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SciDAC-3

ComPASS

Community Project for Accelerator Science and Simulation

James Amundson (*Fermilab*)
for the ComPASS collaboration

with special thanks to Jean-Luc Vay (LBNL) and Cho-Kuen Ng (SLAC)

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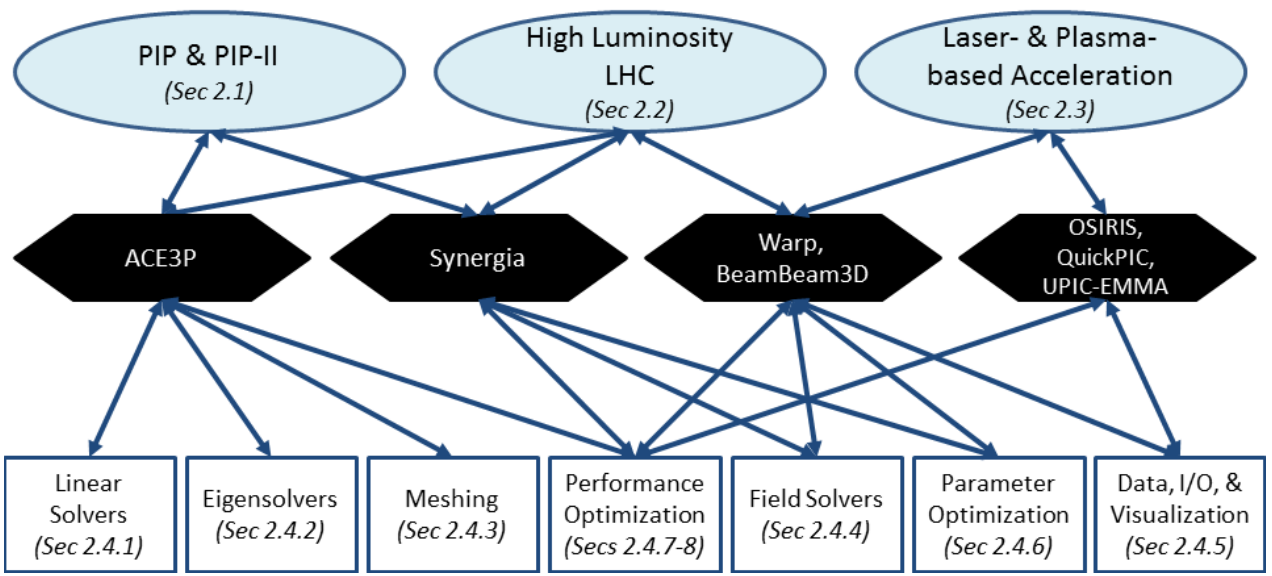
Particle Accelerators and ComPASS

- High Energy Physics relies on particle accelerators for the majority of experimental work
  - Non-HEP applications last year…
  - Frontiers in research involve both high *energy* accelerators and high *intensity* accelerators
    - ComPASS supports both
- HEP partnership with SciDAC Institutes: FASTMath, SDAV, and SUPER
- Cross-cutting activities with LQCD



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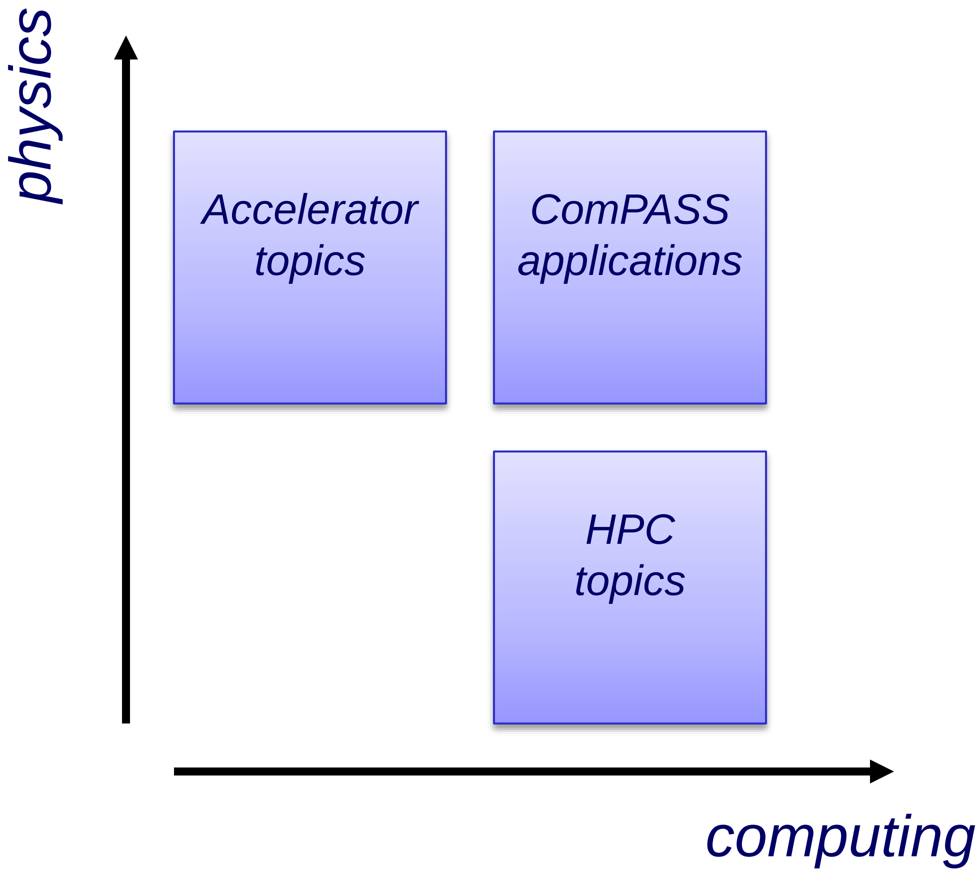
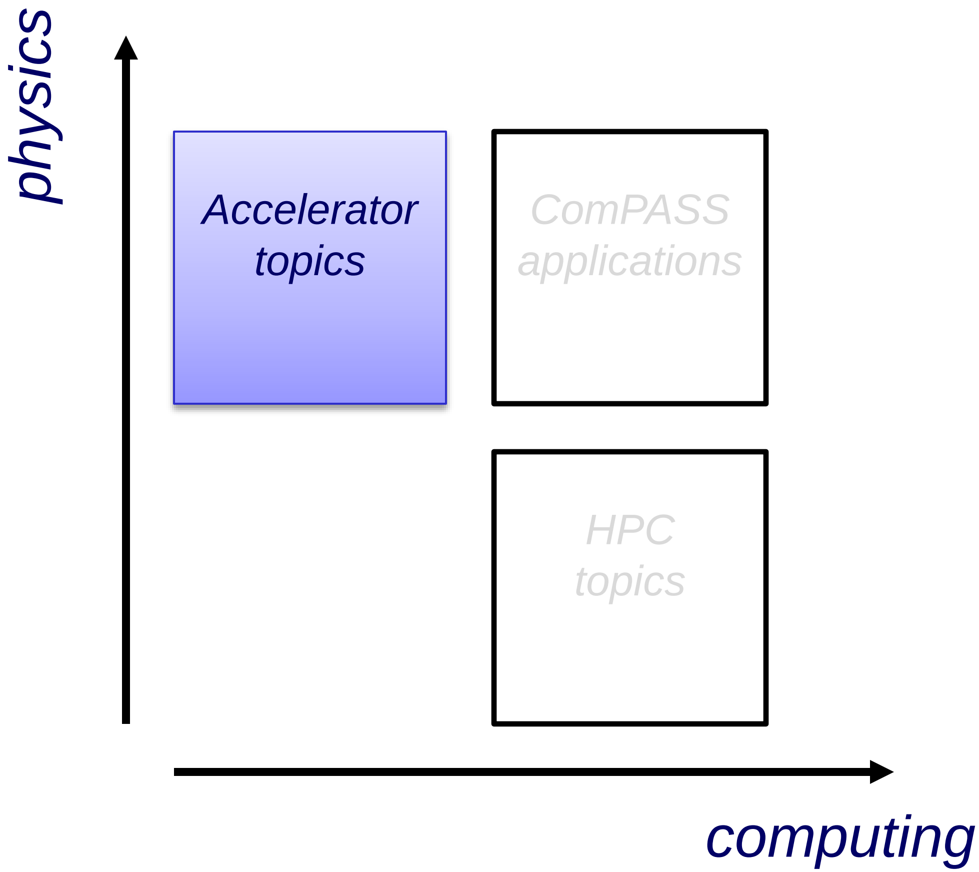
Topics


