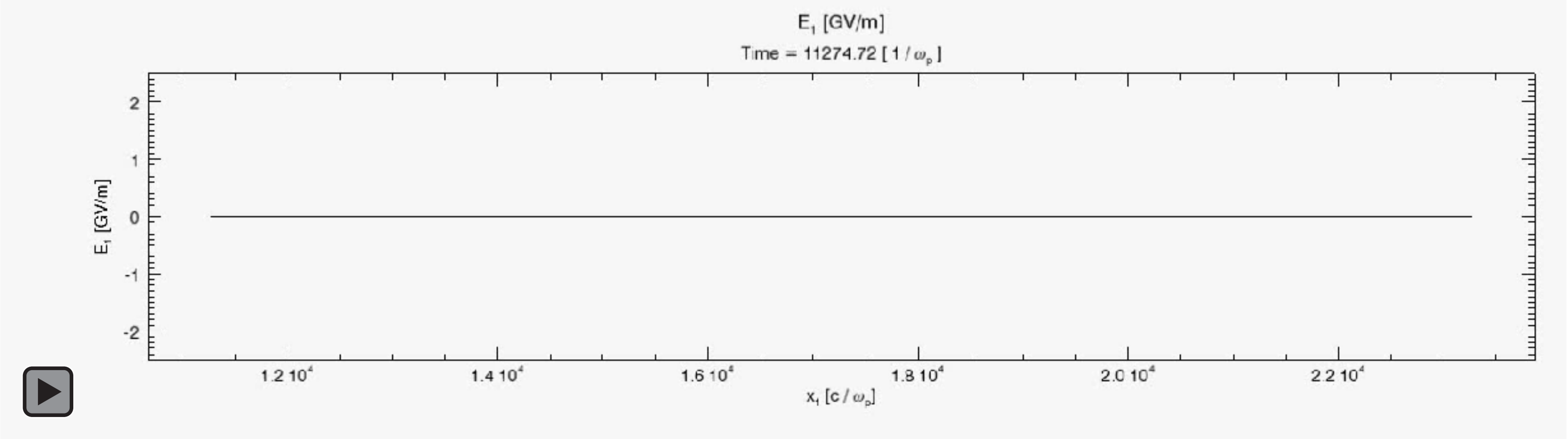
Plasma Denstiy: $n_p = 1 \times 10^{16}$ cm^{-3}

Simulation Results Of SM-PDPWA

Beam Parameters(Set3): N = 1×10^{11}, σ_r = 30 µm, σ_z = 10 cm, ε_N = 0.33 mm mrad
Plasma Denstiy: $n_p = 1 \times 10^{16}$ cm^{-3}

A Movie of the proton beam p1x1 phase space. The propagation distance in the plasma of the beam center is 189.2 cm. The energy modulation on the beam is ΔE > 1 GeV. (The initial energy spread of the beam is set to zero)

