Community Project for Accelerator Science and Simulation 4

ComPASS-4

Eric Stern(FNAL, Deputy-PI)

for

James Amundson (FNAL, PI), Ann Almgren (LBNL), Warren Mori (UCLA), Esmond Ng (LBNL) and Stefan Wild (ANL)

Fermilab UCLA Argonne NATIONAL LABORATORY BERKELEY LAB

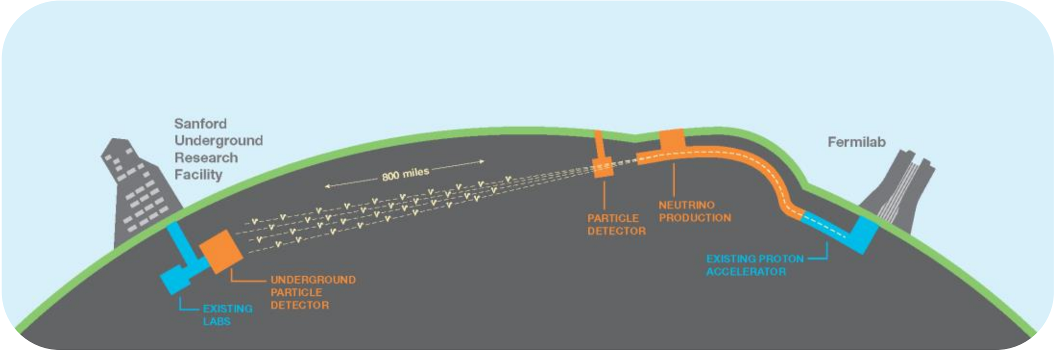
Driven By HEP Priorities from the P5 Report

- Beam Dynamics
  - Conventional accelerator technology
    - [superconducting] RF cavities for acceleration
    - [superconducting] Magnets for steering
  - Intensity-dependent effects are most common limiting factor
- Plasma-based Acceleration
  - Next-generation accelerator technology
  - Could lead the way towards higher energy and more compact accelerators

Both are associated with active programs requiring simulation efforts

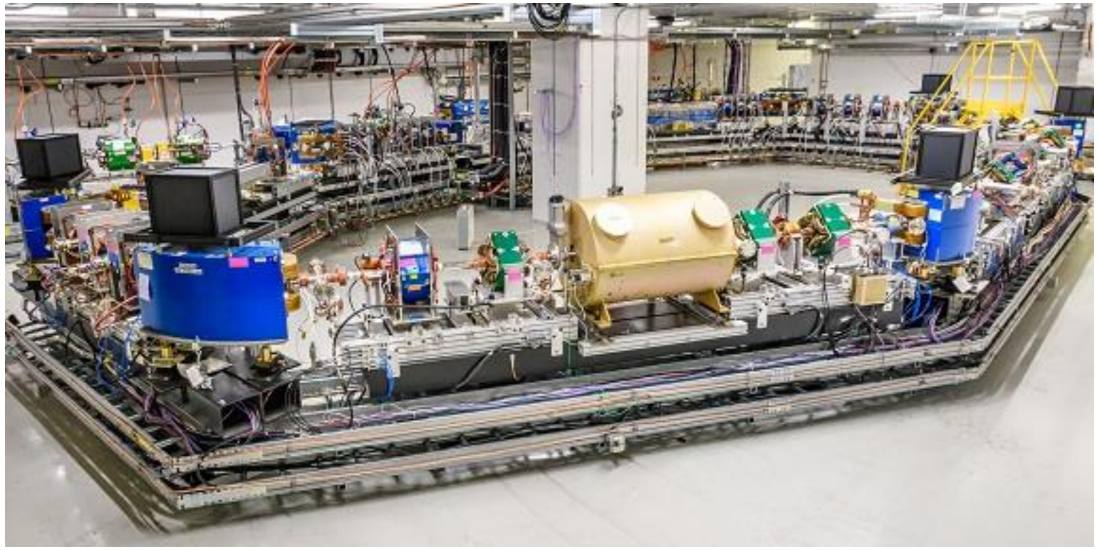
ComPASS4 Supports HEP Accelerator Science

- The US High Energy Physics program is centered on high intensity physics
- The Deep Underground Neutrino Experiment (DUNE) will be the flagship experiment in the US program
- The recently started PIP-II project will increase the intensity of the beams produced by the Fermilab accelerator complex
- High-intensity beams are necessary for the success of DUNE
- Simulations of intensity-dependent beam dynamics and their resulting beam loss are critical for a successful PIP-II implementation
- ComPASS4 is enabling and performing intensity-dependent simulations for PIP-II