physics
Accelerator topics
ComPASS applications
HPC topics
computing

Accelerator topics



Accelerators for High Energy Physics

- 2014 Particle Physics Project Prioritization Panel (P5) report identified these priorities for High Energy Physics
  1. The physics of neutrino mass
     - Fermilab PIP-I,-II and beyond
  2. New particles and interactions
     - Fermilab Muon Program, LHC Upgrades, new machines
  3. Higgs Boson as a tool for discovery
     - LHC and beyond, new machines


Building for Discovery

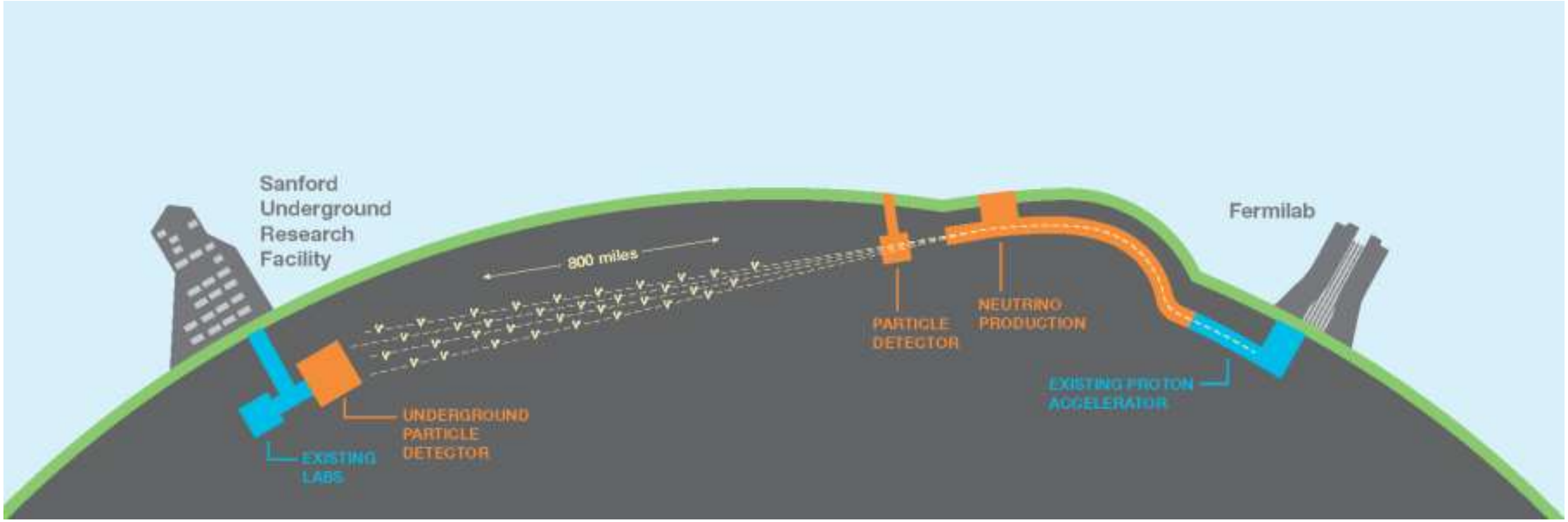
Strategic Plan for U.S. Particle Physics in the Global Context

Report of the Particle Physics Project Prioritization Panel (P5) May 2014

HEP future in the US

- Short term: Fermilab will produce high-intensity beams (PIP)
  - Fermilab Muon Program (g-2 and Mu2e experiments)
- Longer term: Fermilab will produce even higher-intensity beams (PIP-II)
  - Long Baseline Neutrino Facility (LBNF) and the Deep Underground Neutrino Experiment (DUNE)

ComPASS applications support both PIP and PIP-II



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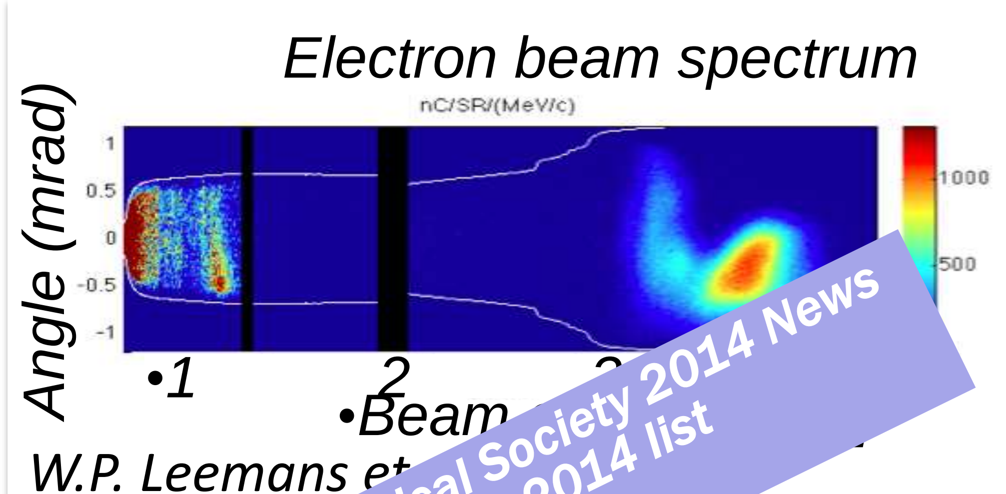
Moving on to future machines Laser-plasma accelerators: shorter and cheaper

Current world record by Berkeley Lab Laser Accelerator

4 GeV in only 10 cm!

First commercial Petawatt laser operating at > 42 J in ~30 fs at 1 Hz



Top 10 American Physical Society 2014 News
Top 20 Scientific American 2014 list

hysicists Break World Record for Compact Particle Accelerator with Powerful Laser