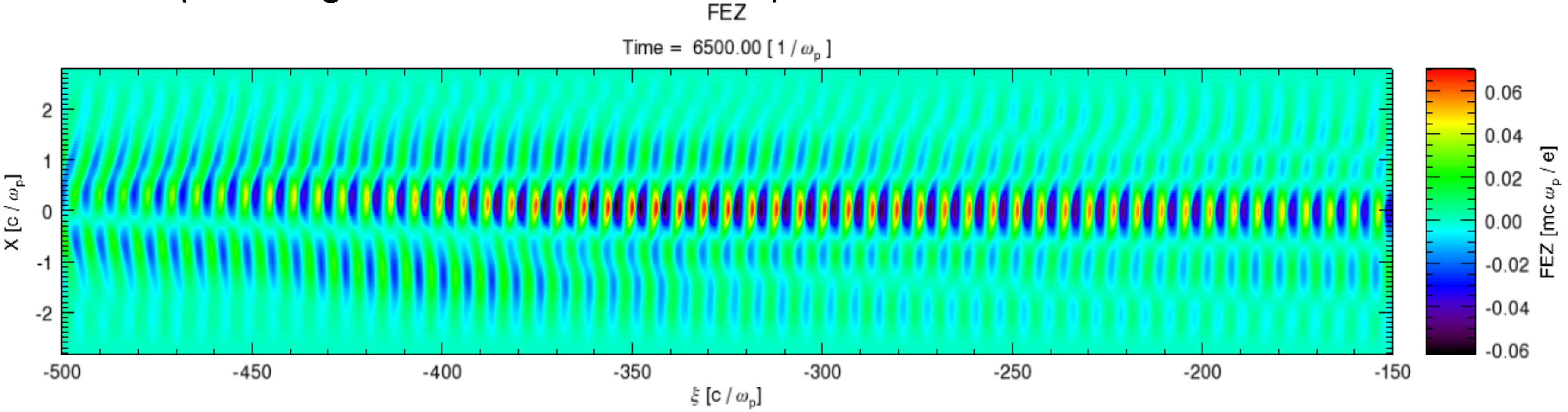


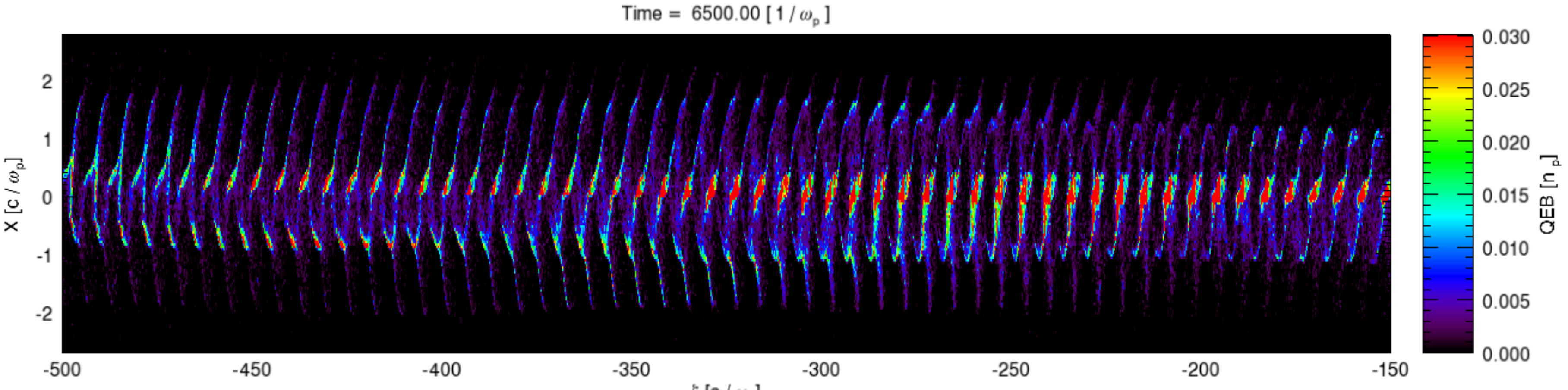


A Movie of the lineout (on the axis) of the wake field E_z. The propagation distance in the plasma of the beam center is 189.2 cm. The maximum E_z reaches 2.5 GV/m.

3D Effects Of SM-PDPWA

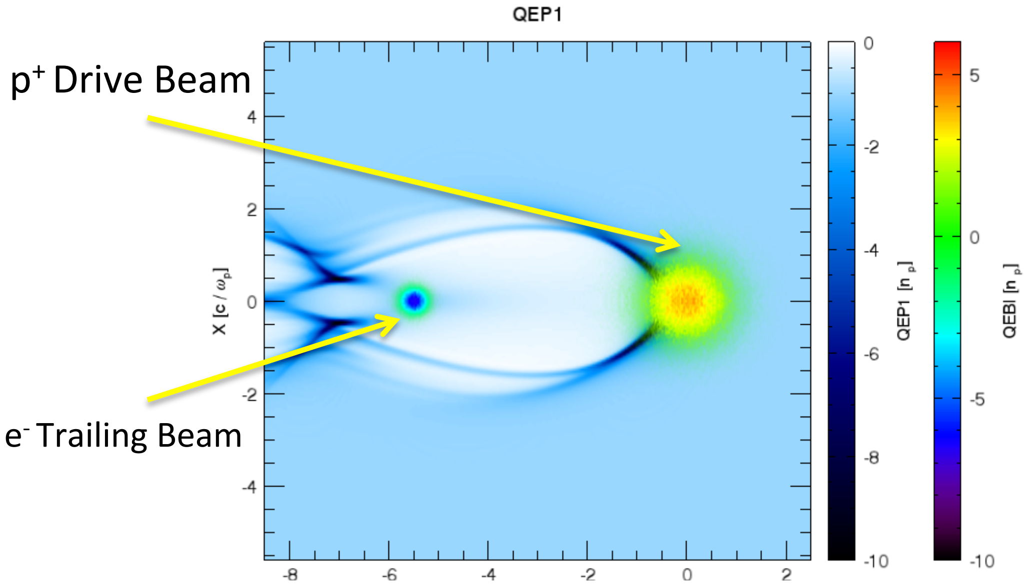
QuickPIC simulation results show that 3D effect may be important. We can find that the proton beam is deflected in a self-modulated regime. More investigation is needed (inculding on the mobile ion effects).

