Advances in Large-Scale Computations of Multi-Particle Beam Dynamics

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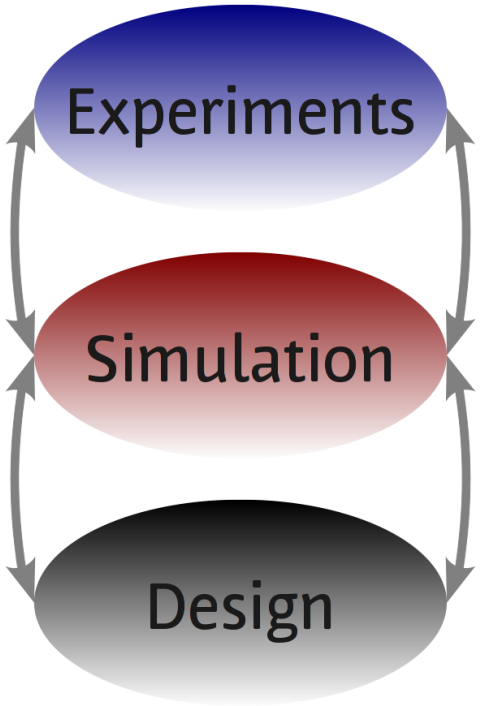
Fermilab
Community Petascale Project for Accelerator Science and Simulation (COMPASS)

SciDAC 2010 Chattanooga

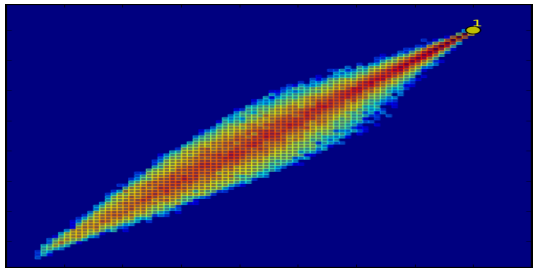
Introduction

- What
  - Advancing the state-of-the-art in particle acceleration
- Why
  - Physics motivation, focus on HEP
- How $\longrightarrow$
- Where we are going
  - Exascale computing

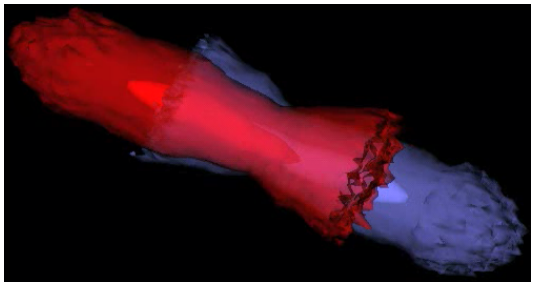


HPC and Beam Dynamics

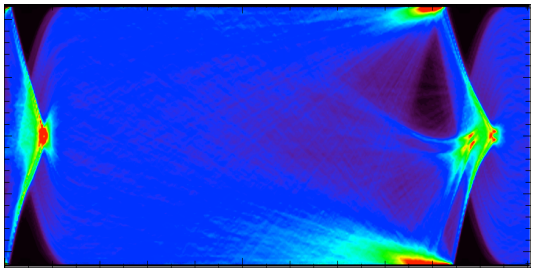
- All accelerator simulations require single particle tracking
- Collective effects require high performance computing



Space charge: interaction of the beam with itself. Requires a field solve and interpolation.



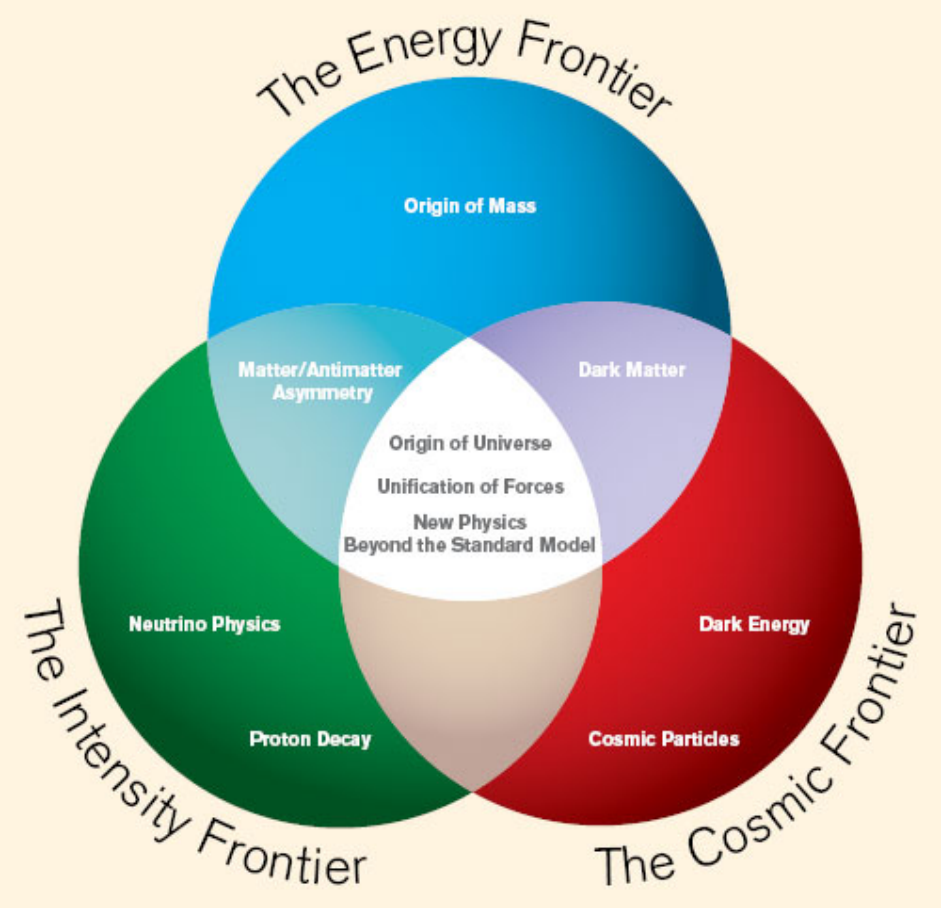
Beam-beam: interaction between two colliding beams. Requires more complex field solve and interpolation.



Electron cloud: Stray electrons are accelerated by passing beam. When they hit the beam pipe, more electrons are generated, causing a cascade.

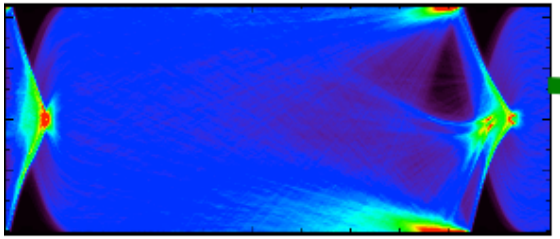
Frontiers of High Energy Physics

- Energy frontier
  - Recently transitioned from Fermilab (Tevatron) to CERN (LHC)
  - Much excitement
    - Read about it in any science periodical
- Intensity frontier
  - Future Fermilab program
  - I will highlight in this talk
  - Bread and butter for HPC accelerator modeling
- Cosmic frontier
  - The universe does the accelerating for us

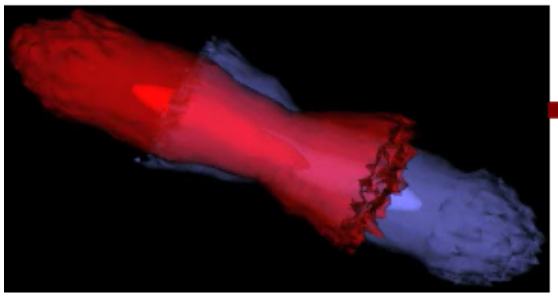


Collective effects in Fermilab accelerators

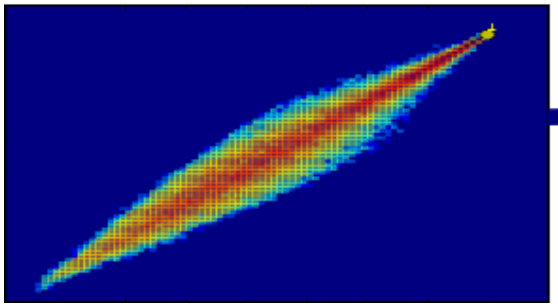
Electron cloud



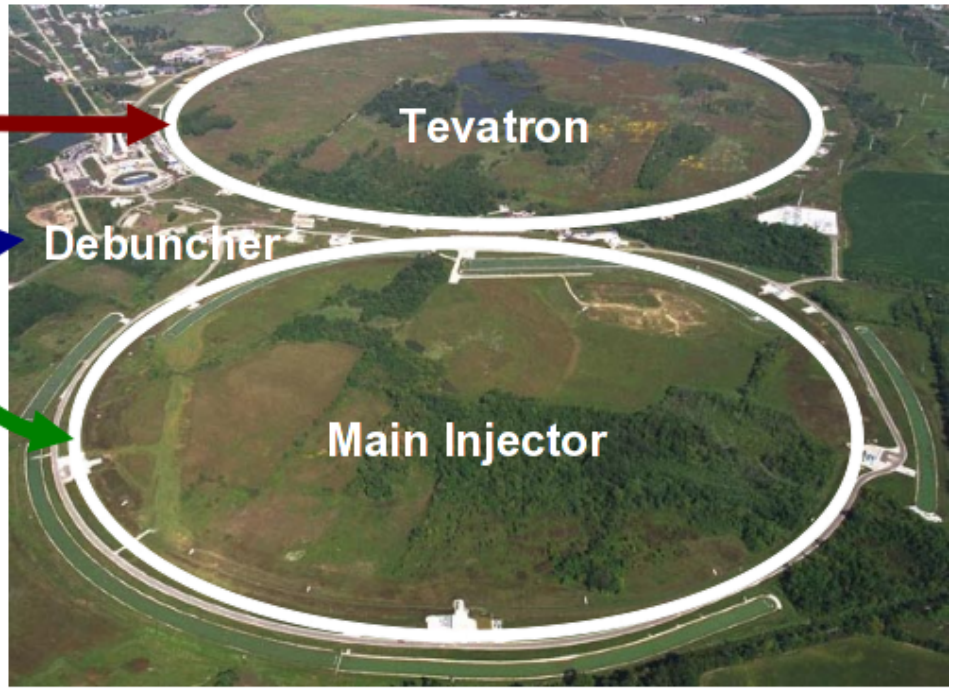
Beam-beam



Space charge

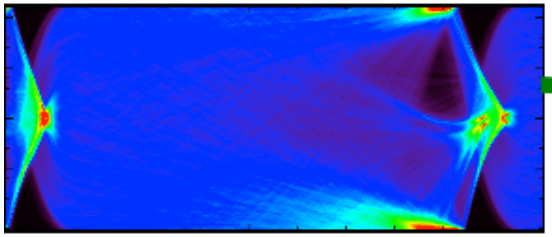


- Electron cloud simulations in the Main Injector for Project-X
- Beam-beam simulations in the Tevatron for Run II
- Space charge simulations in the Debuncher for Mu2e

