FERMILAB-SLIDES-20-078-SCD

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Parallelization for HEP Event Reconstruction

ICHEP 2020, Computing and Data Handling session

July 28, 2020

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This manuscript has been authored by Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359 with the U.S. Department of Energy, Office of Science, Office of High Energy Physics.

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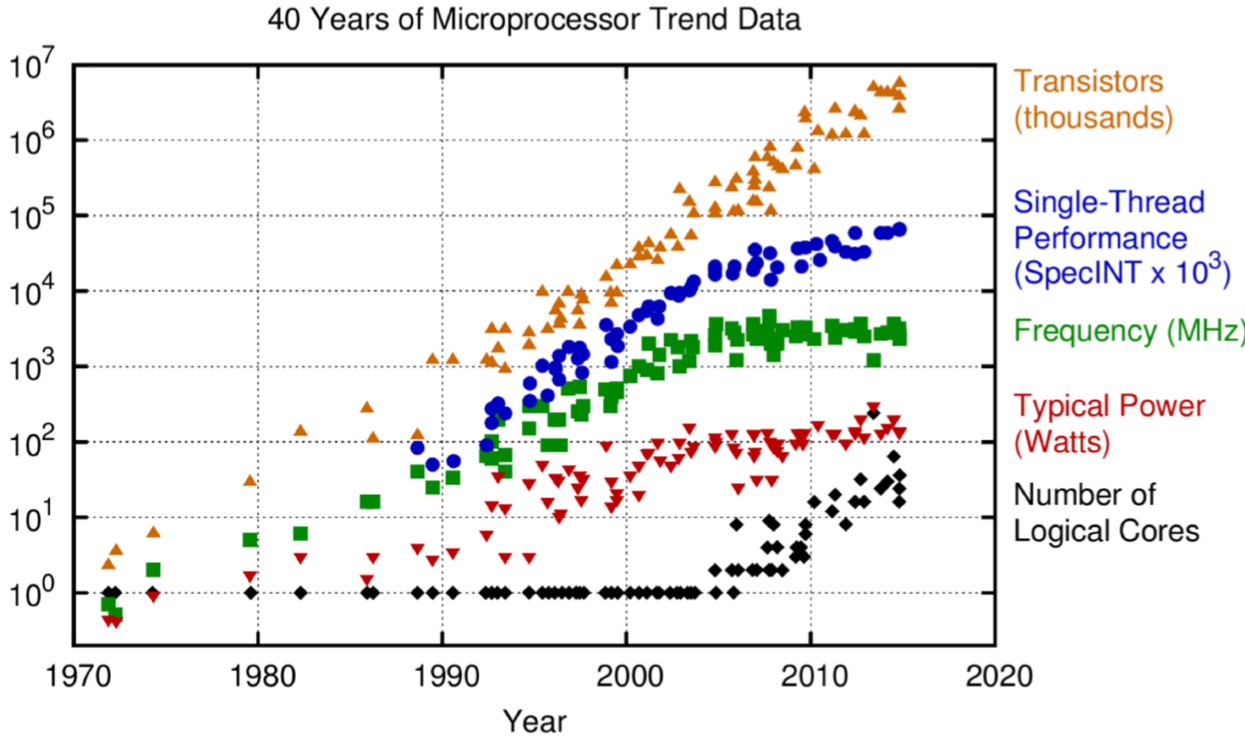
mkFit and SciDAC4-HepReco projects

Recent Changes in the Computing Landscape

- Due to **power** limits, the CPU **frequency** is no longer growing exponentially:
  - nothing for free anymore
  - since 2005, most of the gains in **single-thread performance** come from vector operations
  - growth in number of **transistor** leads to an increase in **logical core** count: multithreading

- Changes can become opportunities:
  - exploit both levels of parallelization to avoid sacrificing physics performance!
  - new technologies dominating the market, e.g. GPU
  - exa-scale machines are being built at HPC centers