Accelerator Science Research

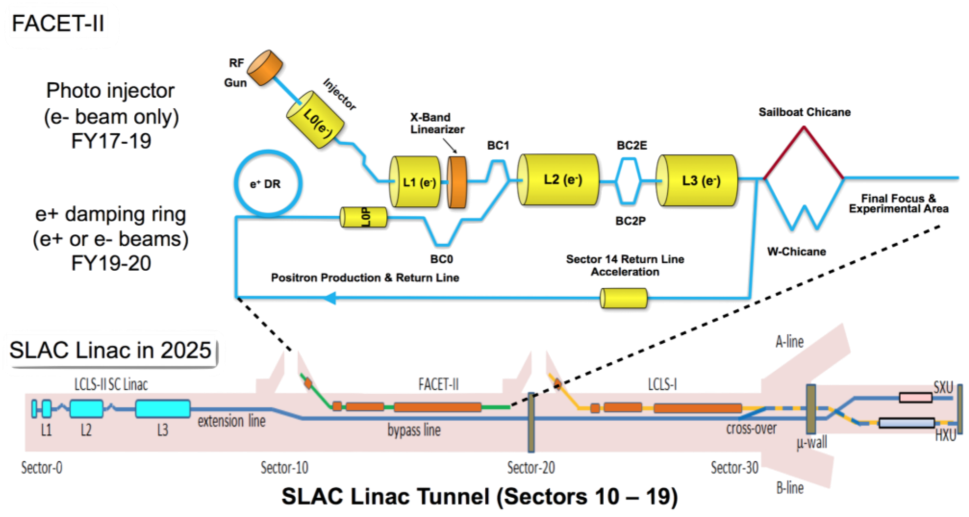
- The Integrable Optics Test Accelerator (IOTA) ring was recently commissioned at the Fermilab Accelerator Science and Technology (FAST) facility for research and development of accelerator technology for the next generation of conventional particle accelerators.
- IOTA will be a testbed for new accelerator instrumentation, control and measurement techniques.
- ComPASS4 simulations are part of the FAST/IOTA program.
- Beam dynamics are simulated with the **Synergia** code developed at Fermilab.



Plasma Acceleration Test Facility: FACET-II

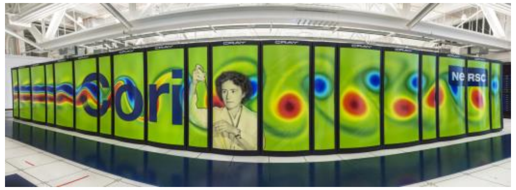
- The FACET-II facility will experimentally investigate plasma wake acceleration with the goal of eventually realizing low-emittance, multi-TeV electron and positron beams for HEP research.

- ComPASS4 simulations will support FACET-II with simulations using the OSIRIS and QuickPIC codes.
- Important simulation issues are:
  - Try to understand emittance growth and develop methods for achieving beams suitable for colliders.
  - Is positron acceleration possible?
  - Multi-stage operation with efficient beam capture between stages.



HEP/ASCR Collaboration in ComPASS4

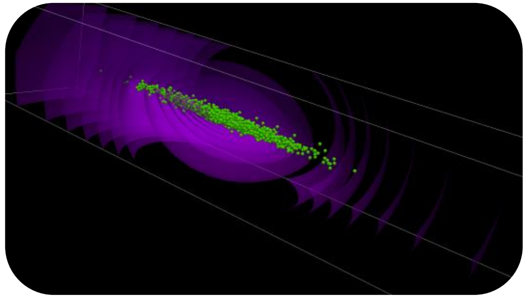
- ComPASS4 accelerator physics efforts partner with ASCR projects in three areas
    1. Advanced Solvers for Accelerator Physics (ASAP) are taking advantage of developments in linear algebra and automatic mesh refinement
    2. PIC methods are being refined for modern computing architectures
    3. Advanced optimization methods are being made available for general accelerator problems in the Platform for Optimization of Particle Accelerators at Scale (POPAS)
- ComPASS4 makes extensive use of DOE scientific computing facilities especially NERSC for large-scale computations
- ComPASS4 takes advantage of other ASCR projects such as Kokkos from ECP