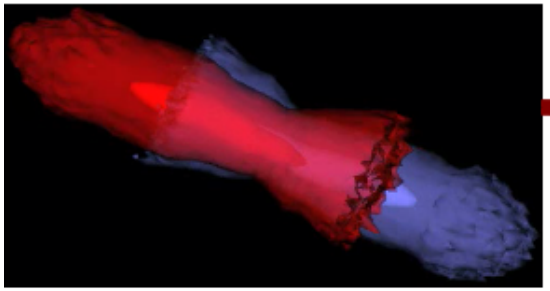


Collective effects in CERN accelerators

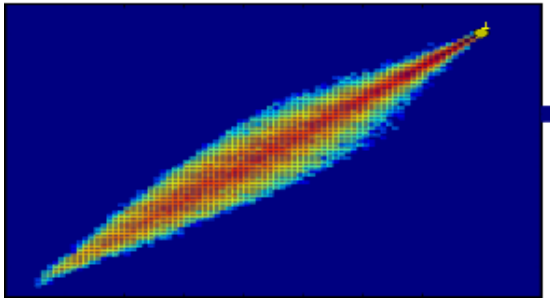
Electron cloud



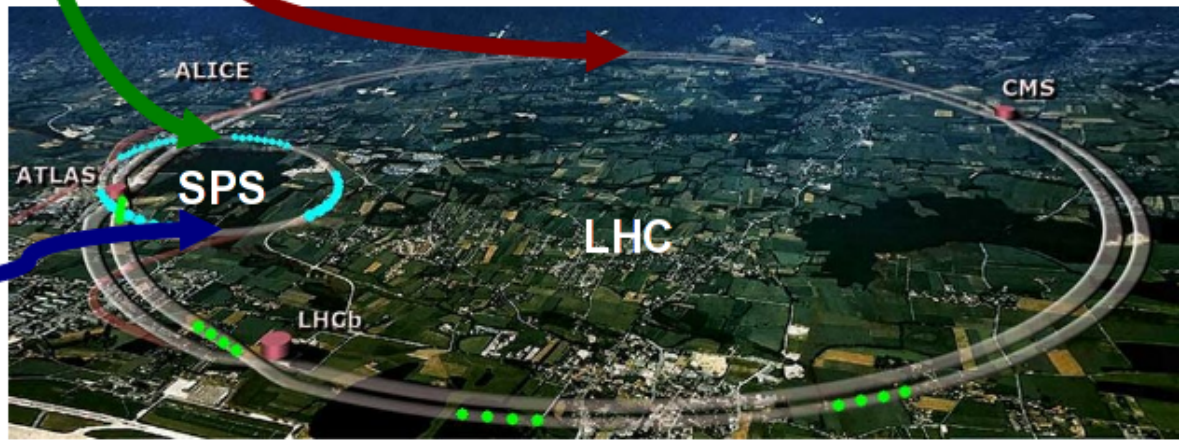
Beam-beam



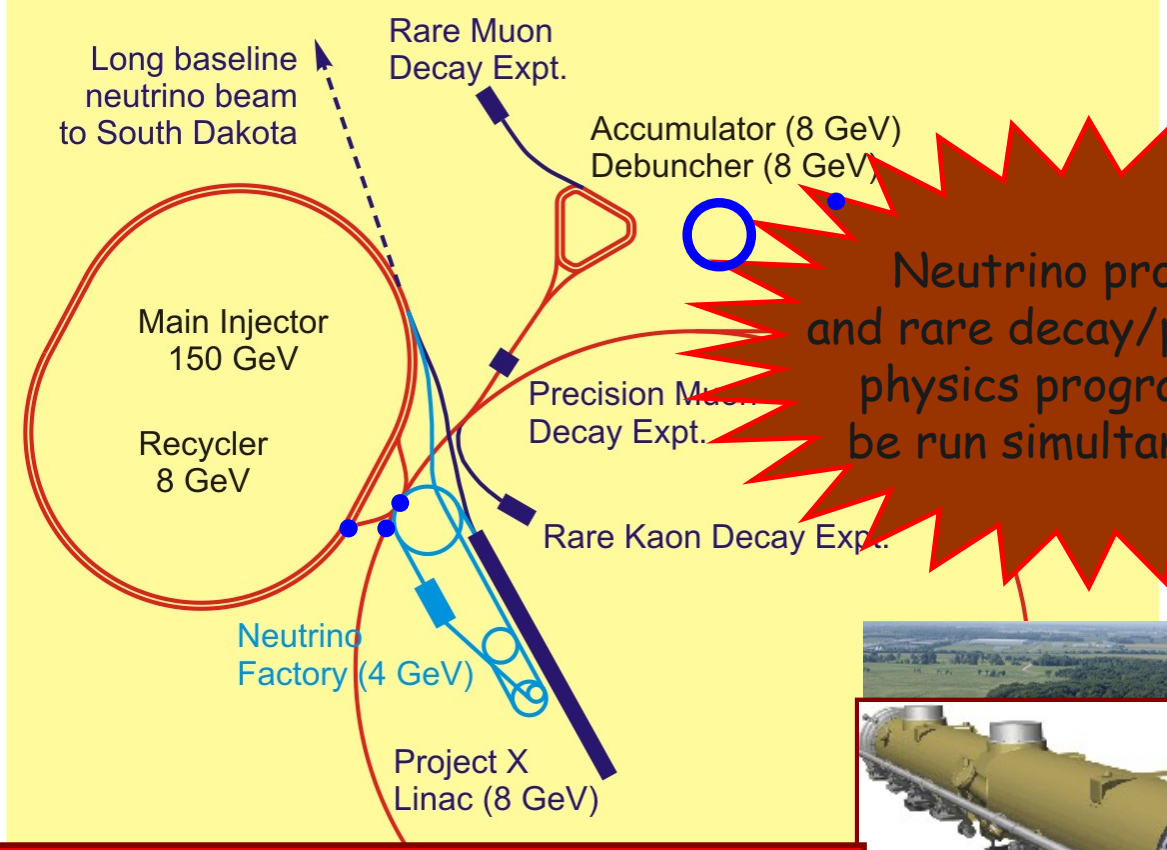
Space charge



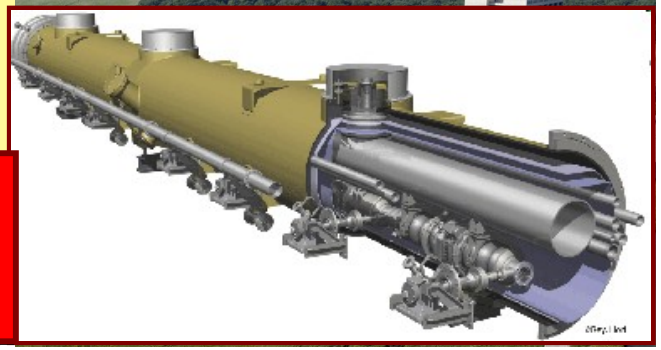
- Electron cloud compensation simulations in the SPS
- Beam-beam simulations in the LHC
- Space charge simulations for PS2 design studies



Project-X at Fermilab (Intensity Frontier)



Neutrino program and rare decay/precision physics program can be run simultaneously!



The Project X linear accelerator would feed a high-intensity neutrino and rare decay/high precision physics program

C. Dukes

Electron Cloud Simulations in the Fermilab Main Injector*

Motivation

- In the Project X era, the Main Injector will have to handle a factor of 3 increase in instantaneous beam current without an increase in beam losses.
- Electron cloud (EC) induced instabilities could interfere with this goal.
- A program to study this effect is underway at Fermilab, and supported in part by these simulations.

*Paul L. G. Lebrun, Panagiotis Spentzouris, John R. Cary, Peter Stoltz, Seth A. Veitzer

Electron Cloud Simulations in the Fermilab Main Injector

Electron cloud production model

- MI beam line (either short, 0.25 m, in a dipole), or long enough to fully handle the microwave absorption experiment, which includes dipoles and one quadrupole
- Secondary electron emission model: "Vaughan" type
- Seed cloud, diffused, following beam profile. Low density compared to the saturation density.
- Proton beam: modeled as a 3D Gaussian, fixed shape, current source.