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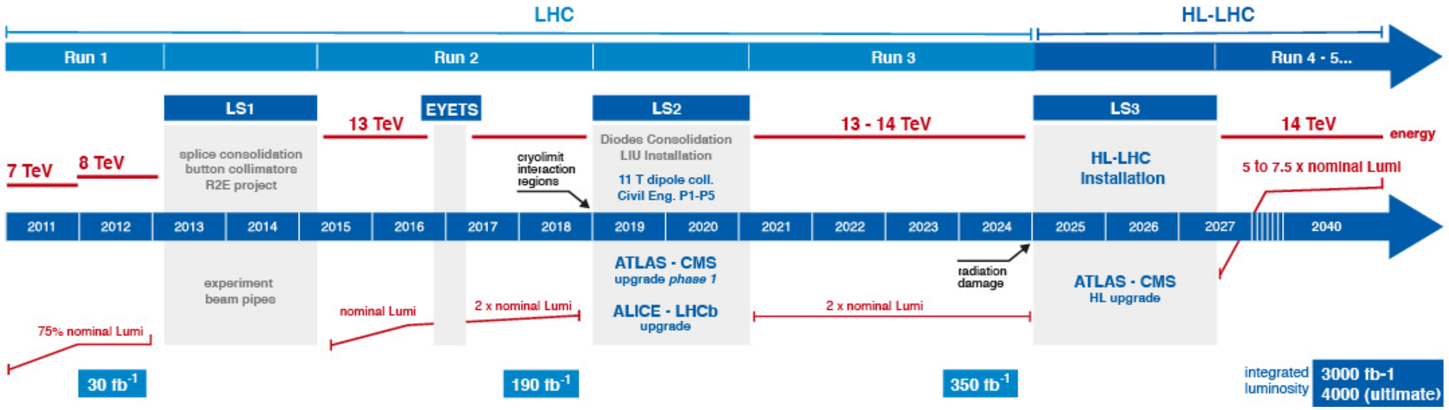
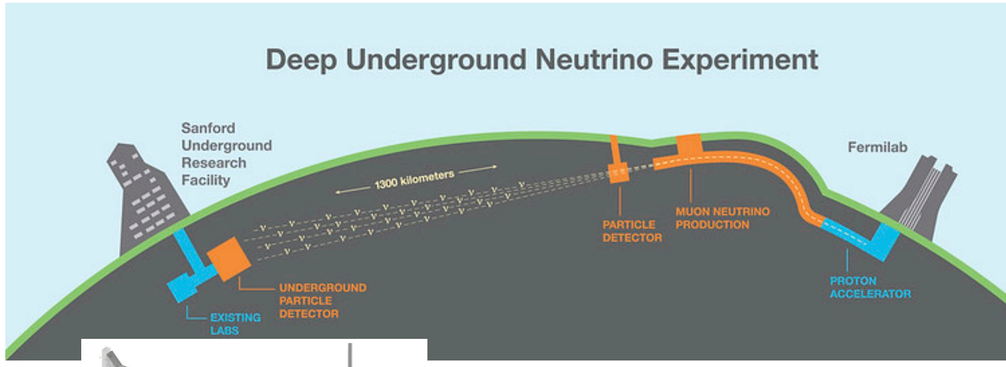
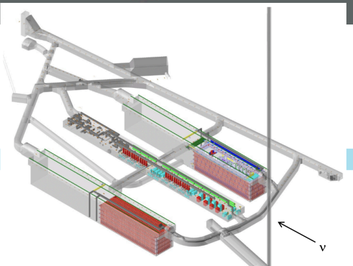
Preparing for the Next Generation of Experiments

- Next generation of HEP experiments will feature **unprecedented** detector **granularity or size**, and will be exposed to beams of unprecedented **intensity**
- These lead to an increase in data volume and corresponding increase in processing time, so exploiting **new computing technologies** is a vital need
- This talk focuses on **computing R&D for reconstruction** in CMS and at LArTPC experiments, with the long term goal of improving the physics reach of **HL-LHC** and **DUNE**



https://project-hl-lhc-industry.web.cern.ch/content/project-schedule





arXiv:2002.02967

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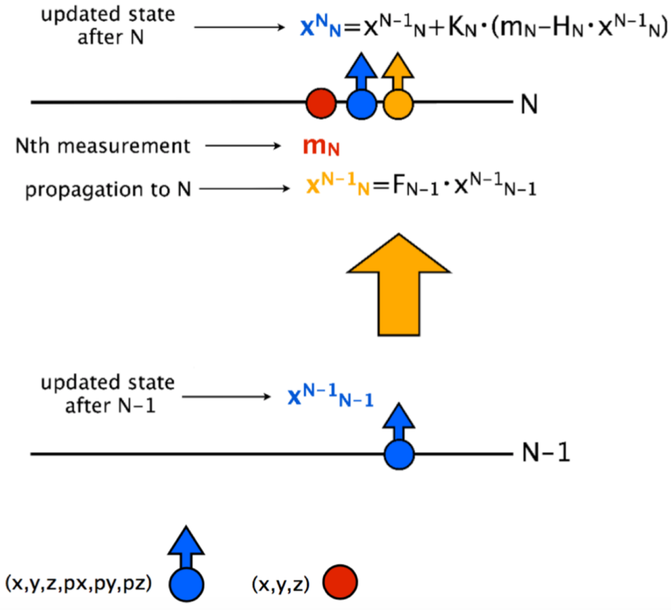
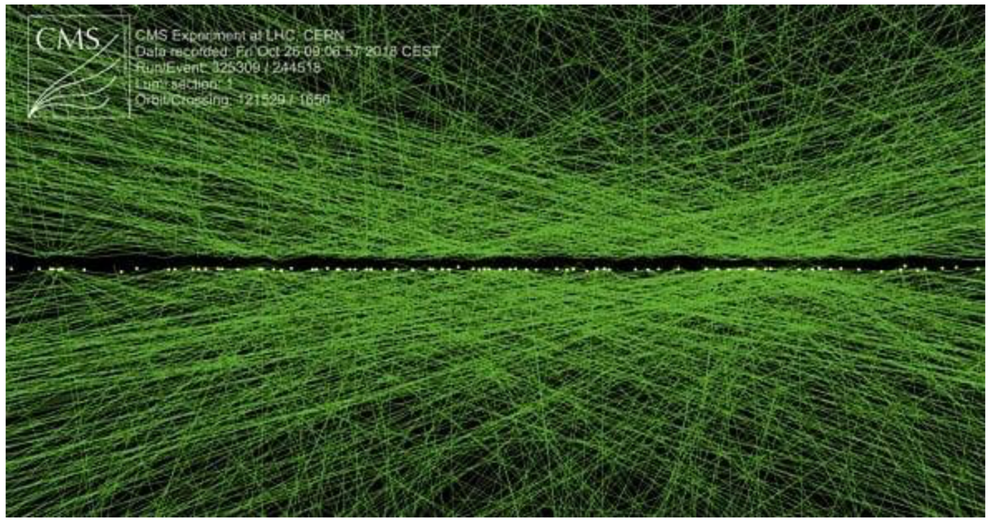
LHC Reconstruction Challenges