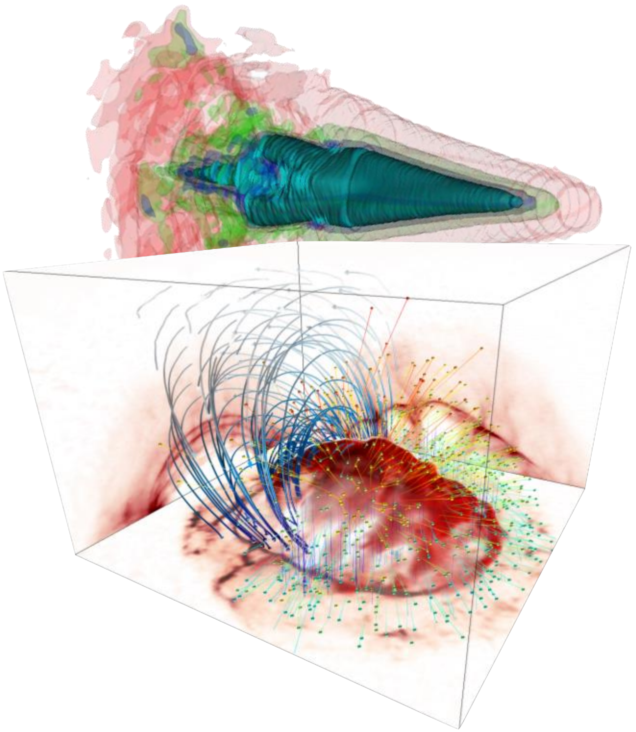


Conventional and Plasma Acceleration Codes

- **Synergia** is the primary ComPASS4 package for conventional beam dynamics
  - Linear and non-linear single-particle dynamics
  - Space charge and general wakefields
  - Tracking of single bunches, bunch trains, and overlapping bunch trains
- **QuickPIC** will be enhanced as part of ComPASS4
  - QuickPIC is a 3D parallel Quasi-Static PIC code, which is developed based on the framework UPIC
    - Pipeline Parallelization in z
    - Laser Module and Field Ionization Module
- Some ComPASS4 physics simulations will utilize **Osiris**
  - Osiris is a full parallel PIC code with state-of-art relativistic EM-PIC algorithm.
    - QED module

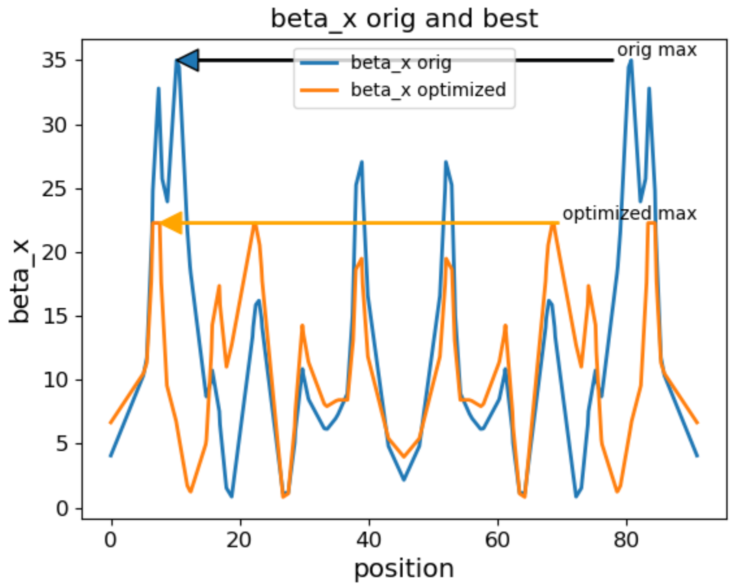
All codes support parallel processing on various architectures