VORPAL

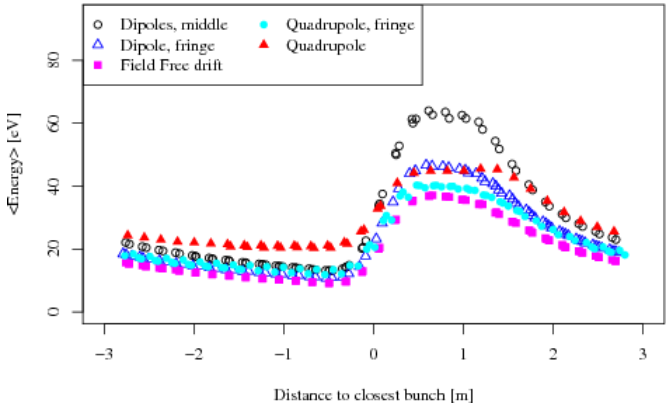
- plasma and beam dynamics
- Fully 3D, self-consistent

Running at ALCF

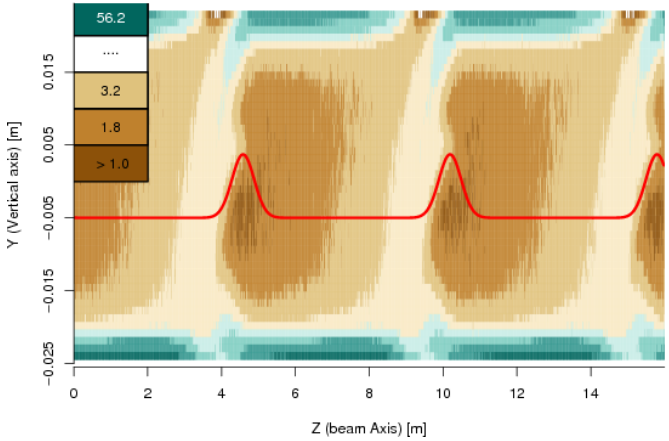
PIC simulation parameters

- Typical grid: $6144 \times 48 \times 48$
  - perfectly matched layers
- Time step: 3.2 ps
  - $\ll$ cyclotron period
- Total time: ≈ 700 ns
- $(5 - 10) \times 10^6$ macro particles

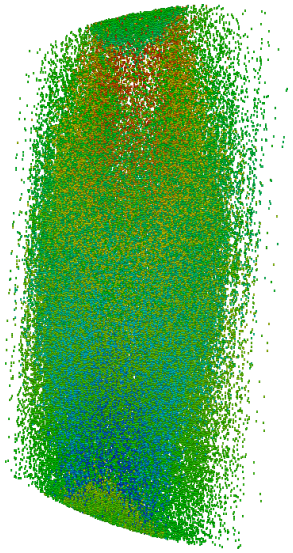
Electron cloud dynamics



Variation of the kinetic energy distribution as function of the distance to the nearest bunch



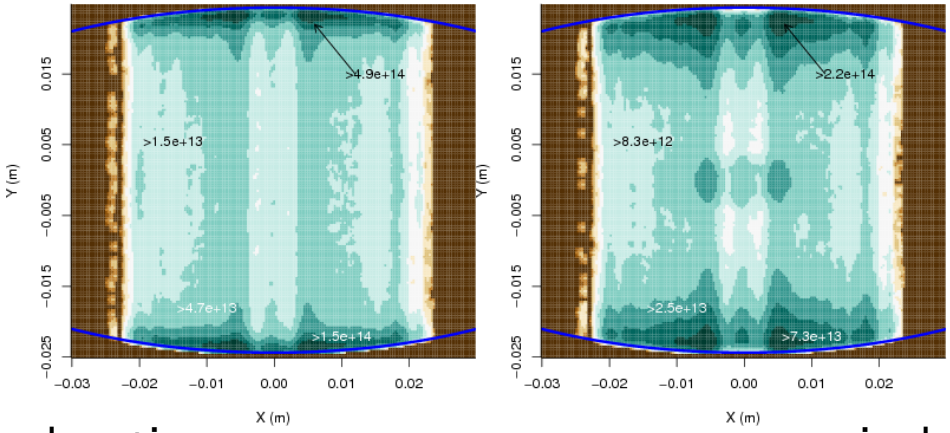
Y-Z projection of EC. The red line depicts the proton beam bunch profile. Here, a continuous dipole field of .234 T is assumed.



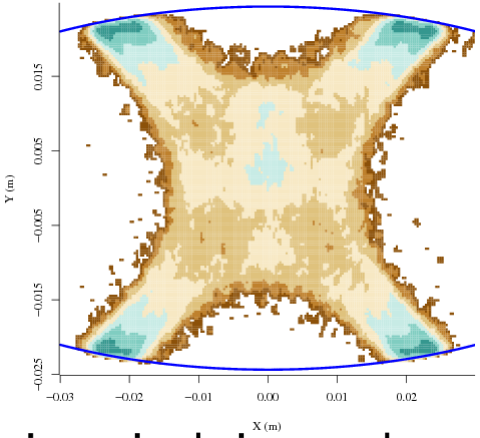
Vislt rendering of a slice of the EC. The color is mapped to v_y/c, showing the weak coherent motion of these electrons

Main Injector Electron Cloud Results

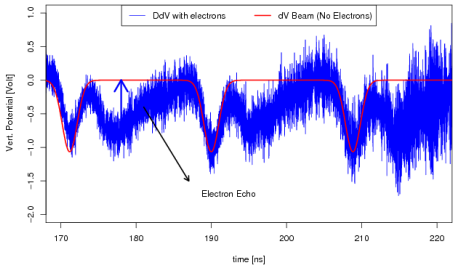
Transverse electron cloud profiles



relaxation pinch



during pinch in quadrupole



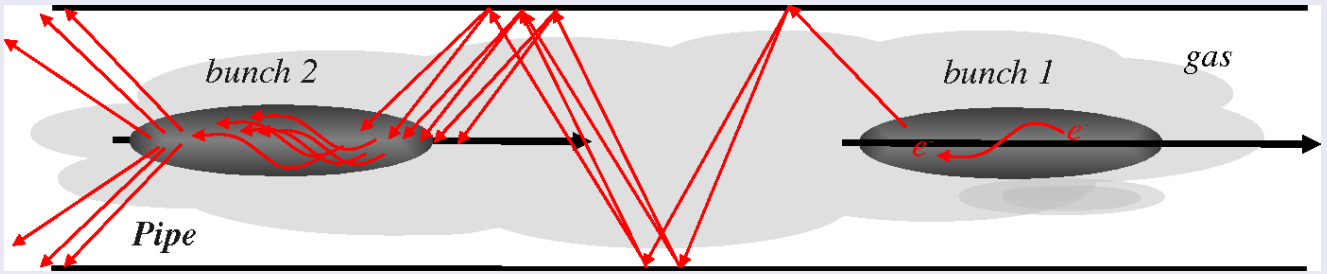
Beam position monitor in a dipole response showing the beam signal and the noise from the EC

Conclusions

- Uncertainties in the phenomenological model of secondary electron emission prevent *ab initio* cloud prediction
- Detailed modeling, including detector, indispensable feedback to experimental program

Electron cloud compensation in the CERN SPS*

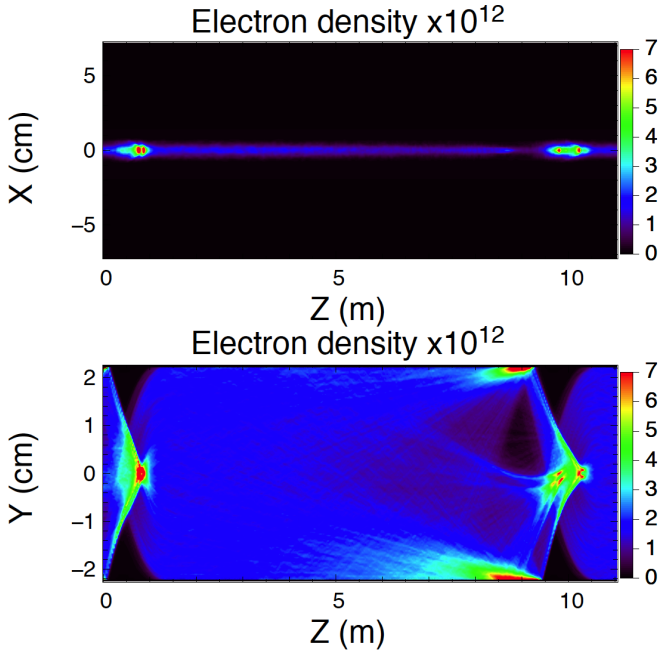
Motivation: Transverse instability observed in SPS beams due to electron clouds



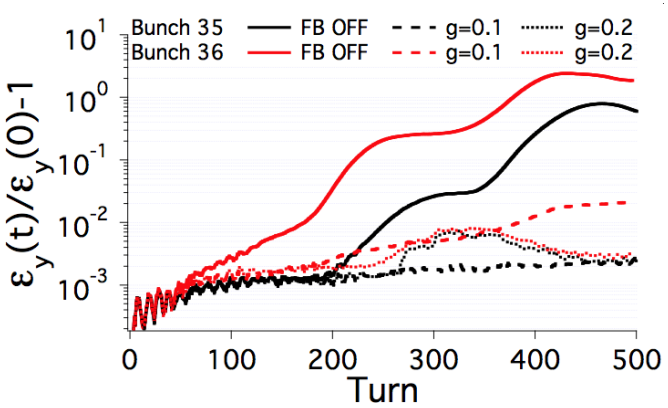
- Feedback system was proposed to control the beam transverse motion
- Use the PIC framework Warp-Posinst to investigate dynamics of instability as well as feasibility and requirements of feedback

*J.-L. Vay, J. M. Byrd, M. A. Furman, R. Secondo, M. Venturini, J. D. Fox, C. H. Rivetta W. Höfle

Electron cloud compensation in the CERN SPS



Electron density around two bunches



Emittance growth with and without compensation

Simulated feedback model

$$\Delta v_y = \frac{q}{\gamma m} \frac{E_f L_f}{v_z}$$

E_f calc based on previous turn + dynamics

Conclusions

- Possible to do detailed modeling of cloud-beam interaction
- Results compared with experiment; qualitative and semi-quantitative agreement