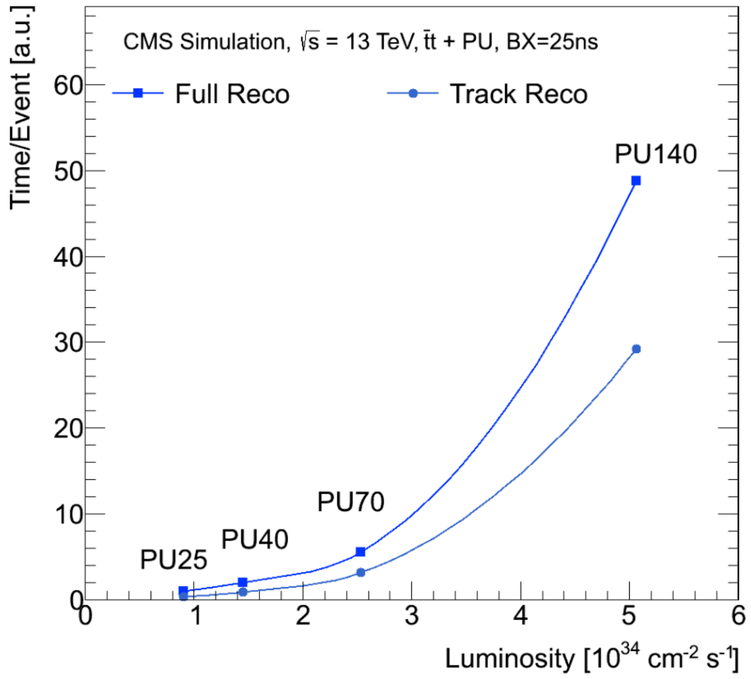
Predicted track state
Detector measurement
Updated track state

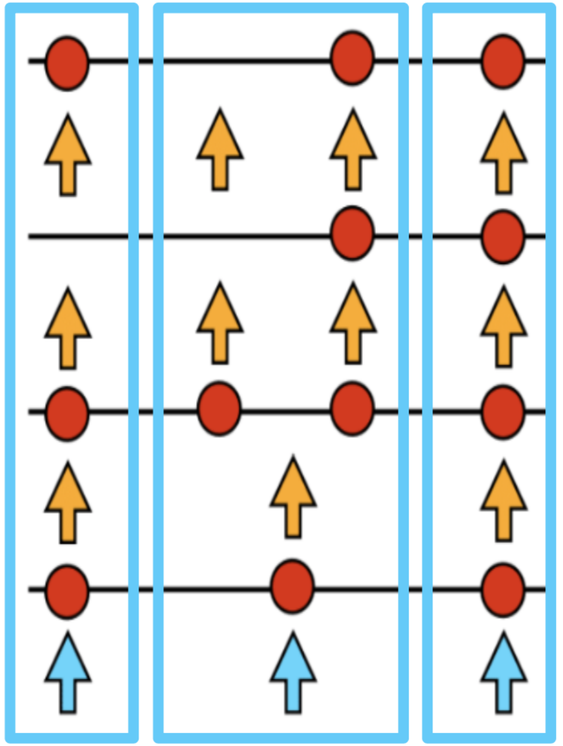


- Increasing pile-up (PU) drives exponential increase in event reconstruction processing time
- **Tracking** is the dominant contributor to the reconstruction time, and it's vital for the physics output of HEP experiments
  - reducing the tracking phase space implies significantly worse physics sensitivity
- **Kalman filter**-based tracking is the "standard" tracking method in HEP
  - demonstrated **high efficiency** physics performance, robust handling of **material effects**
  - track building is a **combinatorial algorithm** traditionally implemented in serial fashion, **challenging to parallelize**



Event display, CMS 2018 high PU run (PU 136)



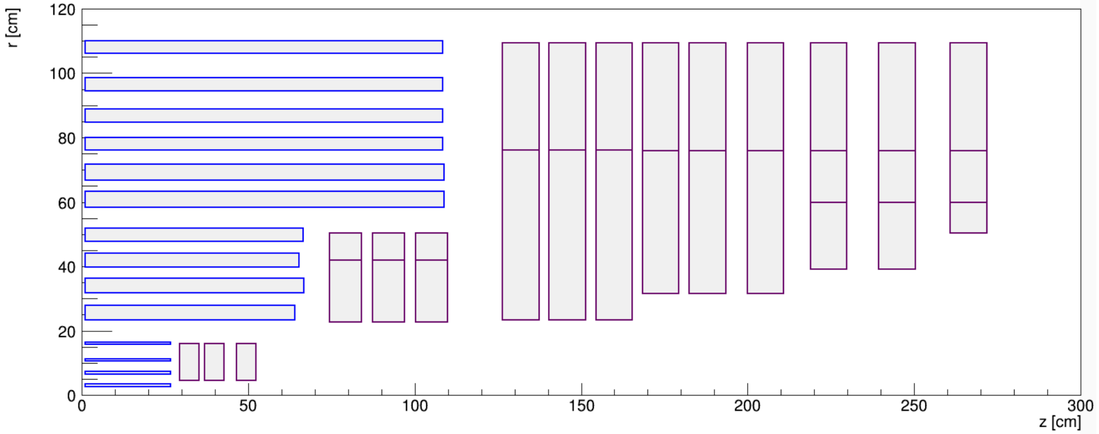


Parallelizing Tracking: the mkFit Approach

- **mkFit** mission: parallelize Kalman filter track building

- **Matriplex** library designed for **SIMD** processing of track candidates
  - bunches of small matrices operating in lock-step, auto-generated vectorized code is aware of matrix sparsity
- mkFit is **multithreaded** at multiple levels with **TBB** tasks: events, detector regions, bunches of seeds
- Reduce memory footprint with **lightweight detector description** (geometry, material, magnetic field)
- Minimize memory operations (number and size) within combinatorial branching
  - bookkeeping of explored candidates, clone only best ranking ones at each layer (with per seed cap)