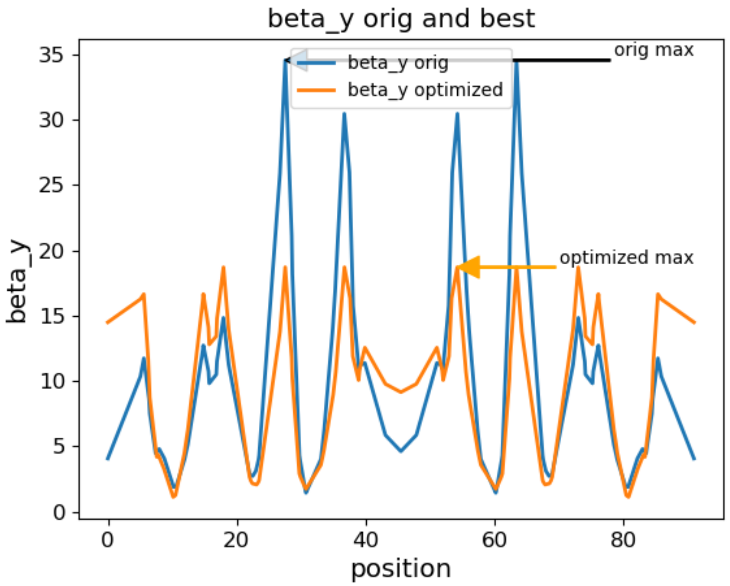




Optimization of an RCS Accelerator with POPAS

- **POPAS** employs Synergia to evaluate candidate RCS design lattices to minimize the largest beta function subject to practical constraints.
- Optimization of 72 accelerator magnet positions, strengths and sizes.
- Reducing the maximum beta function in the lattice design lowers the total cost of the accelerator.



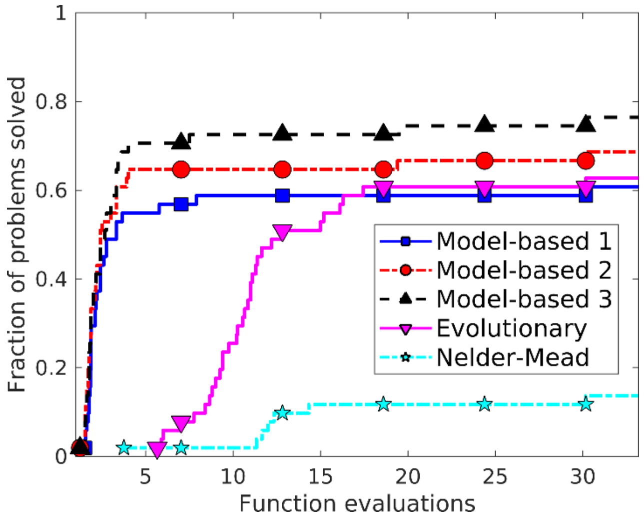


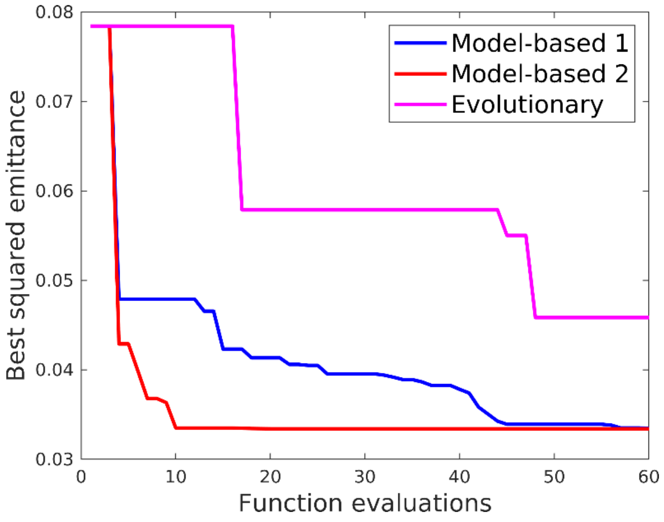
Jeffrey Larson, ANL
Eric Stern, FNAL

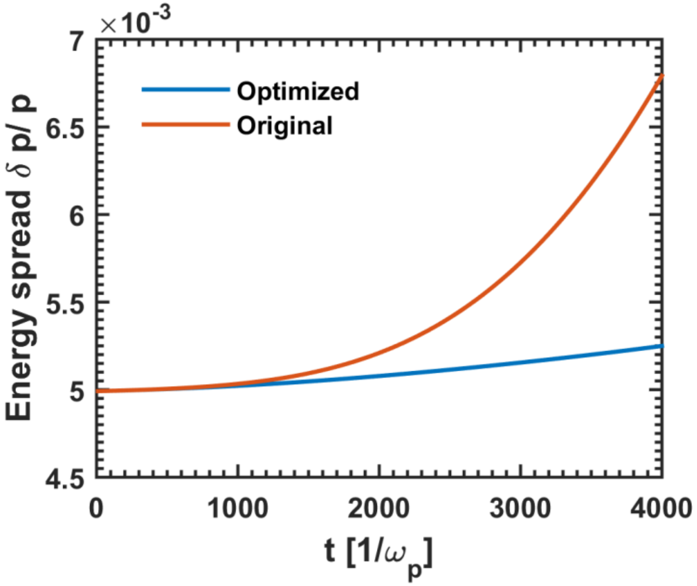
Optimization of positron emittance with POPAS

- Adjust witness beam twiss parameter α_0 and β_0 to minimize emittance growth
- Optimized emittance growth as low as 0.1% in 0.5cm
- Optimized α_0 and β_0 are close to numerical estimation from theory

Energy spread is optimized by adjusting witness beam position and current so that beam loading exactly flattens E_z.