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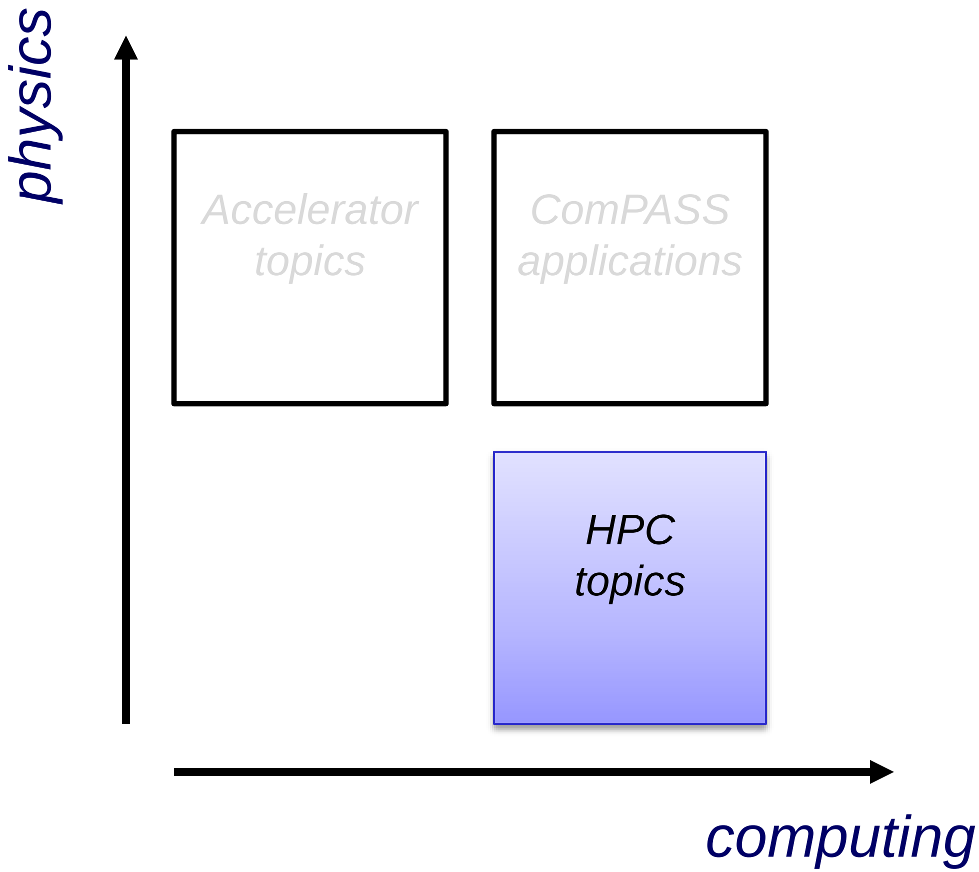
HPC topics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New Machines Coming Soon

- "May you live in interesting times…"
  - OLCF's Summit
    - IBM POWER CPUs
    - NVIDIA Volta GPUs
      - Talked about ComPASS GPU-based efforts in 2013 meeting
  - ALCF's Aurora
    - 3rd Generation Intel Xeon Phi
    - Also, NERSC's Cori
      - 2nd Generation Intel Xeon Phi
    - Work with 1st generation Phi is a valuable building block
      - 8-wide vector instructions
        - Nearly an order of magnitude
        - **Vectorization is not optional**

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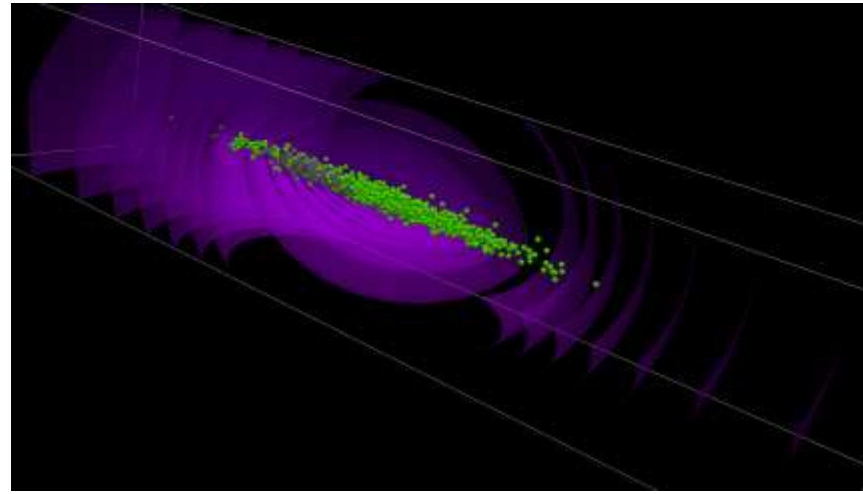
Optimizing Synergia for New Machines

- Synergia
  - beam dynamics
  - C++/Python
  - PIC, including independent particle and collectives
- MPI -> MPI + OpenMP
- Previous optimizations
  - MPI scalability
  - Collective effects
    - Require communication
  - Independent-particles considered trivial



- Code bottlenecks have now shifted
- New optimizations
  - Vectorization
  - Many-threaded OpenMP
  - Independent-particles not so trivial

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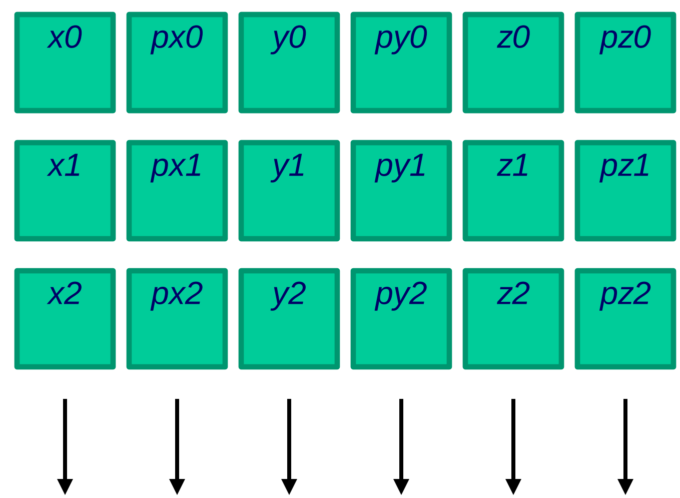
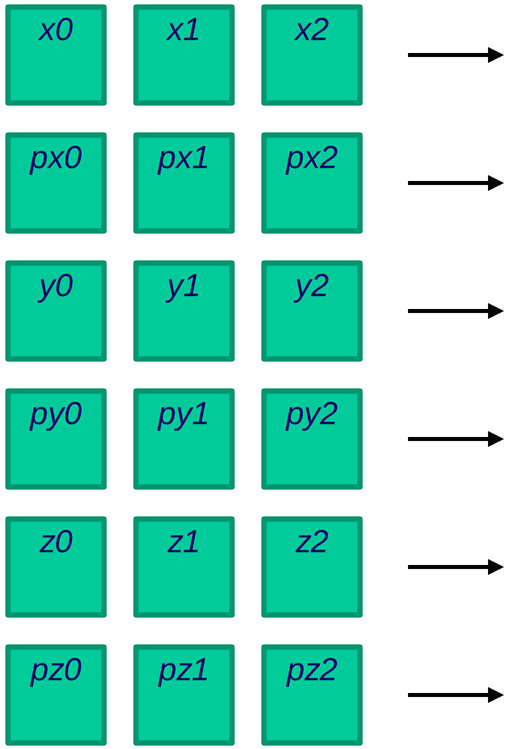
Vectorization in Synergia 1