Matriplex memory layout



mkFit geometry representation

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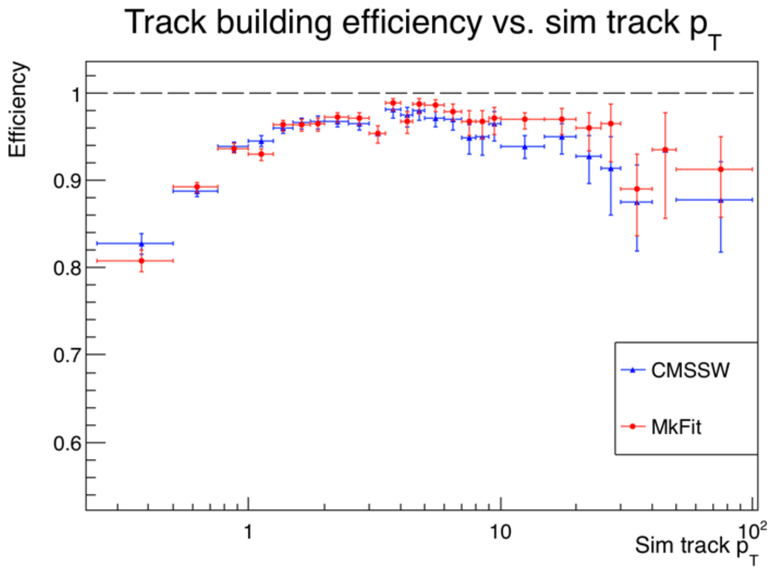
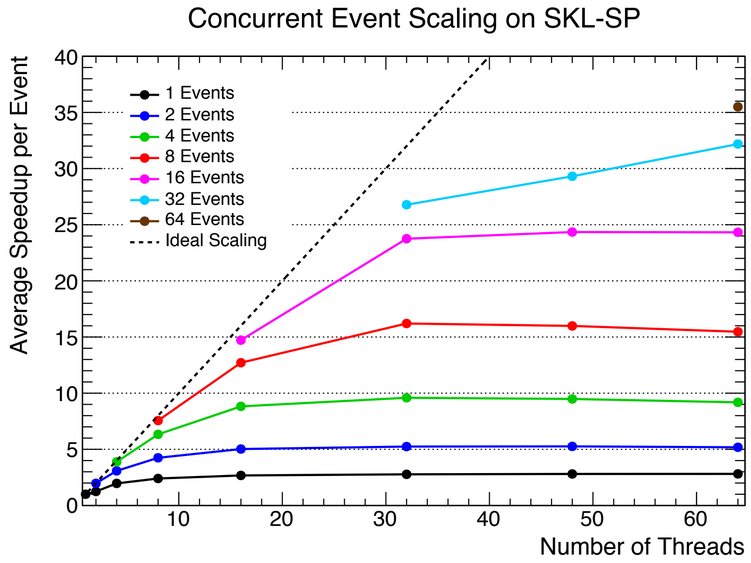
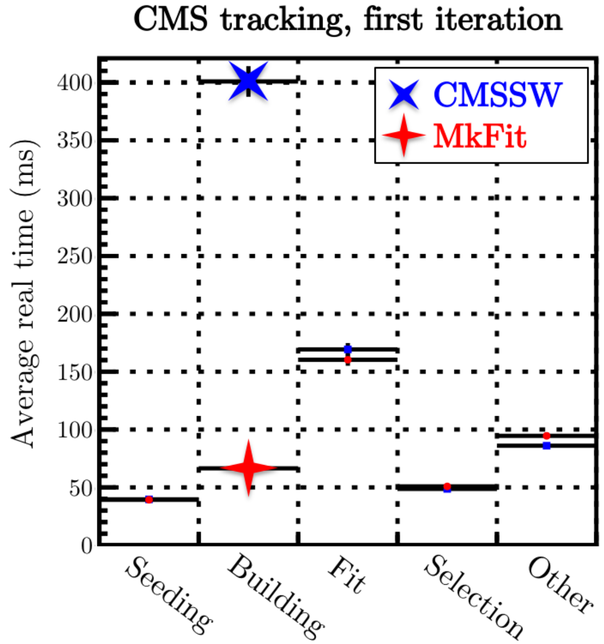
mkFit Physics and Computing Results

- mkFit track building achieves **comparable physics performance** as standard CMS tracking (first iteration)
- Standalone application achieves **speedups** of up to **3x from vectorization** and up to **35x from multithreading** across multiple collision events
  - vectorization speedup computed on main track building function only, evaluated on Intel Skylake Gold processor
- mkFit is **integrated in CMS framework** (CMSSW), with a single threaded application it is **6x faster**
  - mkFit compiled using icc and AVX-512 extensions
  - track building with mkFit is faster than CMSSW track fitting!
  - integration of mkFit in CMS workflows is currently under investigation







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mkFit paper — hot off the press!