Beam-Beam at the LHC*

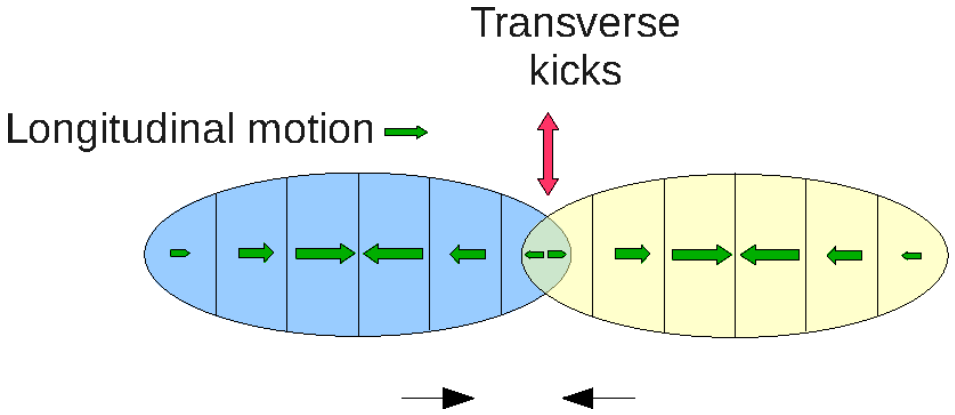
Motivation

- Offset collisions are unavoidable due to the different bunch collision schemes at LHC
- Such offset collisions might cause emittance growth that degrades luminosity lifetime and experimental conditions

*Ji Qiang

BeamBeam3d

- Beam-Beam forces – integrated, shifted Green function method with FFT
- Multiple-slice model for finite bunch length effects



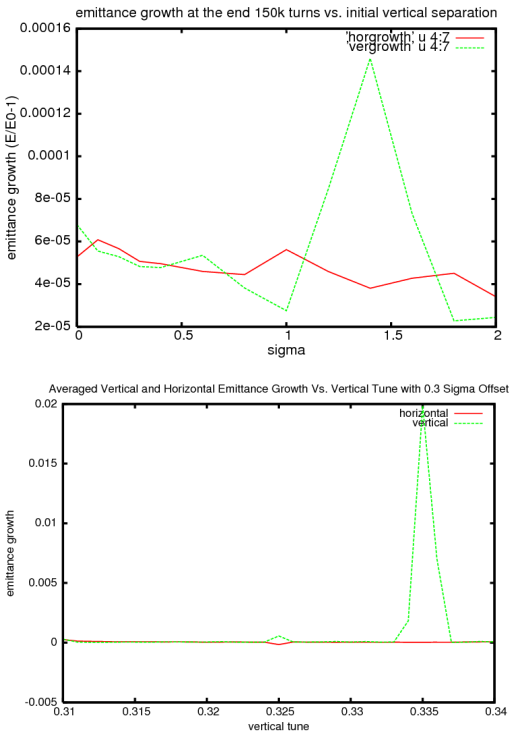
- Parallel particle-based decomposition to achieve optimum load balance
- Lorentz boost to handle crossing angle collisions
- Multiple bunches, multiple collision points
- Linear transfer matrix + one turn chromaticity + thin lens sextupole kicks + thin lens multipole kicks
- Symplectic element by element tracking
- Conducting wire, crab cavity, and electron lens compensation

Parallel scans of Beam-Beam at the LHC

Parallel scans

- Accelerator design typically involves scanning a parameter space (quad gradients, RF cavity phases, RF cavity dimensions, etc.) to explore and optimize the design
- Typical beam dynamics simulation of a single point in parameter space involves parallel modeling using
  - 100 - 1000 processors
  - 10 million - several billion macro particles
- One would like to perform 100's to 1000's of these simulations to scan the parameter space

Results



Emittance vs. offset and tune

Simulations for this study required 2.5 hours. Would have required 78 hours without parallel scan.

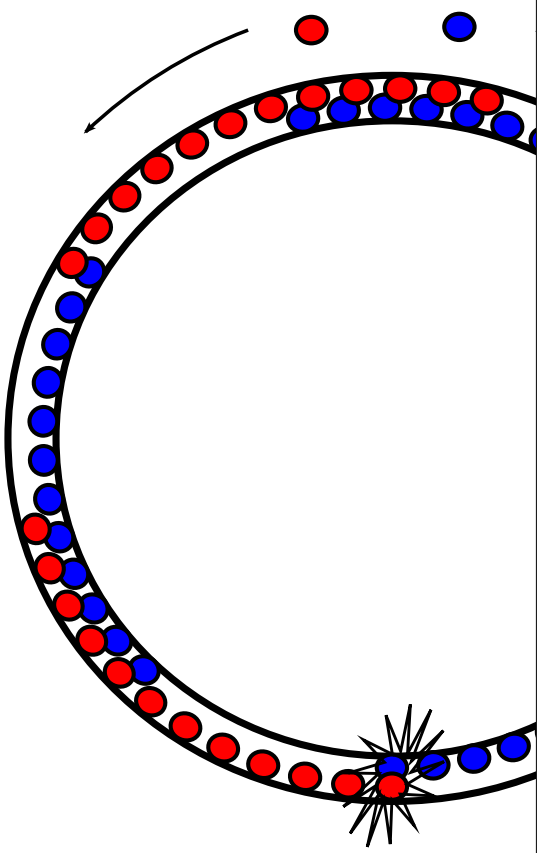
Beam-beam and chromatic effects in the Tevatron*

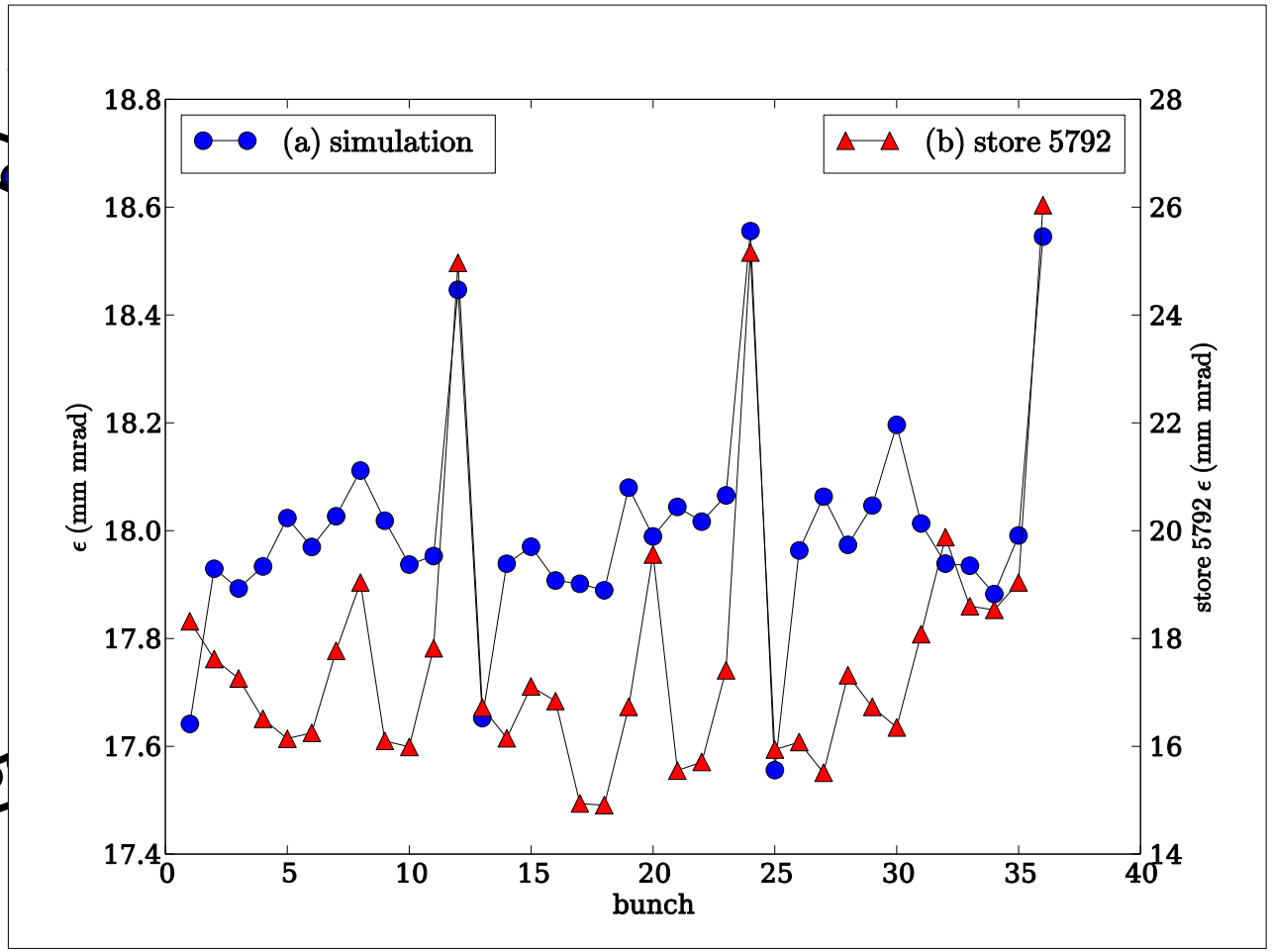
Motivation

Maximizing total integrated luminosity for Run II has required the Tevatron to operate reliably at high beam intensities.

*E. Stern, J. Amundson, P. Spentzouris and A. Valishev

A SciDAC Breakthrough Presentation (Eric Stern)





Pattern reproduced by the simulation

Space Charge in the PS2*

Motivation

One option in the scenario of upgrades of the LHC accelerator complex is to replace the existing CERN Proton Synchrotron (PS) by a new and larger synchrotron (PS2). Space charge studies are necessary for the design process.