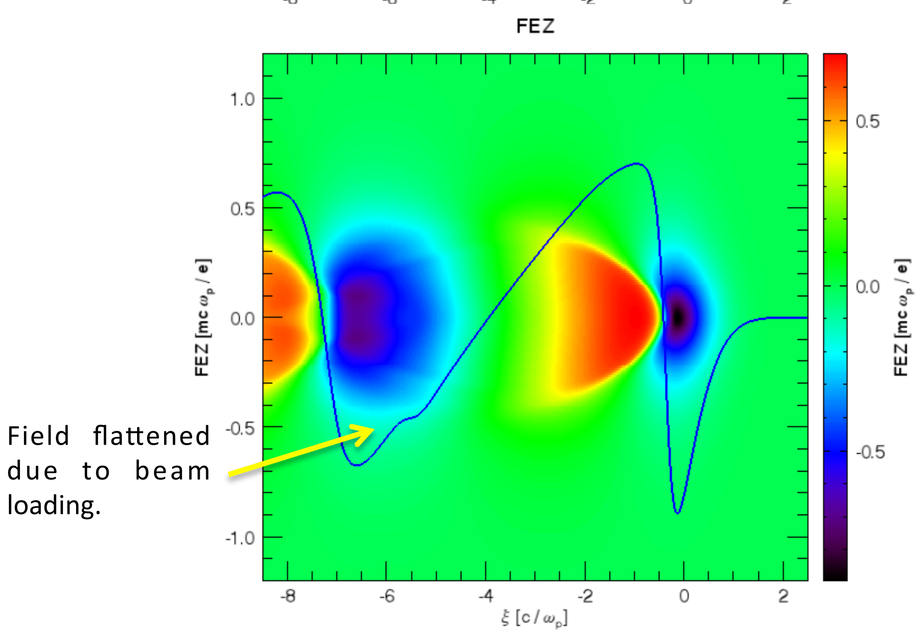




Partially Enlarged E_z and beam density plot after 35 cm propagation in the plasma. The plot is a 2D slice from a 3D data along the transverse direction x (at y = 0).

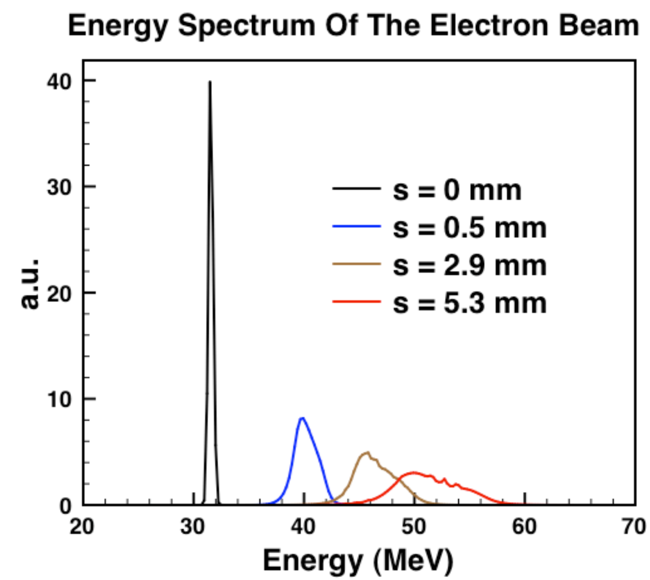
Plasma Wake Field Driven By A Compressed Proton Beam





Beam Parameters: $E = 8$ GeV, $N = 1 \times 10^{11}$, $\sigma_r = 30\ \mu m$, $\sigma_z = 10$ cm, $\varepsilon_N = 3.33$ mm mrad

Plasma Denstiy: $n_p = 1 \times 10^{15}\ cm^{-3}$

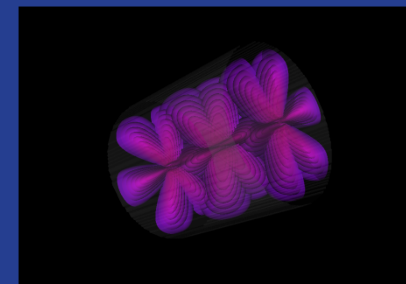


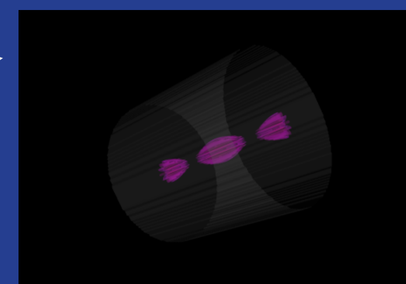
This preliminary simulation shows that the trailing electron beam can obtain 20 MeV energy gain within 5.3 mm propagation in a $10^{15}\ cm^{-3}$ plasma. The energy gain is limited by the dephasing. Exploring energies between 8 and 120 GeV is ongoing.