- Original data layout
  - Cache-friendly data locality
    - All coordinates for a single particle are contiguous
    - Not vectorization-friendly
  - Data stored in dense 2d array
    - Boost MultiArray
  - Independent particle code has per-particle overhead
    - Small*
    - Perfectly scalable



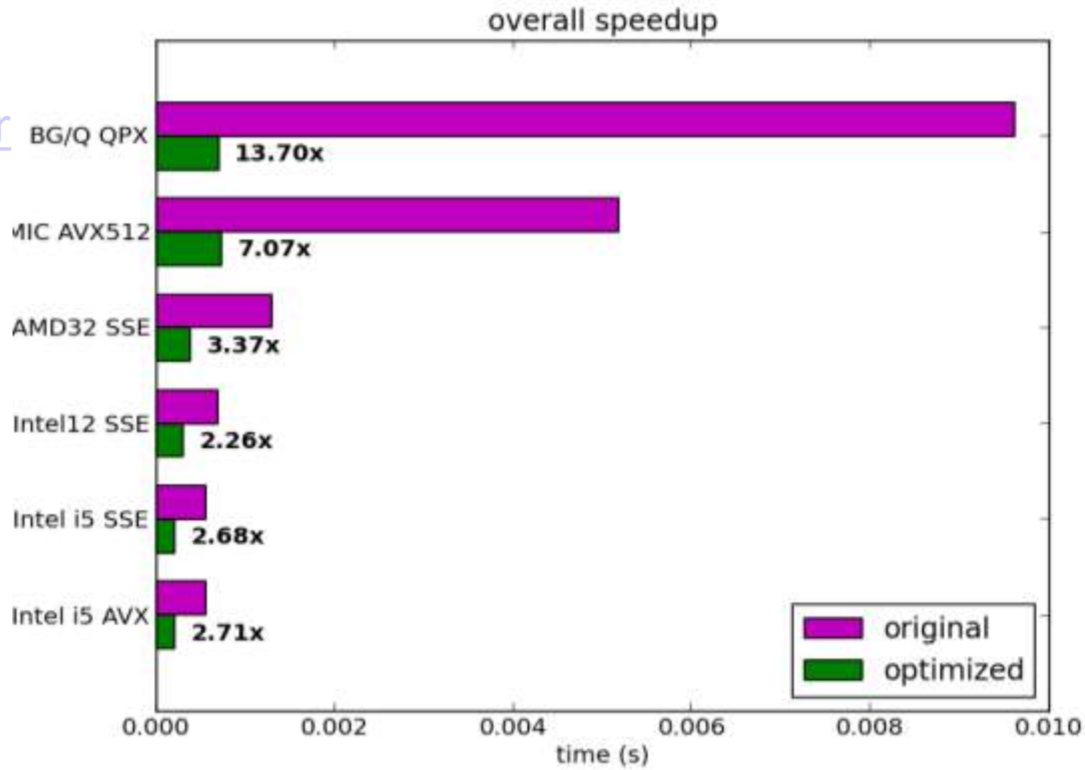
Vectorization in Synergia 2

- New data layout
  - Vectorization-friendly data locality
    - Each coordinate is contiguous
    - Always wins vs. original
  - Data still stored in dense 2d array
    - Boost MultiArray with Fortran ordering
      - Minimal code changes
  - New independent particle code has no per-particle overhead



Explicit Vectorization

- C++ template-based
  - vectorclass
    - http://www.agner.org
  - GSVector
    - Generalized SIMD Vector
    - Part of Synergia
    - Compile-time vectorization model choice
      - double to AVX512



Accessing Array Data

- No standard (yet) for multi-dimensional arrays in C++
- We use Boost MultiArray for particle data
  - Dense 2d array
- Consider multiple ways to access the *y* (index=2) value of particle *i* :
- MultiArray: particles[i][2]
- Manual index calculation: data[i+stride*2]
- C-style array: double * y = … ; y[i];
- Restricted array: double * __restrict__ y = … ; y[i];
  - language extension

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Performance vs. Access Type

- Performance is highly platform- and compiler-dependent

BG/Q	orig	manual index	array	restricted array	explicit vectorization
gcc	1.00	0.99	0.99	0.99	NA
xlc	1.87	1.87	1.87	3.75	7.78
bgclang	3.63	3.77	3.77	3.77	6.73
Intel Xeon					
gcc	1.00	1.00	1.00	1.00	2.00
icc	1.00	2.02	1.00	2.02	2.02
Intel Phi					
icc	1.00	9.48	1.27	9.37	6.99

A single version of the code produces optimal performance on all platforms using GSVector

Observations on C++ in HPC

- Abstraction invaluable in low-level optimization
  - Changed data ordering with a flag, not by switching indices throughout the code.
  - Explicit vectorization with templates is easy.
    - Rewriting expressions with function calls is a nightmare.
- GCC and Clang are great for C++03
  - icc requires workarounds to compile our code
  - xlc requires more workarounds, still stuck on Boost Serialization
- HEP experiments have moved to C++11/C++14
  - Much better
  - C++17 on the horizon
- Multiple proposals for multi-dimensional arrays for C++17
  - Finally!
  - No evidence of input from HPC community
- Need real C++ support on next-generation machines

Spectral solver parallelization

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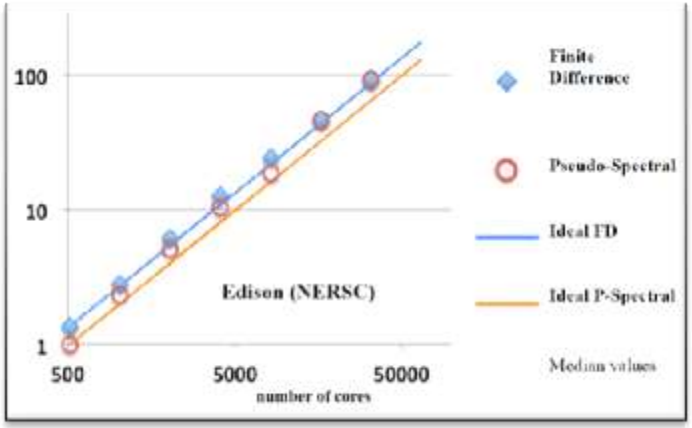
- *Novel paradigm for parallelization of spectral solvers promises large scalability*

•Uses finite speed of light to enable domain decomposition with local FFTs:
➔ direct scaling to many cores.