- More details about the mkFit algorithm and results in our paper
  - arXiv:2006.00071, recently accepted for publication in JINST

Speeding up Particle Track Reconstruction using a Parallel Kalman Filter Algorithm

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Abstract: One of the most computationally challenging problems expected for the High-Luminosity Large Hadron Collider (HL-LHC) is determining the trajectory of charged particles during event reconstruction. Algorithms used at the LHC today rely on Kalman filtering, which builds physical trajectories incrementally while incorporating material effects and error estimation. Recognizing the need for faster computational throughput, we have adapted Kalman-filter-based methods for highly parallel, many-core SIMD architectures that are now prevalent in high-performance hardware. In this paper, we discuss the design and performance of the improved tracking algorithm, referred to as mkFit. A key piece of the algorithm is the Matriplex library, containing dedicated code to optimally vectorize operations on small matrices. The physics performance of the mkFit algorithm is comparable to the nominal CMS tracking algorithm when reconstructing tracks from simulated proton-proton collisions within the CMS detector. We study the scaling of the algorithm as a function of the parallel resources utilized and find large speedups both from vectorization and multi-threading. mkFit achieves a speedup of a factor of 6 compared to the nominal algorithm when run in a single-threaded application within the CMS software framework.

Keywords: Data processing methods; Pattern recognition, cluster finding, calibration and fitting methods; Performance of High Energy Physics Detectors.

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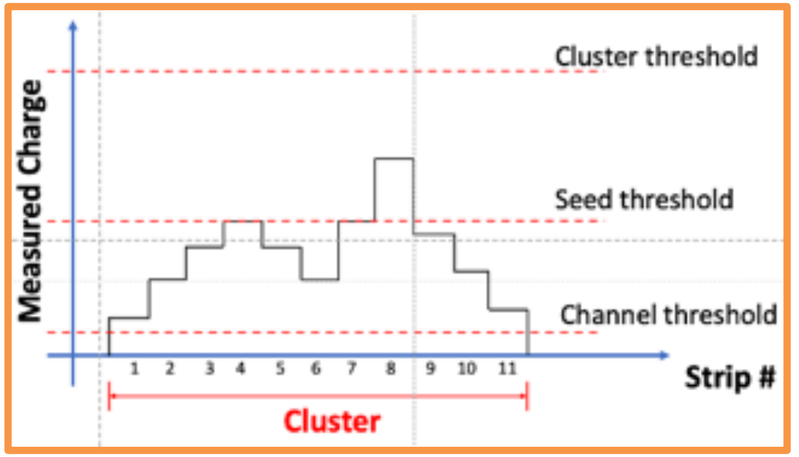
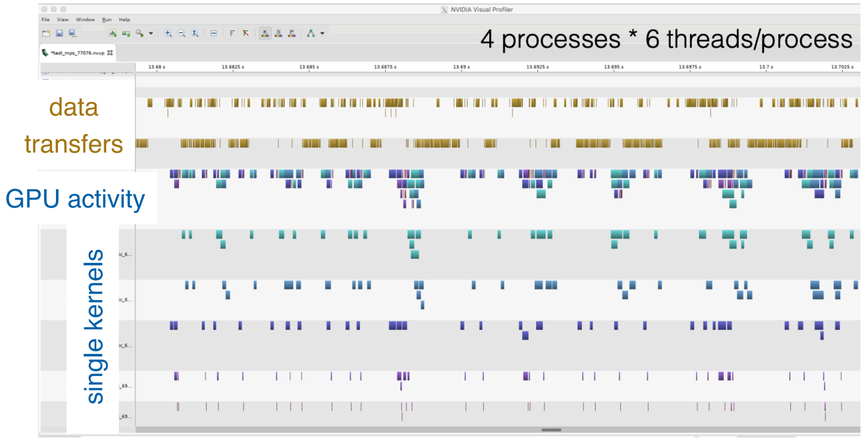
Next Steps: Strip Unpacking and Clustering on GPU

- **Silicon Strip Hits** are the main input to the mkFit algorithm
  - producing them can be a limiting factor to using mkFit in CMS trigger
- **GPUs** can help to speed up the processing of Si-Strip data
  - Unpacking of raw data from CMS Silicon Strip with SoA format
  - Parallelized implementation of “three threshold” clustering algorithm
  - Initial standalone version: multi-event processing using **OpenMP** with nested parallelism in CPU, and **CUDA** streams in GPU
- Recently developed a **CMSSW producer**, with CUDA application as “ExternalWorker”
  - time split roughly evenly between data transfers and computations
  - workload is not enough to saturate a GPU, multi-processing is being studied to achieve better utilization
  - achieve an aggregate throughput ~1.15 KHz, projected to be 50% faster than CPU-only equivalent process
- Next steps: evaluate hit positions on the GPU, produce hits in mkFit data format