Weiming An, UCLA, Jeffrey Larson, ANL

Accelerator Simulation unified GPU/CPU code

- **Synergia** being upgraded to use Kokkos Views to hold particle data.
- Supports CPU and GPU parallel processing and reduction with same code base.

52M particles, FODO lattice, 20 iterations

Processor	Cost	Time [s]
Intel Xeon@3.2 GHz, 32 threads	$2000	82.9
nVidia Tesla V100 GPU@1.53 GHz, 5120 threads	$10000	0.2

It's not surprising that the GPU can process a lot of data very fast. The point is that we can achieve a huge performance boost with just changing compilation flags. No code change necessary.

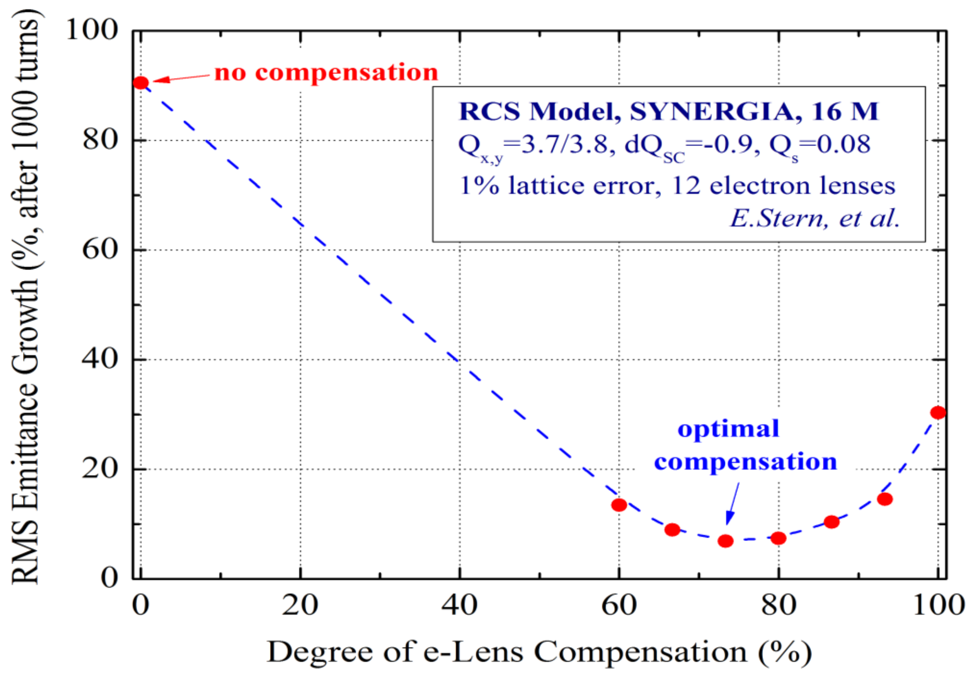
The GPU system was like "Summit", and similar to resources that will be available on "Perlmutter".

Q. Lu, E. Stern, FNAL

Simulation of space charge compensation with an electron lens

- **Synergia** simulations of an electron lens in a high current beam show the first evidence of compensation in a realistic particle-in-cell code.

- Simulations used 16M macro-particles to achieve precision required running at NERSC.
- At high intensities, space charge effects produce unacceptable beam loss. Some form of compensation is required. These simulations show that electron lenses may be an option.