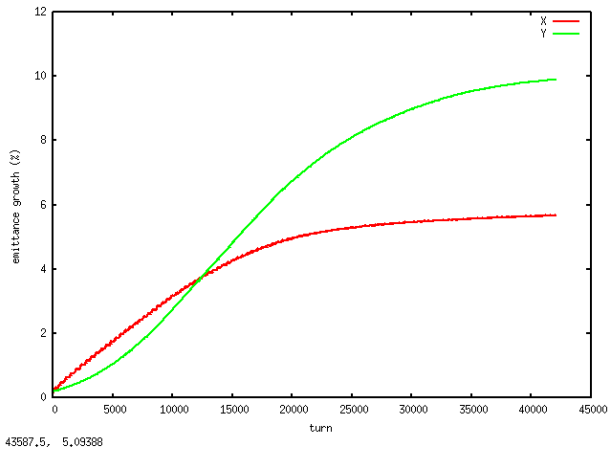
*J. Qiang

Space Charge in the PS2

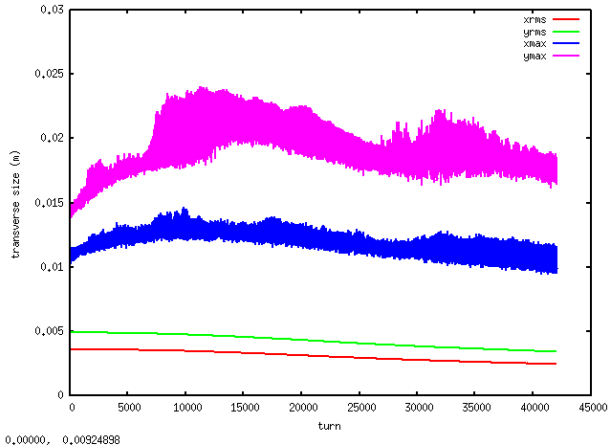
IMPACT

- Detailed RF accelerating and focusing model
- Multiple 3D Poisson solvers
  - Variety of boundary conditions
  - 3D Integrated Green Function
- Multi-charge state
- Machine error studies and steering
- Wakes
- CSR (1D)
- Multiple turn tracking
- Thin lens kick for nonlinear elements
- Lumped space-charge

Results



Emittance growth

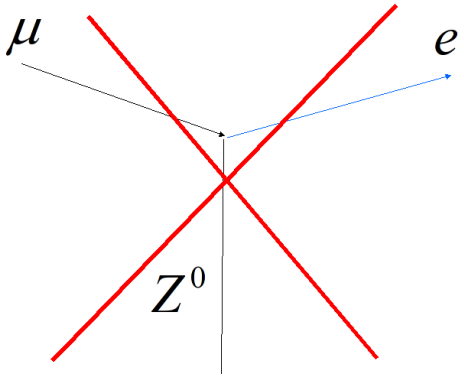


Beam sizes and maximum amplitude

The Mu2e Experiment at Fermilab (Intensity Frontier)

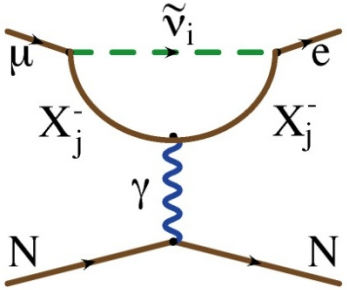
The Mu2e experiment will search for $\mu \rightarrow e$ transitions

First order (tree-level) flavor-changing neutral currents



- Forbidden in the Standard Model

Higher-order ("penguin") graph

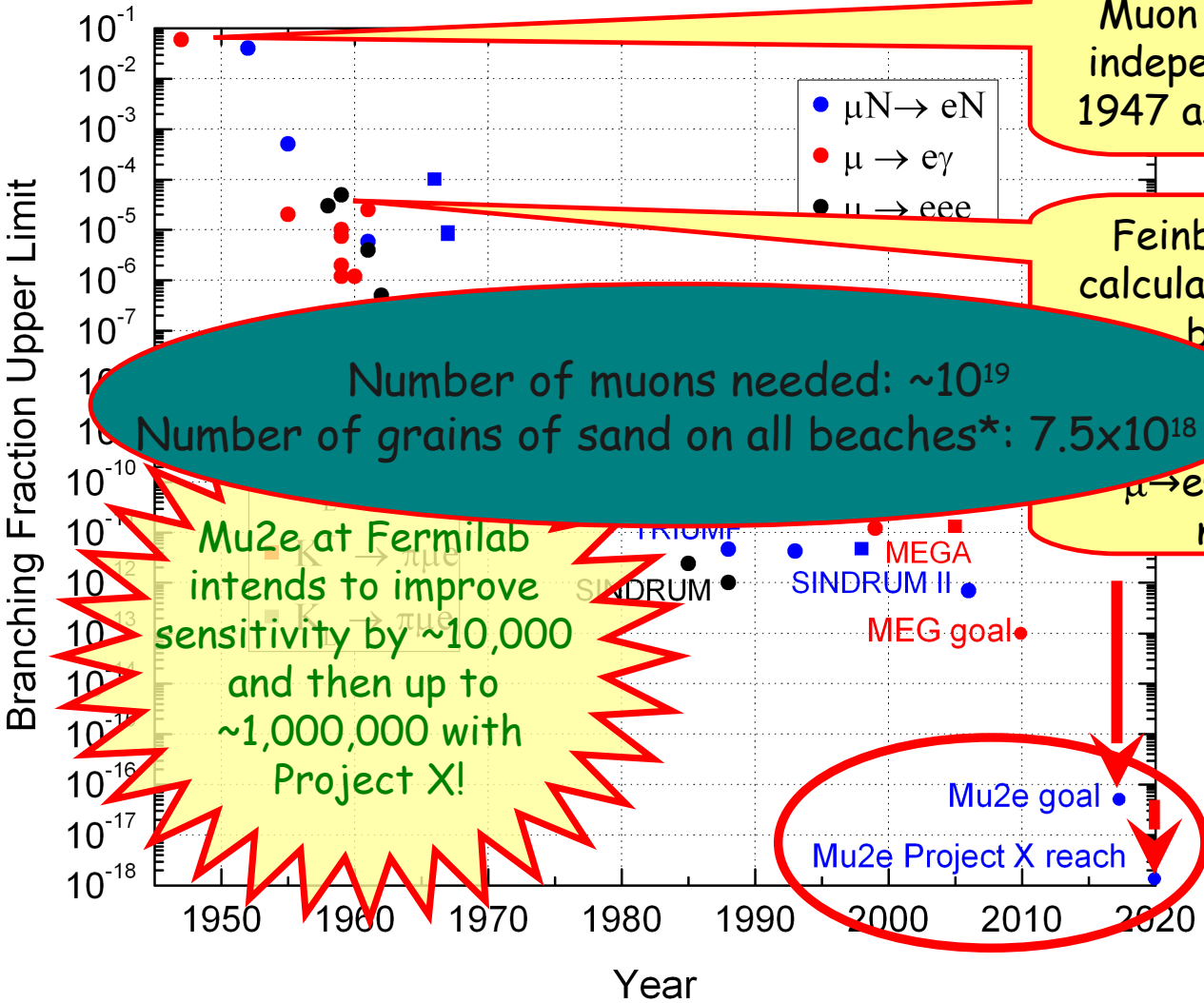


- Observation of neutrino masses means this process is non-zero
- Photon can be real ($\mu \rightarrow e\gamma$) or virtual ($\mu N \rightarrow eN$)

Standard-model prediction is ridiculously small

$$Br(\mu \rightarrow e\gamma) = \frac{3\alpha}{32\pi}\left|\sum_{i=2,3} U^*_{\mu i} U_{ei} \frac{\Delta m^2_{1i}}{M^2_W}\right|^2 < 10^{-54}$$

History of Lepton Flavor Violation Searches



Muon established as independent lepton in 1947 as μ→eγ not seen

Feinberg 1958 loop calculation: μ→eγ must be 10^{-4}-10^{-5}

Number of muons needed: ~10^{19}
Number of grains of sand on all beaches*: 7.5x10^{18}

servation of μ→eγ implies two neutrinos!

Mu2e at Fermilab intends to improve sensitivity by ~10,000 and then up to ~1,000,000 with Project X!

C. Dukes

* http://www.hawaii.edu/suremath/jsand.html

Space charge and nonlinear optics studies for Mu2e*

Motivation

- Beam to be extracted from Fermilab Debuncher using (nonlinear) resonant extraction
- Accumulator/Debuncher required to handle 10^5 times more particles than current operating conditions
  - Space charge is the biggest worry.

*J. Amundson, A. Macridin, L. Michelotti, C. S. Park, P. Spentzouris, E. Stern

Accelerator/Beam parameters

Accelerator physics

Particles in a beam bunch behave like glorified harmonic oscillators. The particle *tune* is the oscillation period in units of revolution time.

Beam parameters from original Mu2e proposal

- 8 GeV
- 1.2×10^{13} protons/bunch
- 20π emittance
- 40 nsec longitudinal RMS
- (Laslett) space charge tune shift is ~ 0.08

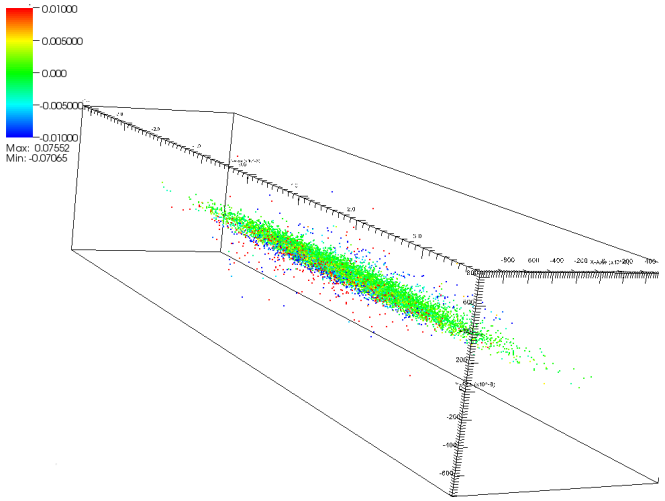
Simulation details

Space charge simulations utilizing Synergia

- PIC code
- Fully three dimensional
- Space charge included via split-operator technique

- Single-particle physics from CHEF
  - Existing single-particle simulation immediately
  - All the realism "you care to model"