“Three threshold” clustering



NVPROF screenshot



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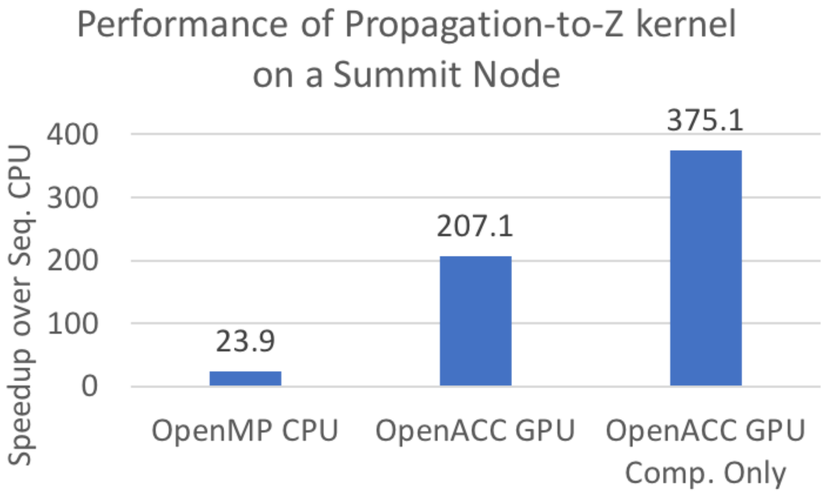
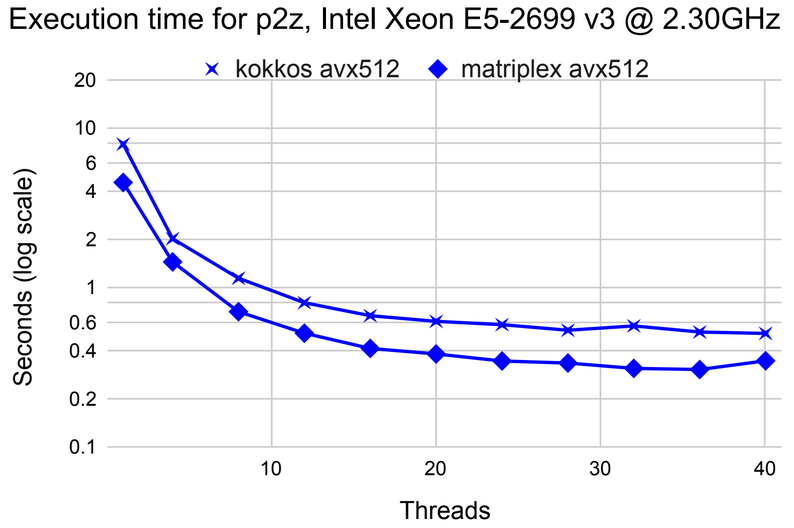
Next Steps: Portable Code Explorations

- NVIDIA and CUDA are the current leaders in the GPU market, but the future will bring GPUs from a variety of vendors and possibly different **heterogeneous solutions**
- Need to explore solutions for **code portability** across platforms to avoid re-writing software for each platform
  - many different options are emerging, mainly compiler directives or libraries
- Started an effort to **test** different **portable implementations** using a single function from the mkFit code
  - function is the propagation of track parameters to a given position along the z axis
  - representative of full code in terms of math operations types; main limitation is that it does not include combinatorics
- Early tests using **OpenACC** and **Kokkos** give promising results
  - on a Summit Node OpenACC GPU application almost 10x faster than OpenMP application fully loading the CPU
  - performance of Kokkos CPU version is similar to nominal implementation with dedicated Matriplex library
- Ongoing work towards a more completed suite of measurements, including OpenMP, OpenACC, Kokkos, Alpaka, Eigen, as well as different compilers





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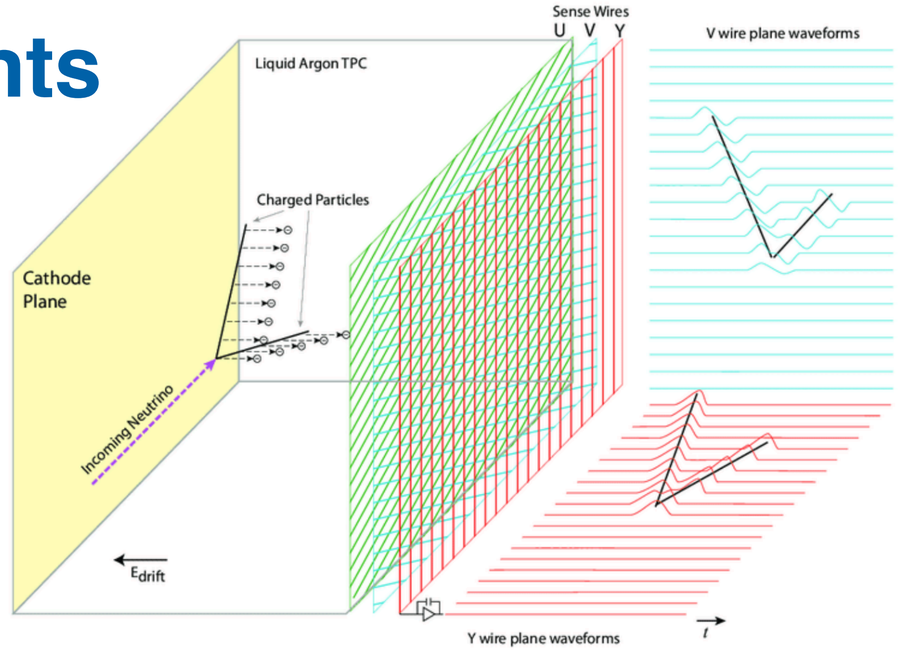
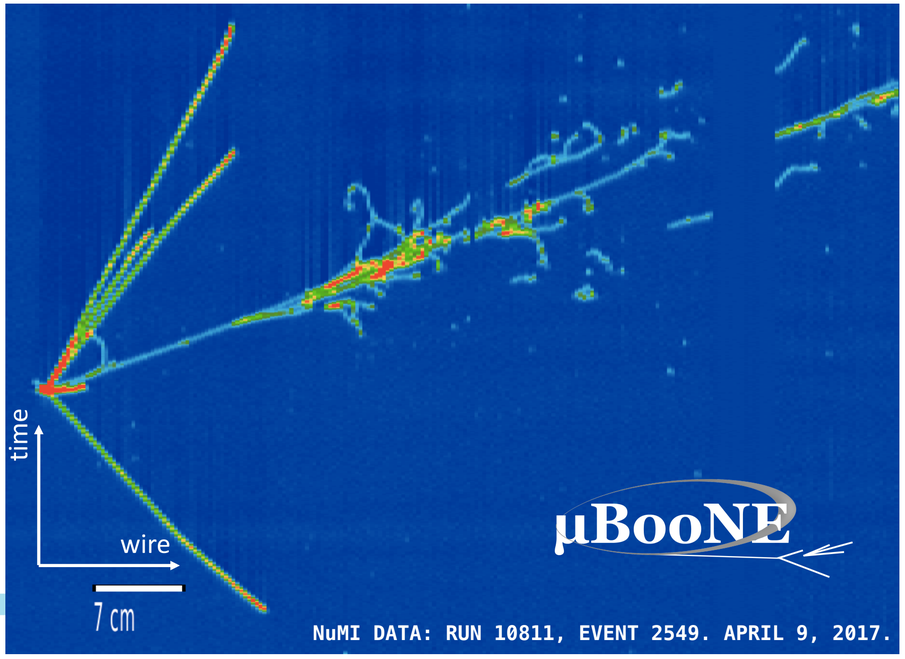
Reconstruction for LArTPC ν experiments