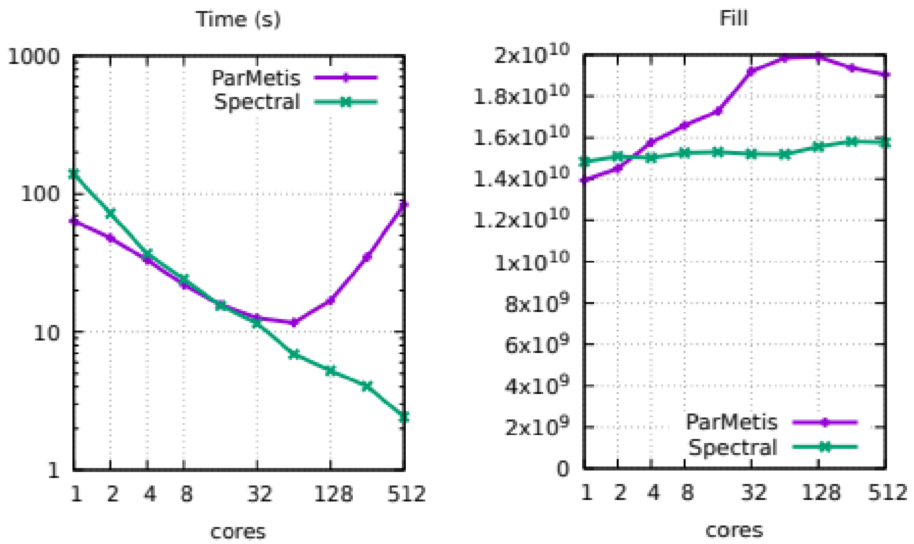
0.8M MPP hours used on Cori

E. Stern, FNAL

ASAP: New spectral solver using improved partitioning for improved scalability and quality*

- Parallel scalable nested graph-dissection code for sparse matrix fill-reducing ordering has been developed.
- Improved result quality and scalability.
- Sparse matrices are used in many HPC codes such as SuperLU, PETSc.

*see P. Ghysels poster

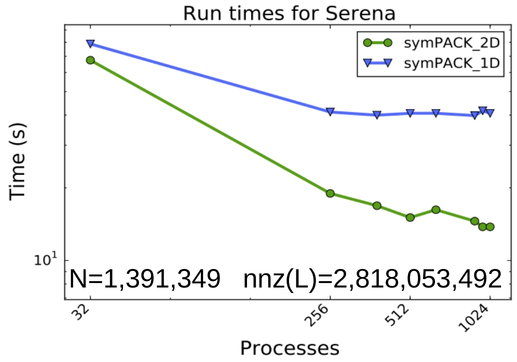


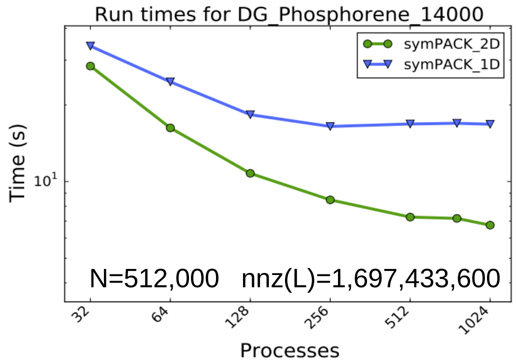
Results for the Queen_1417 matrix with 4.1M rows and columns and 333M nonzeros from Tim Davis' sparse matrix collection: (left) Our new spectral nested-dissection code scales much better than the widely used ParMETIS. (right) The fill in a sparse solver (~ memory usage) is similar to that obtained with ParMETIS when running on 1 core, but is less when running at scale, since the quality of ParMETIS degrades with increasing amounts of parallelism. Results obtained on NERSC Cori, Haswell, using 32 MPI processes per node.

Work was performed at LBNL: P. Ghysels, M. Jacquelin, E. Ng, R. Van Beeumen
Universiteit Antwerpen, Belgium: Siegfried Cools

ASAP: New 2D task-based SymPACK

- A new highly scalable 2D data distribution for the symPACK solver, a direct linear solver for sparse symmetric matrices was developed. The new distribution leads to much improved strong scalability and significant speedups over the previous 1D data distribution.
- Sparse direct linear solvers are at the heart of many HPC codes. When matrices are symmetric, fewer storage and computations are required.
- Factorization is a crucial preprocessing step to PEXSI, a library used in electronic structure computations.





Strong scalability on Cori Haswell:
- Up to **3x** speedup for Serena
- Up to **2.5x** speedup for DG_Phosphorene_14000

Work was performed at LBNL M. Jacquelin and E. Ng

Conclusions

- ComPASS4 is optimizing capabilities in the major US accelerator programs as defined by P5
  - Fermilab PIP-II and IOTA/FAST programs (Synergia)
  - SLAC FACET-II program (QuickPIC)
- ASCR collaboration with FASTMath develops and uses
  - Advanced Solvers for Accelerator Physics (ASAP)
  - Platform for Optimization of Particle Accelerators at Scale (POPAS)
- ComPASS4 codes track computing developments for efficient computation
- The Computing Facilities provide important resources for this work
  - conventional sim: 0.8M NERSC hours, plasma sim: 12.7M NERSC hours

Thanks!

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