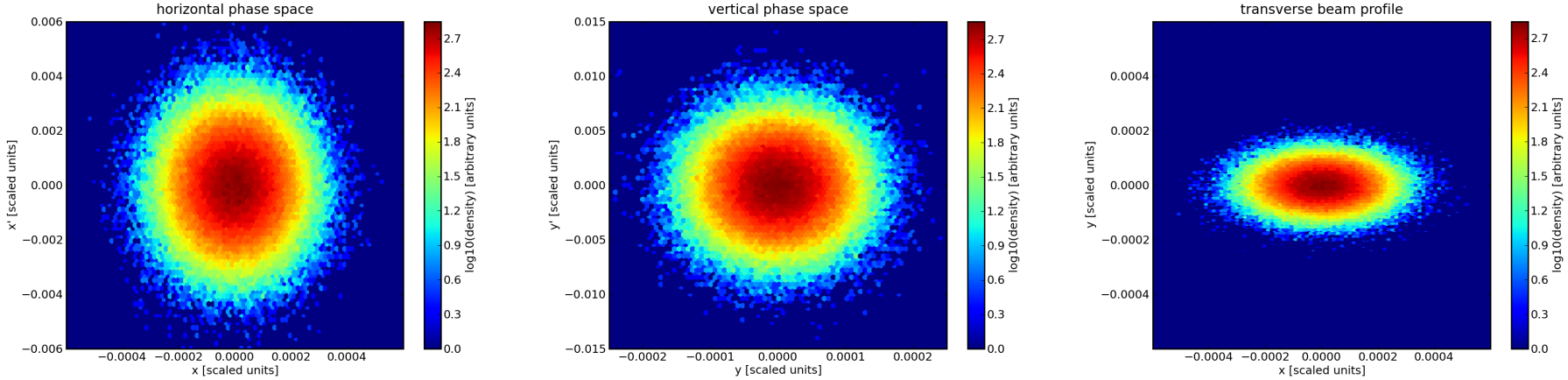
- $64 \times 64 \times 64$ space charge grid (typical)
- 240 kicks per turn
- 3×10^6 particles
- Fully three-dimensional transverse dynamics
  - Full 3D bunch shape
  - Full 3D field calculation
  - *Transverse* space charge kicks



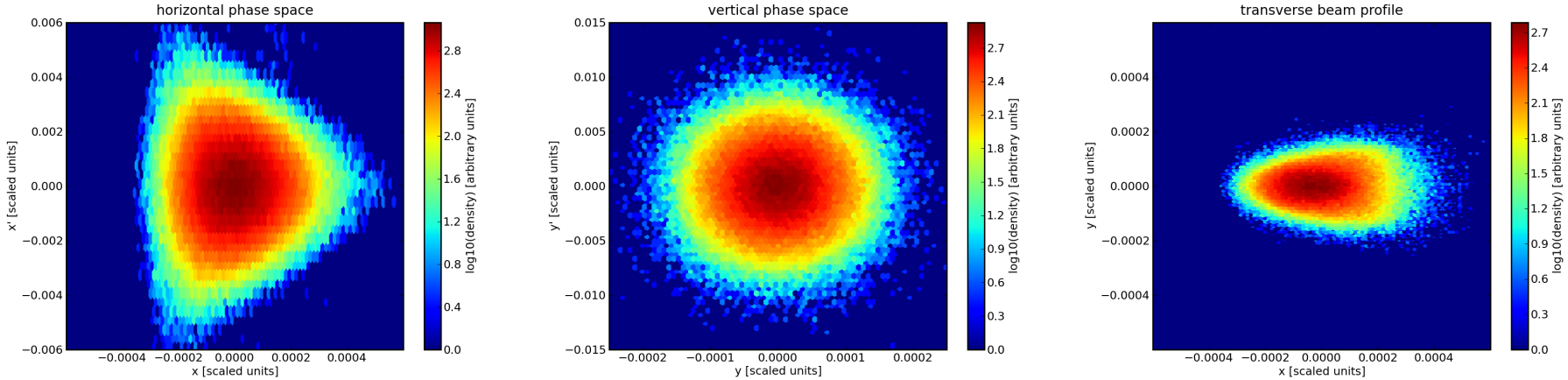
Simulating 1000 turns takes roughly 20 hours on 128 processors on Hopper.

Sextupoles without space charge

Beam with linear magnets only



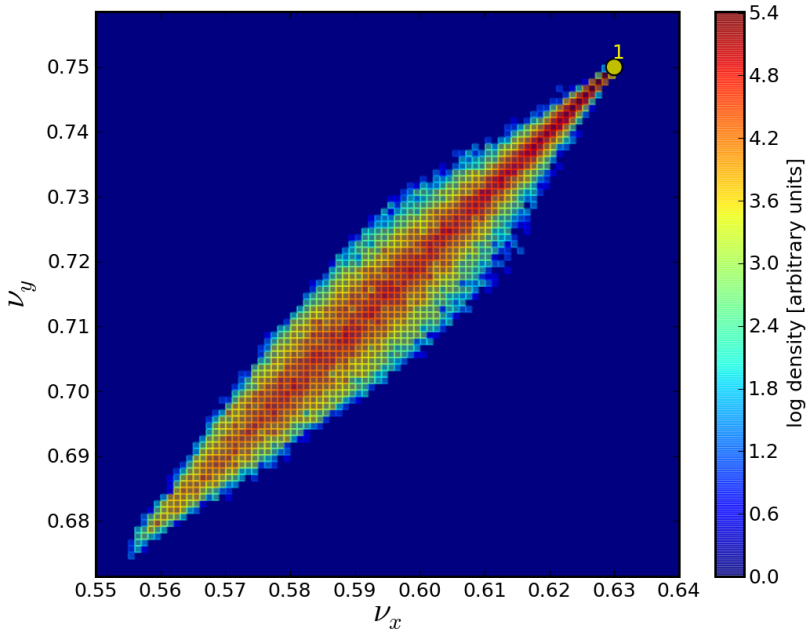
Beam with (nonlinear) sextupoles

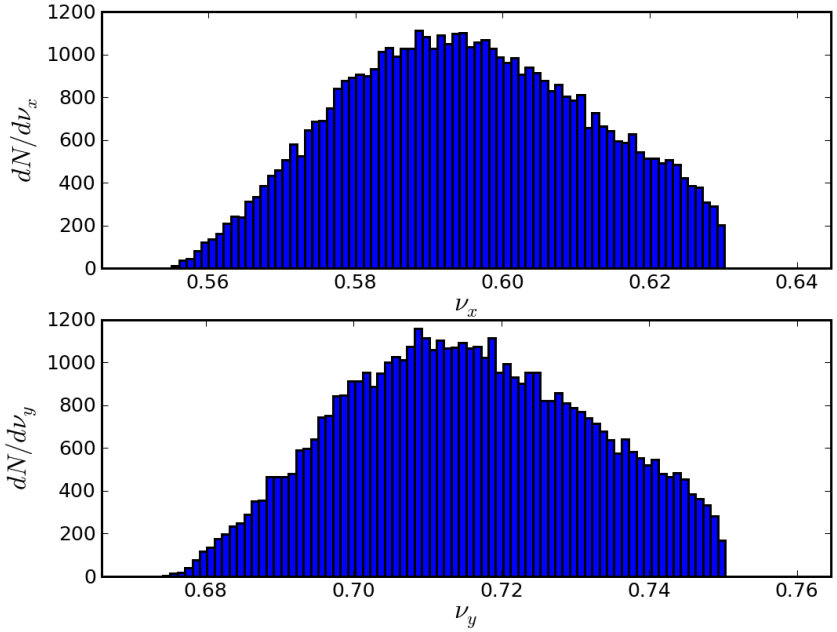


Nonlinear magnets distort the phase-space structure of the beam.

Effects of space charge without sextupoles

- In a fully linear linear problem, all particles have the same ("bare") tune.
- Space charge creates a "tune footprint"

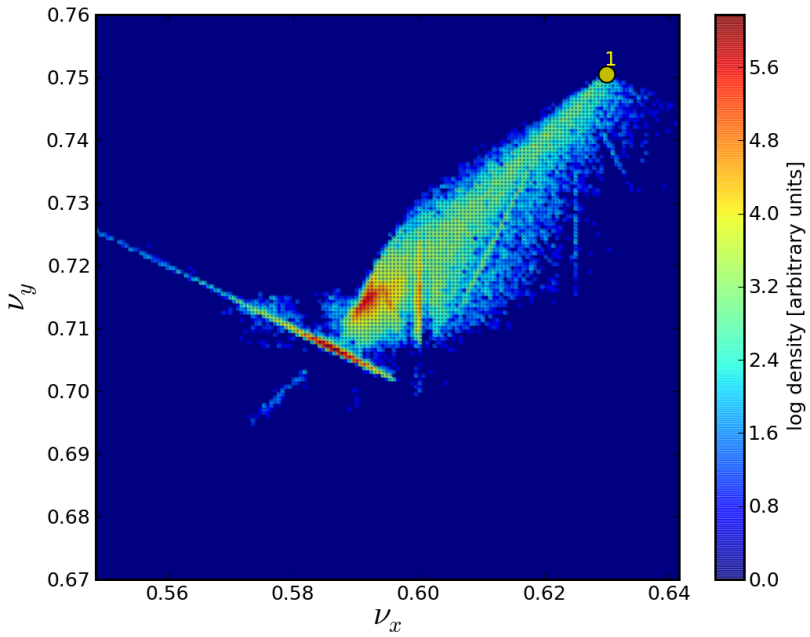


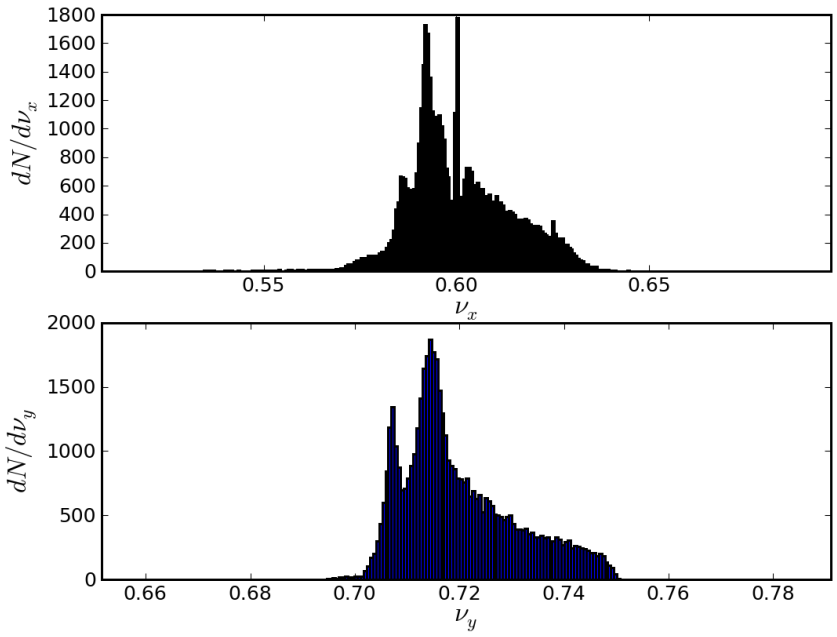


- Two-dimensional densities (colors) are plotted on a logarithmic scale
- One-dimensional densities are plotted on a linear scale
- Bin sizes are one unit of tune resolution