- Charged particles produced in neutrino interactions ionize the argon, ionization electrons drift in electric field towards anode planes
- Sense wires detect the incoming charge, producing beautiful detector data images

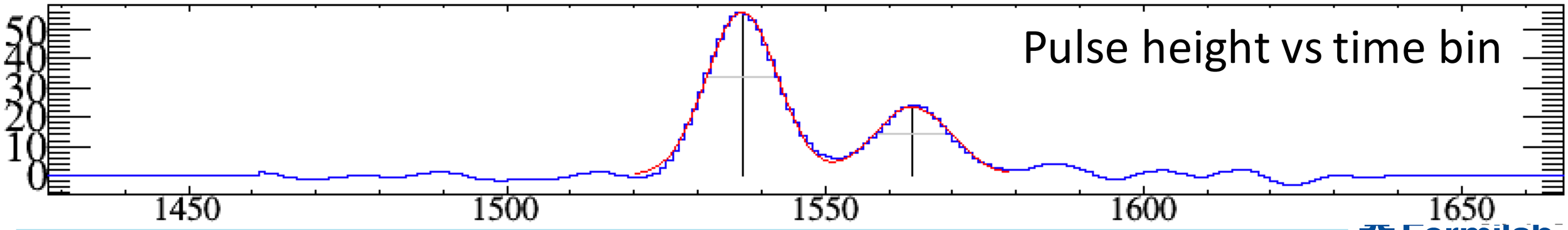
- Reconstruction in LArTPC experiments is **challenging** due to unknown interaction point, many possible topologies, noise, contamination of cosmic rays
  - Takes O(minutes)/event in MicroBooNE
  - ICARUS ~5x bigger, DUNE Far Detector O(100)x bigger
- LArTPC detectors are modular in nature ➔ **parallelism**!



Parallelization of HitFinder Algorithm

- **Hit finding**: identify pulses and determine their peak position and width
  - takes a significant fraction of the reconstruction workflow (few to few tens of %, depending on the experiment)
- Wires can be independently processed: suitable to **demonstrate speedup potential** by parallelizing LArTPC reconstruction

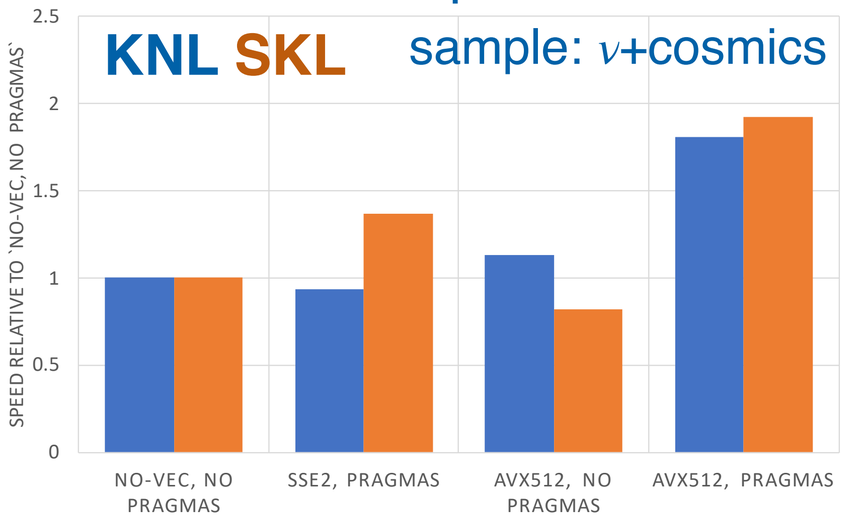
- Hit finder algorithm has been **successfully parallelized**:
  - replaced Gaussian fit based on Minuit+ROOT with a local implementation of Levenberg-Marquardt minimization
    - early tests showed this lead to ~8x speedup in the minimization code already
  - **vectorize specific loops** within the minimization algorithm, typically across data bins
    - main limitations: only a subset of the code is vectorized, number of bins is same order as vector unit size
  - two-level **nested multithreading** parallelization over **events** and regions of interests in **wires**