Summary

- A 120 GeV FNAL proton beam (with ε_N = 0.33 mm mrad) leads to GV/m gradient within 1 meter of a 10^{15} cm^{-3} plasma.
- Energy modulation $\Delta E > 1$ GeV can be seen in the proton beam.
- Simulations in which σ_r, ε_N and n_p are varied are still required.
- The ultimate goal is an experiment using a compressed proton beam.

Accelerator design: multi-scale, multi-physics problem

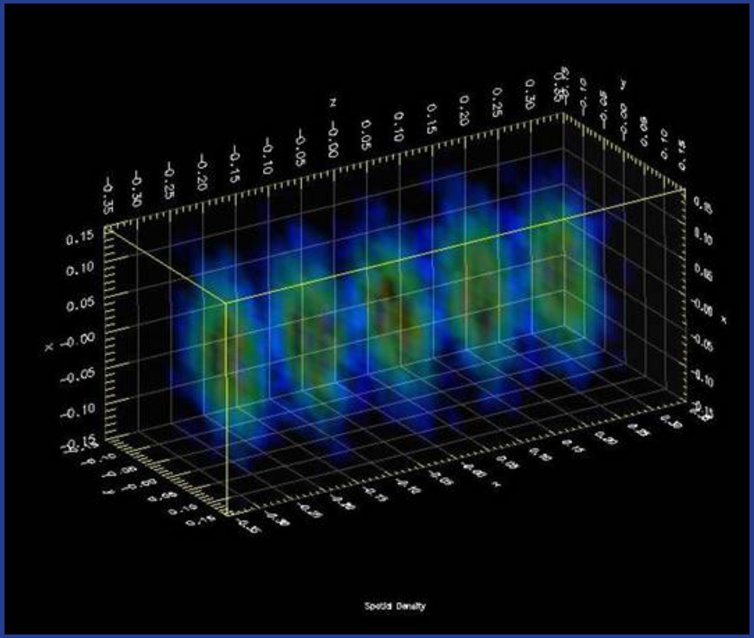


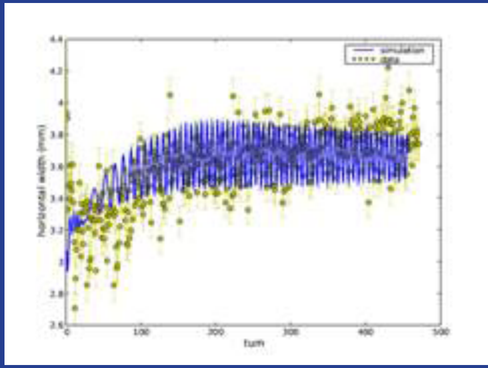


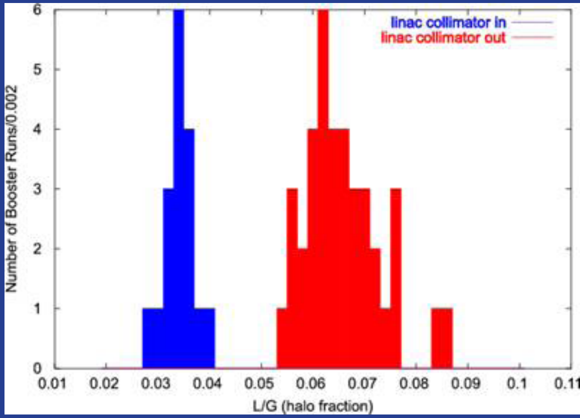
- Wide range of scales:
  - accelerator complex (10^3m) → EM wavelength (10^2-10 m) → component (10-1 m) → particle bunch (10^{-3} m) → PIC (10^{-12})
  - Simulations need to connect scales and allow inclusion of multiple physics effects at each level
  - Requires efficient utilization of HPC

Synergia applications: FNAL Booster

- Extensive modeling of the Booster with Synergia
  - 400 MHz structure debunching and 37.7 MHz capture
  - Including machine ramping
- Emittance growth and halo formation studies
  - Including comparison with experiment
  - Used to help optimize operating parameters
    - Work with AD proton source department personnel
  - NIMA570:1-9,2007







Fermilab