Combining sextupoles and space charge

Highly non-trivial interaction between the two effects...



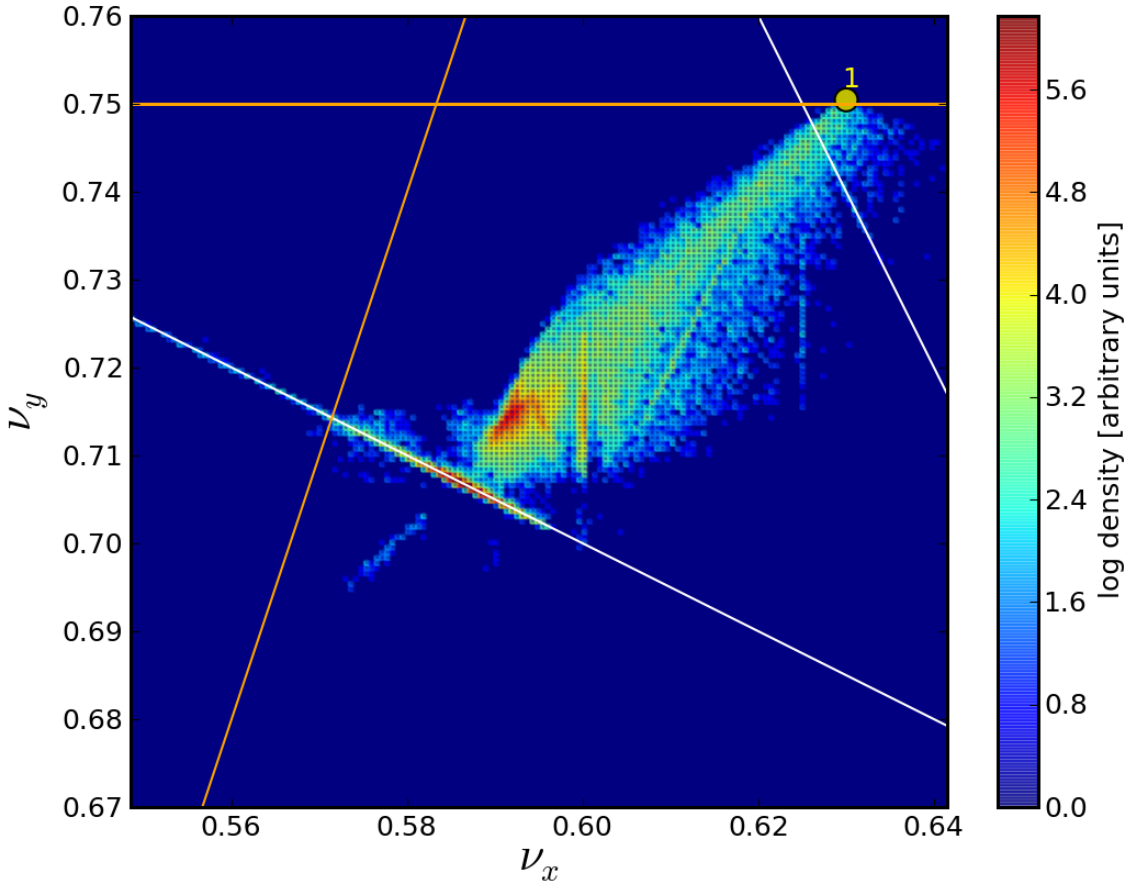


...leading to unacceptably large losses. Results are understood in terms of resonance theory. Resonances occur when

$$m + l\nu_x + q\nu_y = \nu_x$$

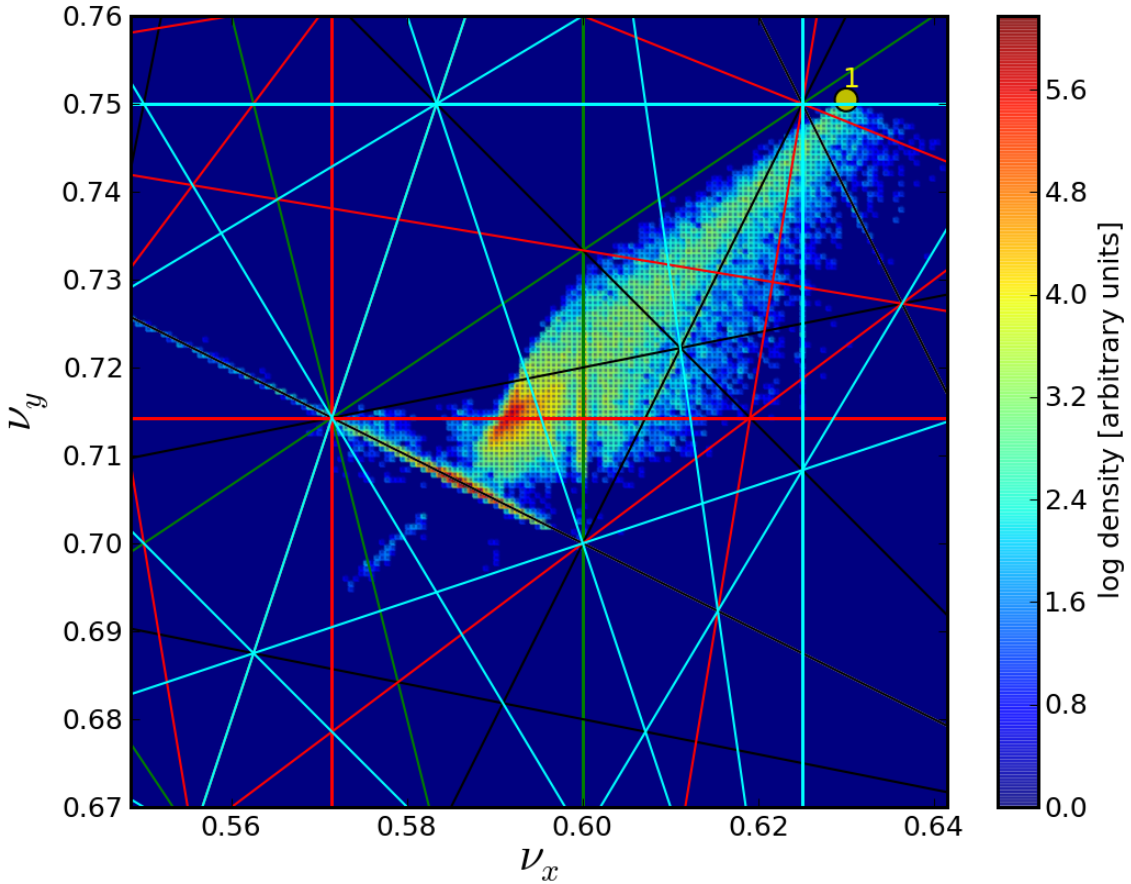
for integer m,l,q.

Resonance lines in the tune footprint



white	3rd-order	black	6th-order
orange	4th-order	red	7th-order
green	5th-order	cyan	8th-order

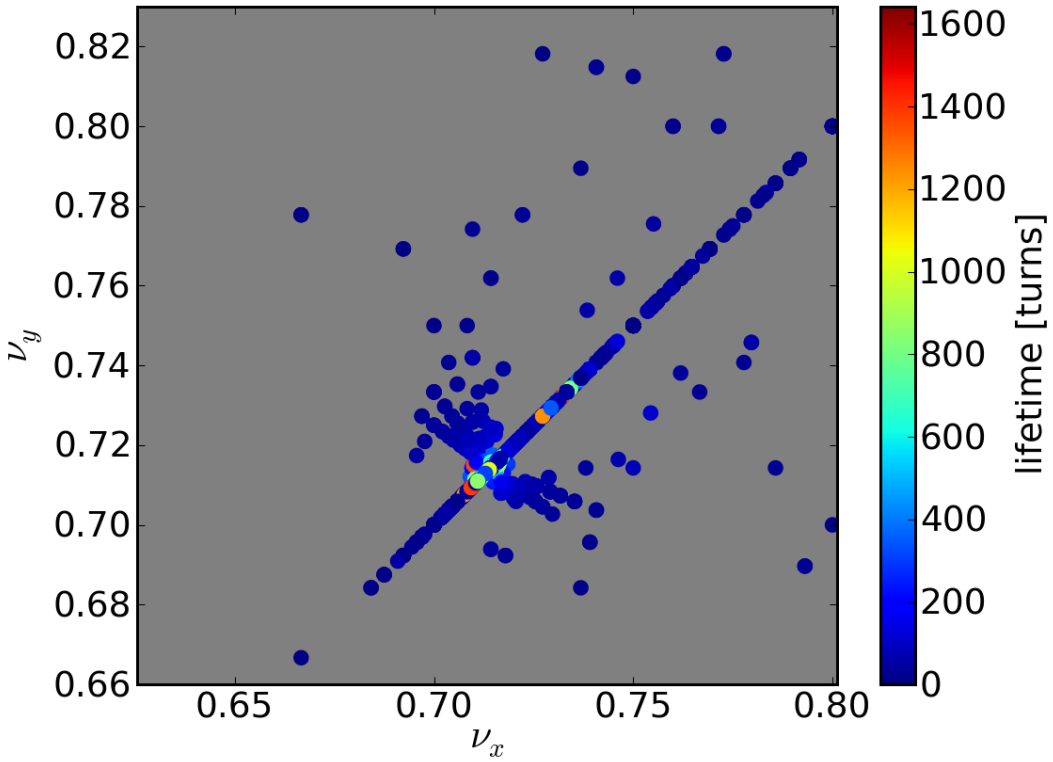
Resonance lines in the tune footprint



white	3rd-order	black	6th-order
orange	4th-order	red	7th-order
green	5th-order	cyan	8th-order