*•J.-L. Vay, I. Haber & B. B. Godfrey, J. Comp. Phys. **243** (2013)*
•J.-L. Vay, L. A. Drummond, A. Koniges, B. B. Godfrey & I. Haber, poster SC'14, New Orleans, LA.
•2014 NERSC Innovative Use of HPC Achievement award

•Warp FDTD/spectral-PIC (strong scaling)



- *Demonstrated analytically and numerically efficiency of Perfectly Matched Layers for open boundaries with spectral Maxwell solvers*

spurious reflections

*•P. Lee, J.-L. Vay, Comp. Phys. Comm. **194**, 1-9 (2015)*

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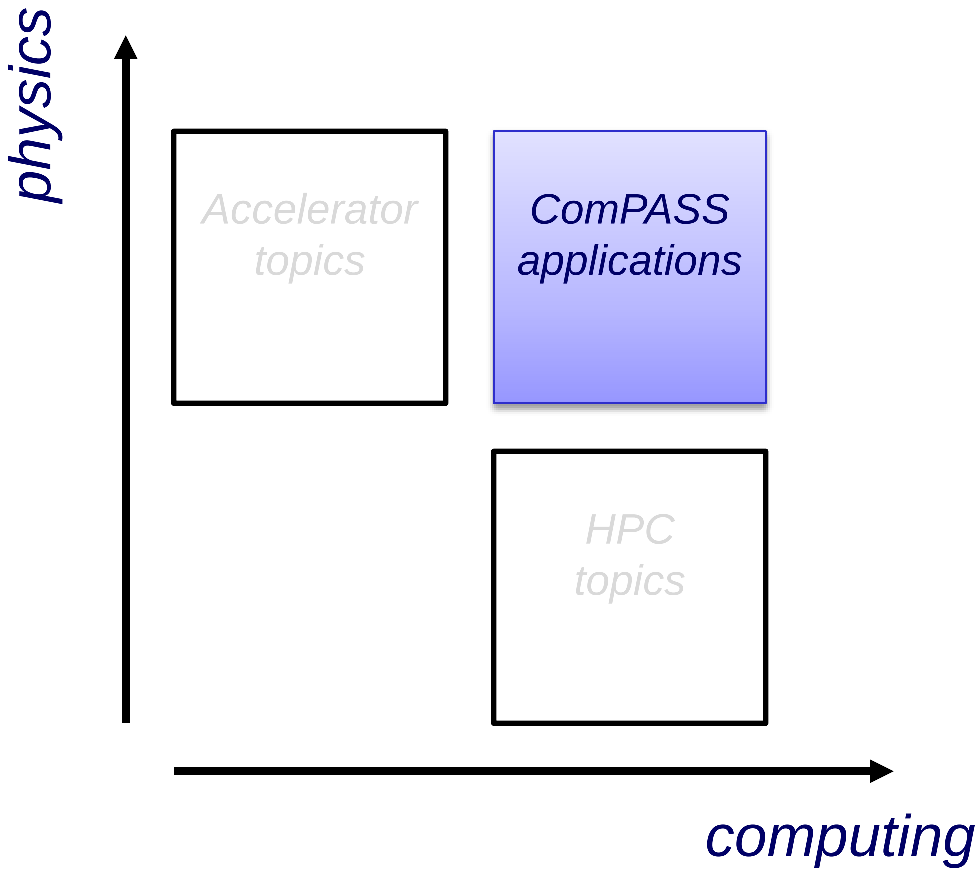
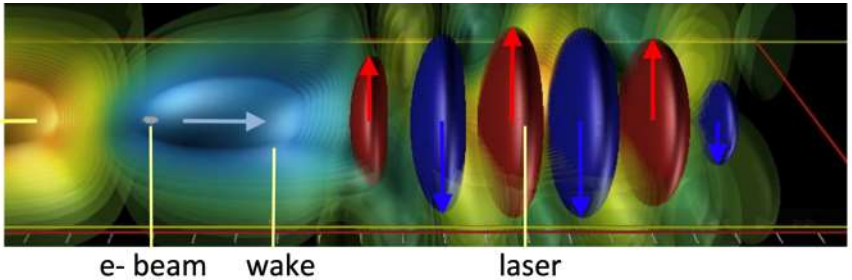
ComPASS Applications

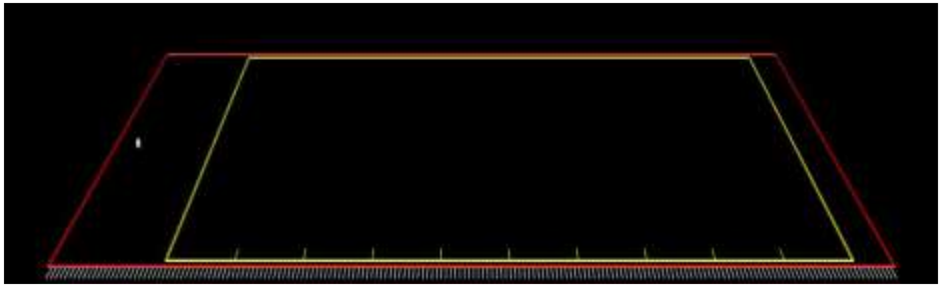


Challenges in first-principle models

Electron beams surf on plasma waves that support very high electric fields.



For a 10 GeV stage:

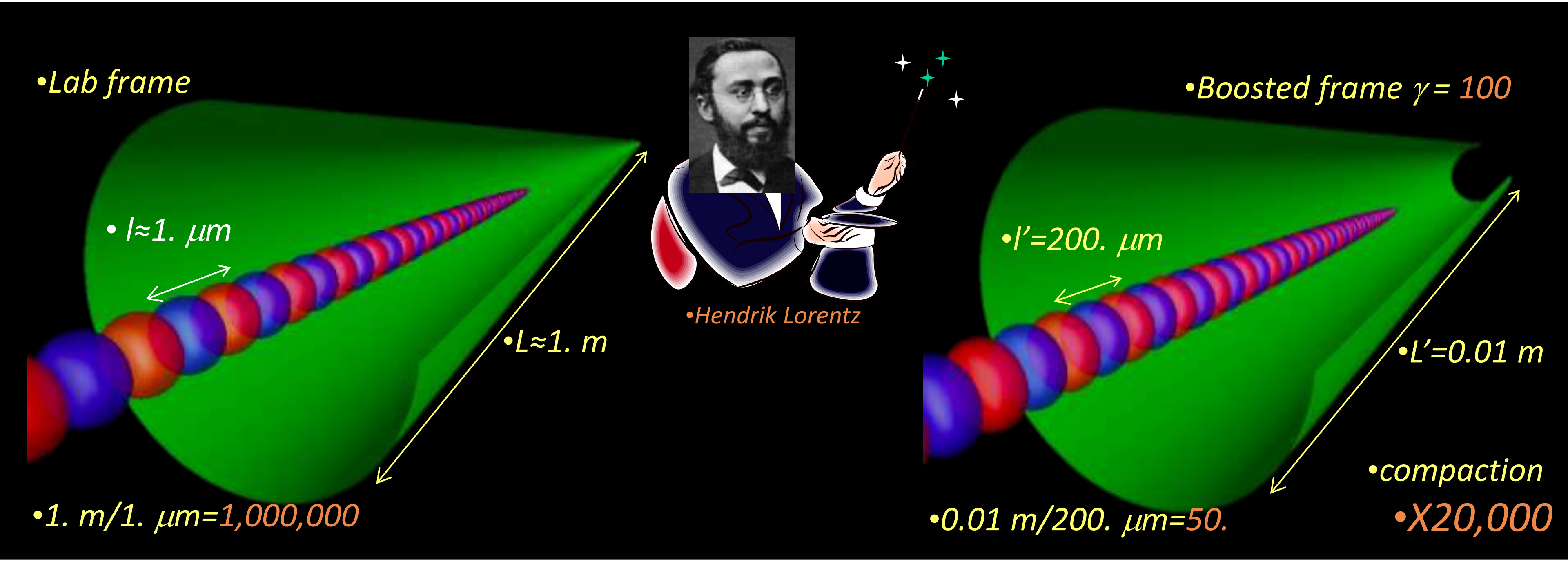


~1μm wavelength laser propagates into ~1m plasma

➔ millions of time steps needed

(similar to modeling 5m boat crossing ~5000 km Atlantic Ocean)