Resonance structure of lost particles

Since we track all particles, we can also examine losses in detail



- Particles fall neatly on resonance lines
- An example of "resonance streaming" predicted 20 years ago

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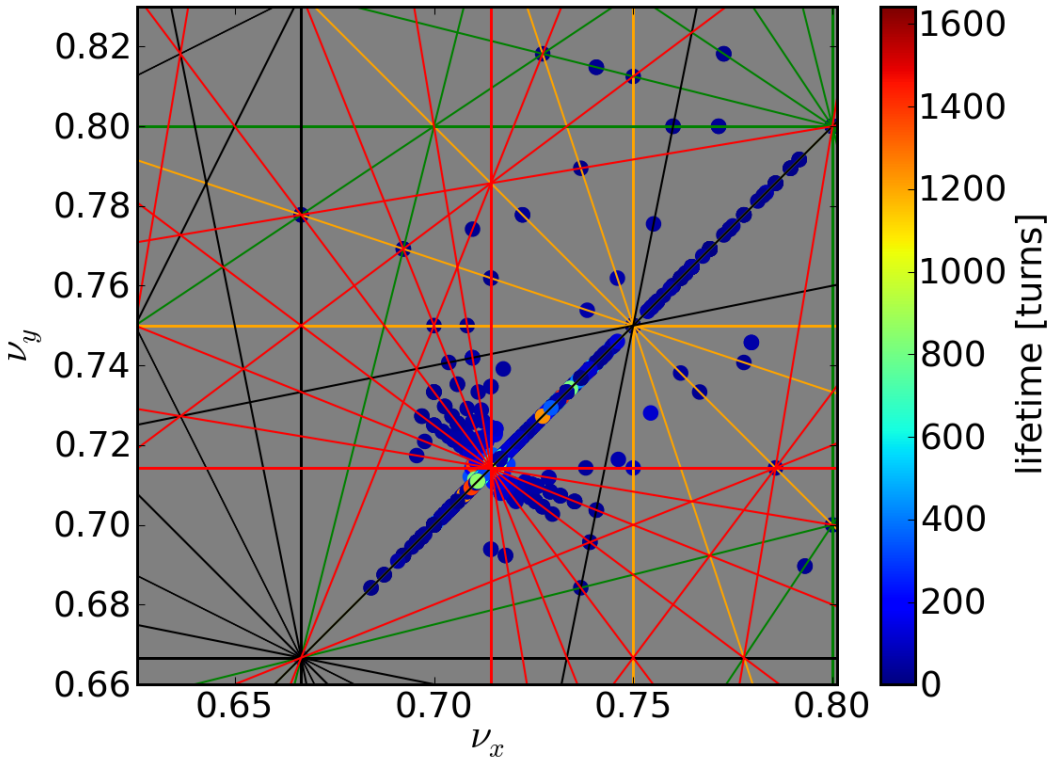

- Particles fall neatly on resonance lines
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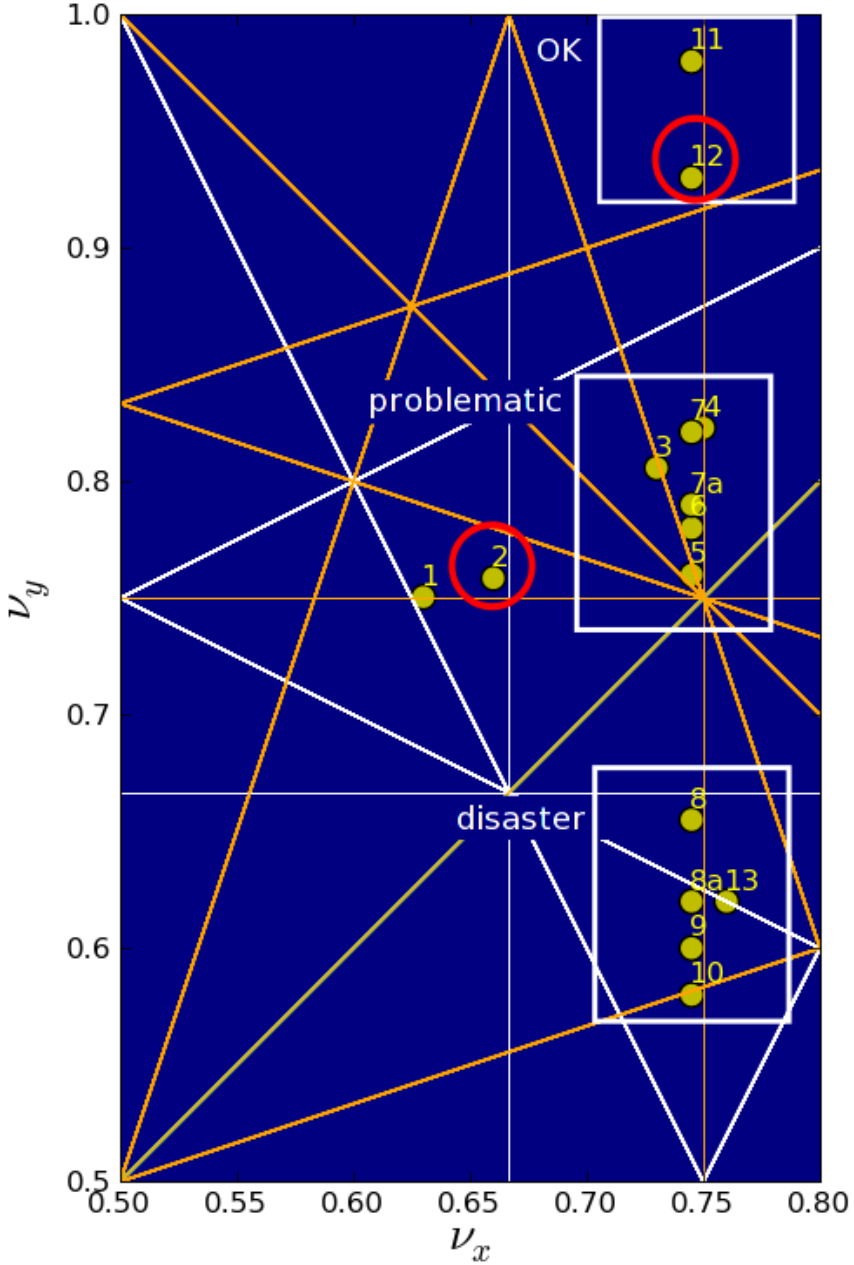
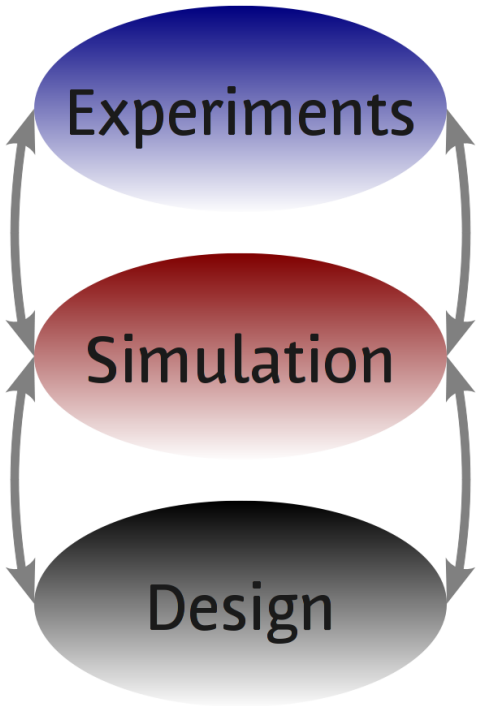
Conclusions from Mu2e simulations



- Performed tune scan
  - A few points better
  - Most much worse
  - None good enough
- Conclusion: beam will experience unacceptable losses before extraction process begins
  - Experiment decided to look at lower-intensity options
  - Simulation work in progress
- This problem very amenable to automatic optimization strategies
  - Again, work in progress

Preparing for the Exascale

- First step: realize how ingrained current architecture assumptions are in models
- Next step: start explorations of different architectures
  - Generic PIC simulations abstracted and parameterized; good performance obtained when applied to GPUs
- Strong scaling is limited
- Find new ways to exploit weak scaling
  - Effective parallel optimization
  - New algorithms for longer time steps
- Some weak scaling is easy
  - Typical particle bunches in accelerators run $10^{10} - 10^{13}$ particles – simulations could be done with real (not macro-) particles
- New decomposition strategies
  - Dynamic 6d decomposition – grid follows phase space, minimizing communication
- Application people working with CS/AM people and hardware vendors

Summary

- SciDAC Beam Dynamics codes
  - BeamBeam3d
  - VORPAL
  - IMPACT
  - Synergia
- HEP applications
  - The Energy Frontier
  - The Intensity Frontier
- Feedback between experiments, simulations and design
- Preparing for next generation of HPC