One approach: Boosted Frame



- *BELLA-scale w/ ~ 5k CPU-Hrs: 2006 - 1D run ➔ 2011: 3D run*
- *Other possibilities include quasi-static/laser envelope solvers*

However "numerical Cherenkov" instability limits speedup!

•*J.-L. Vay, Phys. Rev. Lett. **98**, 130405 (2007)*

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Progress on Numerical Cerenkov

- ***Analysis of Numerical Cherenkov has been generalized:***
  - ***to finite-difference PIC codes ("Magical" time step explained):***
    - *B. B. Godfrey and J.-L. Vay, J. Comp. Phys. 248* ***(2013)*** *33.*
    - *X. Xu, et. al., Comp. Phys. Comm., 184* ***(2013)*** *2503.*
  - ***to pseudo-spectral PIC codes:***
    - *B. B. Godfrey, J. -L. Vay, I. Haber, J. Comp. Phys., 258* ***(2014)*** *689.*
    - *P. Yu et. al, J. Comp. Phys. 266* ***(2014)*** *124.*

- ***Efficient suppression techniques were recently developed:***
  - ***for finite-difference PIC codes:***
    - *B. B. Godfrey and J.-L. Vay, J. Comp. Phys. 267* ***(2014)*** *1.*
    - *B. B. Godfrey and J.-L. Vay, Comp. Phys. Comm.,* ***in press***
  - ***for pseudo-spectral PIC codes:***
    - *B. B. Godfrey, J.-L. Vay, I. Haber, IEEE Trans. Plas. Sci. 42* ***(2014)*** *1339.*
    - *P. Yu, et. al., arXiv:1407.0272* ***(2014)***

Applications to relativistic laboratory and space plasmas

SciDAC ComPASS collaboration played a key role

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ComPASS Applications

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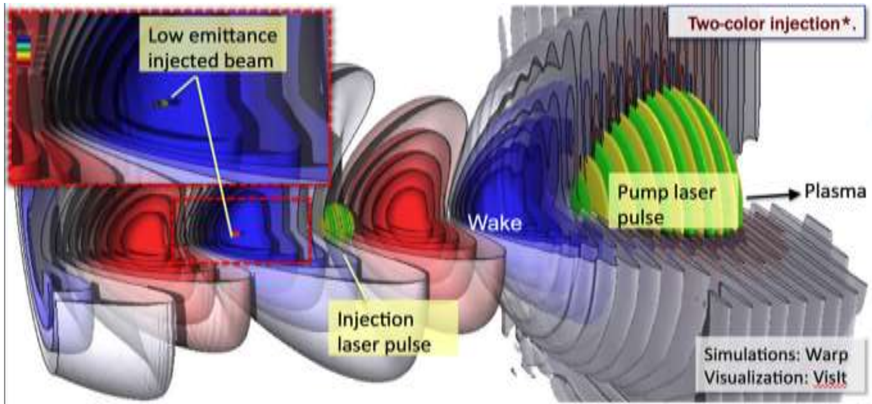
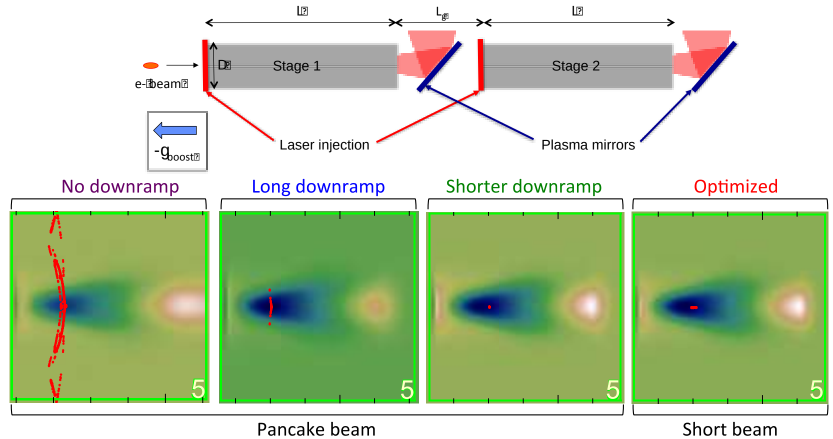
•*Validation of a new concept of injection of high-quality beam*



•*L.-L. Yu, et al, Phys. Rev. Lett.* ***112****, 125001 (2014)*

•*C. Schroeder, et al, Phys. Rev. ST-AB* ***17****, 101301 (2014)*

•*Optimization of beam quality in chained stages for colliders studies*



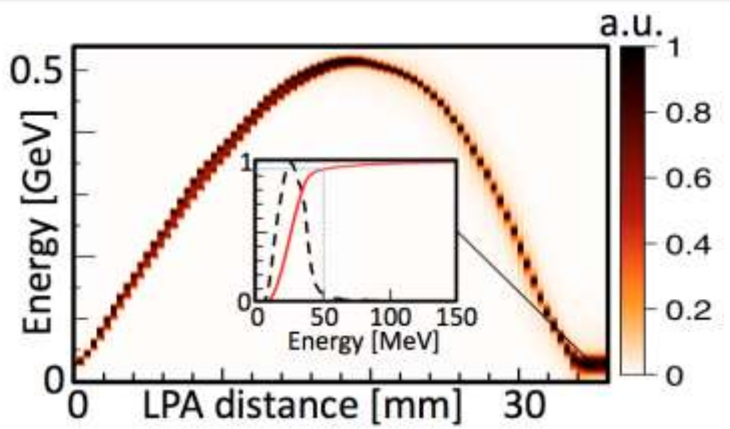
•*J.-L. Vay, et al., Proc. 2014 Advanced Accelerator Concepts*

•*Design of efficient accel-decel stages for portable radiation sources*

•*J.-L. Vay, et al, Proc. NPNSP14 (2015)*

•*C. G. R. Geddes, et al, Nucl. Instr. Meth. Phys. B* ***350*** *(2015)*

•*S G Rykovanov, et al, J. Phys. B: At. Mol. Opt. Phys.* ***47*** *(2014)*



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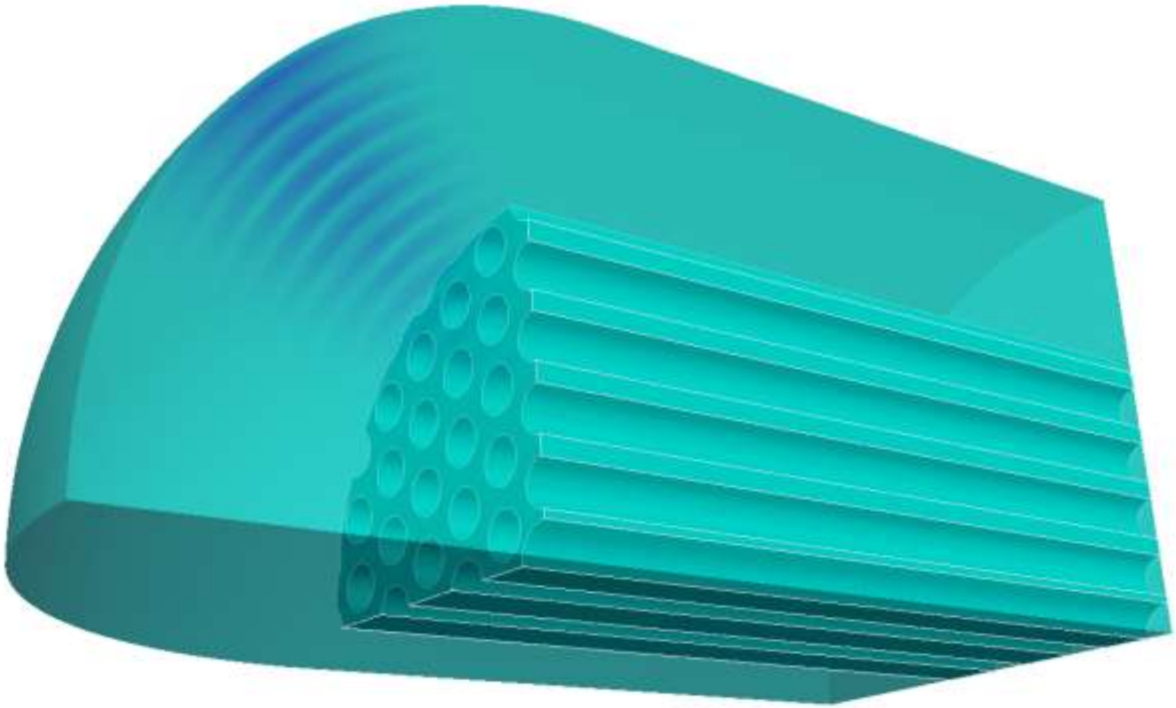
Dielectric Laser Acceleration



- *Excitation of accelerating mode in photonic bandgap (PBG) fiber using laser beam from free space*
- *ACE3P used to investigate coupling mechanism for optimum power transfer form laser to accelerating mode in PBG fiber*

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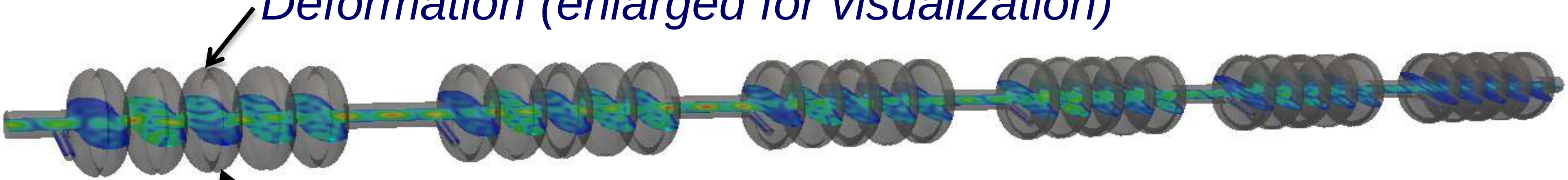
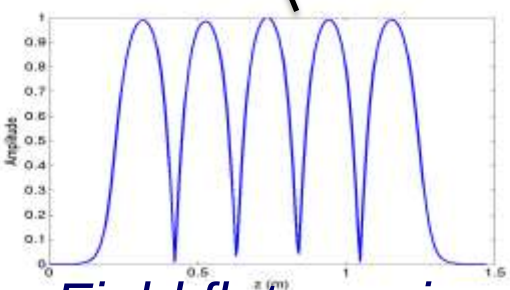
PIP-II Linac Cryomodule

Deformation (enlarged for visualization)





Field flatness in cavity

Higher-order mode (HOM) in the PIP2 650 MHz cryomodule (consisting of 6 superconducting cavities) with deformations at equators of cavity cells. The electric field pattern is shown on a cut plane.

- *Using ACE3P, deformed cavities in the cryomodule tuned to provide the designed frequency and field flatness across the cavity cells for the accelerating mode*
- *Deviations of HOM frequencies in deformed cryomodules evaluated for studying their effects on beam stability*

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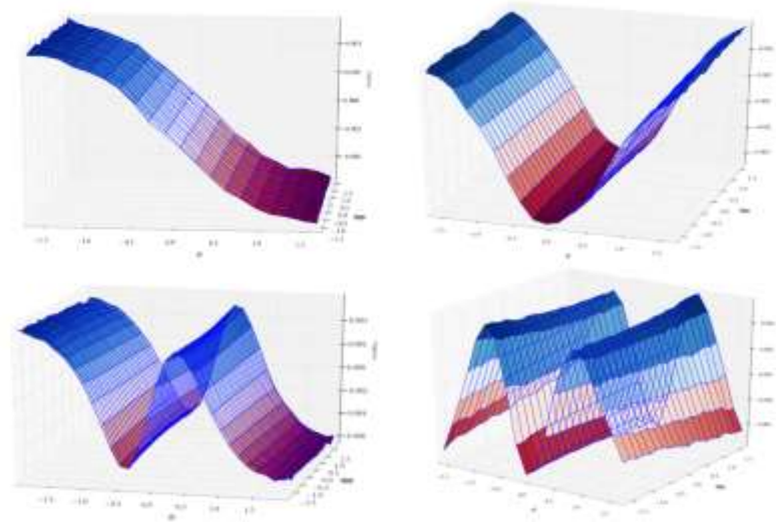
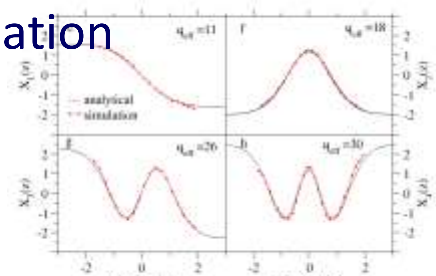
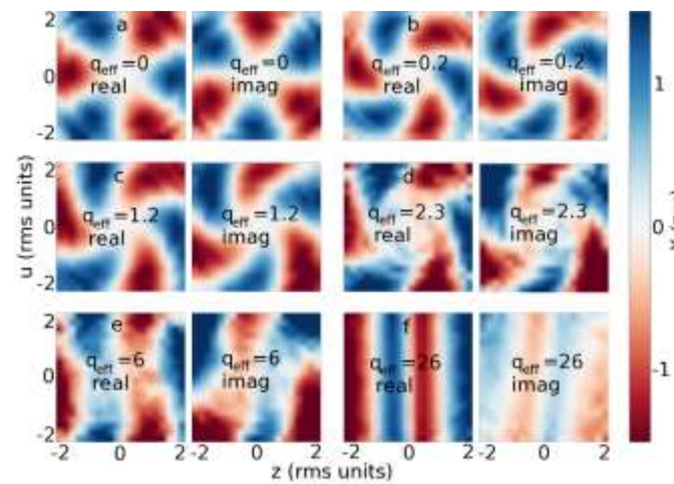
Applications to Accelerator Theory

- Space charge modes provide theoretical framework for space charge studies
  - A. Burov, PRST-AB 12, 044202 (2009), PRST-AB 12, 109901, (2009).
- Difficult to modes from noise in realistic simulation
- First use of Dynamic Mode Decomposition (DMD) in Beam Dynamics
  - ComPASS: Macridin, et al., PRST-AB *to appear in 2015.*
- Excellent theory/simulation agreement







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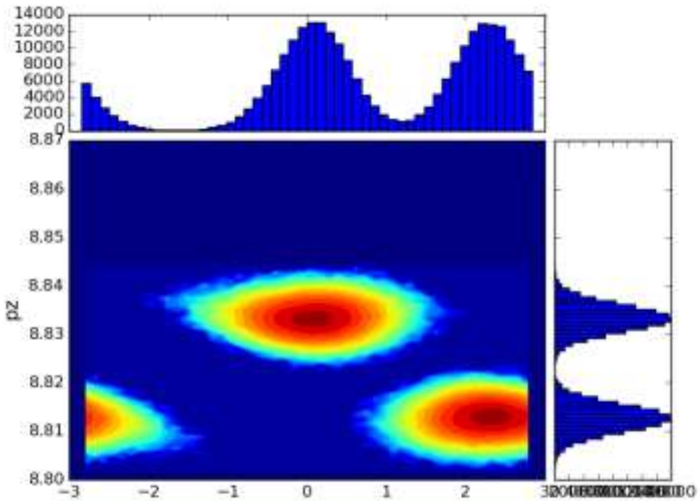
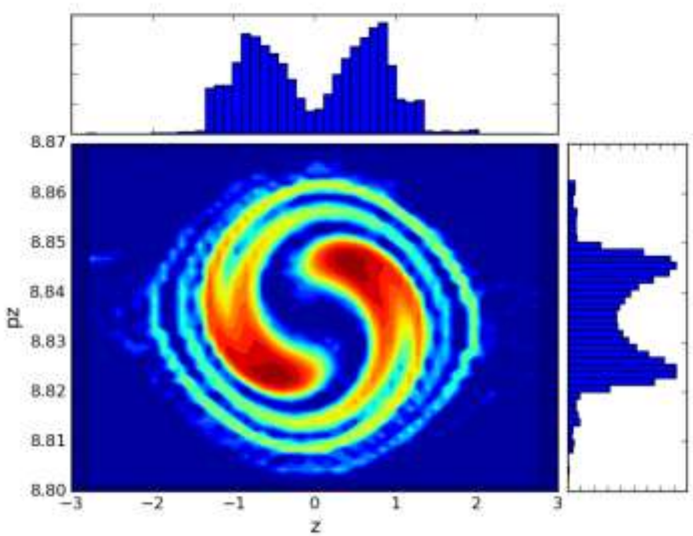
Application to Fermilab PIP-II

- Slip stacking
  - Used at Fermilab to create high-intensity beams
    - Pairs of bunches combined
  - Synergia simulations of single pairs require O(1000) cores
    - Periodic boundary conditions mimic other pairs
  - Realistic simulations will include O(500) pairs
    - Non-trivial structure observed in operation
    - Bunch-bunch wake field interactions
- Truly a leadership class computing problem.
  - Work in progress!





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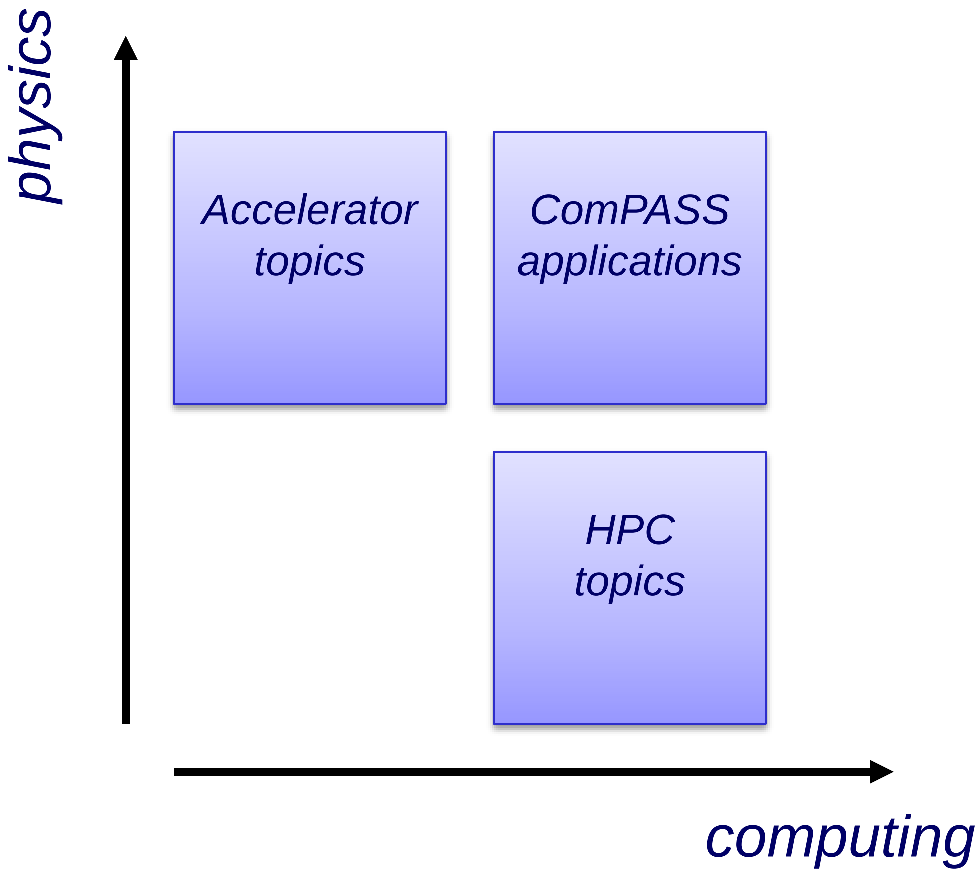
Conclusions



- Accelerator Topics
  - ComPASS working on P5 Priorities
  - Especially PIP-II, et al. at Fermilab for LBNF and DUNE
- HPC Topics
  - New machines
  - Vectorization
  - Scalable spectral solvers
- ComPASS Applications
  - Boosted Frame/Cerenkov problem
  - New accelerator problems
  - Theory/Simulation and DMD
  - Slip Stacking