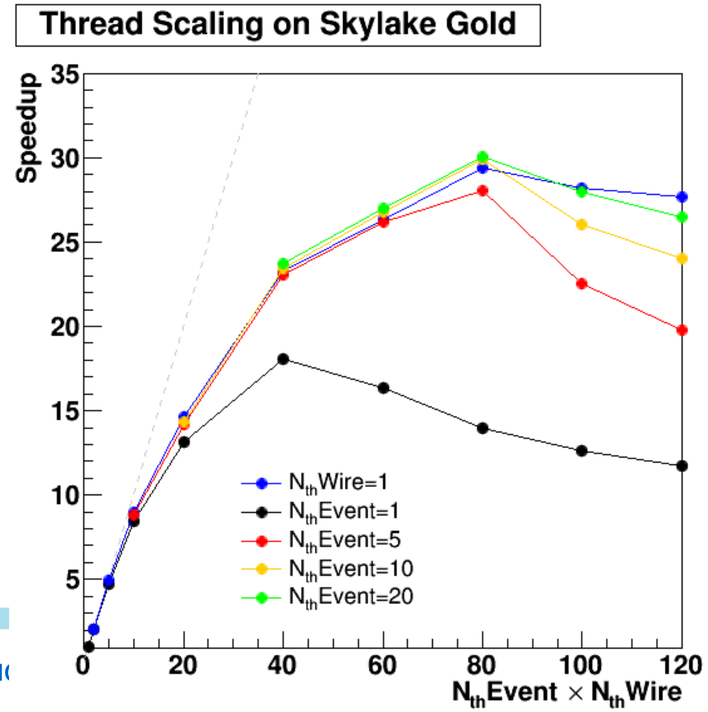


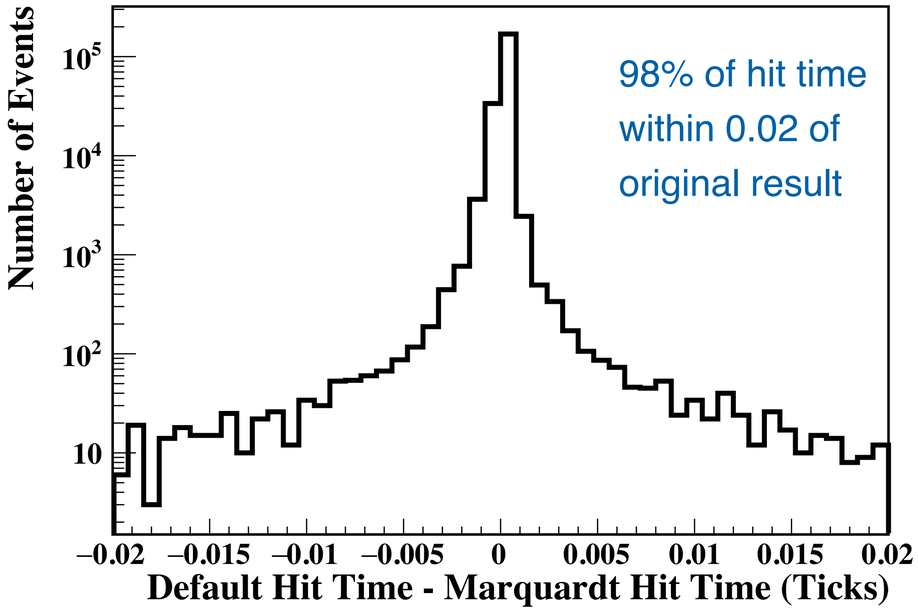
Parallel HitFinder Results

- **Vectorization** gives **~2x speedup** when compiling with icc+AVX512 (both Skylake Gold and KNL)
- OpenMP **multi-threading** shows near ideal scaling at low thread counts, with speedups increasing **up to 30x** (95x) for 80 (240) threads on Skylake Gold (KNL)
- Physics output nearly identical to original algorithm
- New version integrated in the experiment codebase (larsoft) and **adopted by ICARUS and DUNE**
  - Single-threaded application up to 10x faster than previous version, significant impact on reco time of experiments!

Vectorization performance

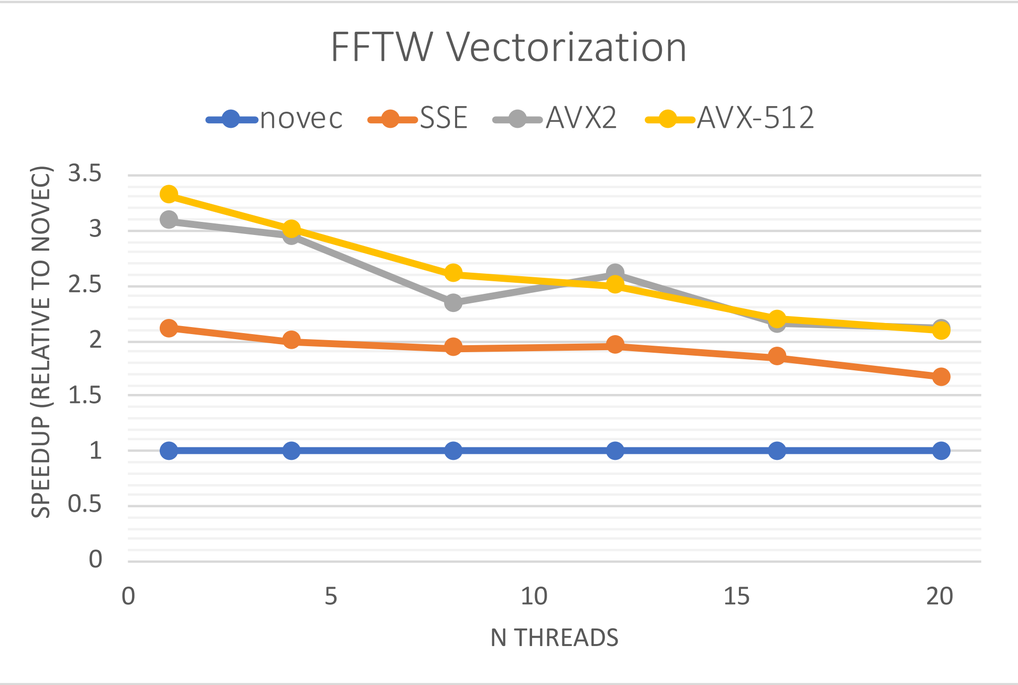


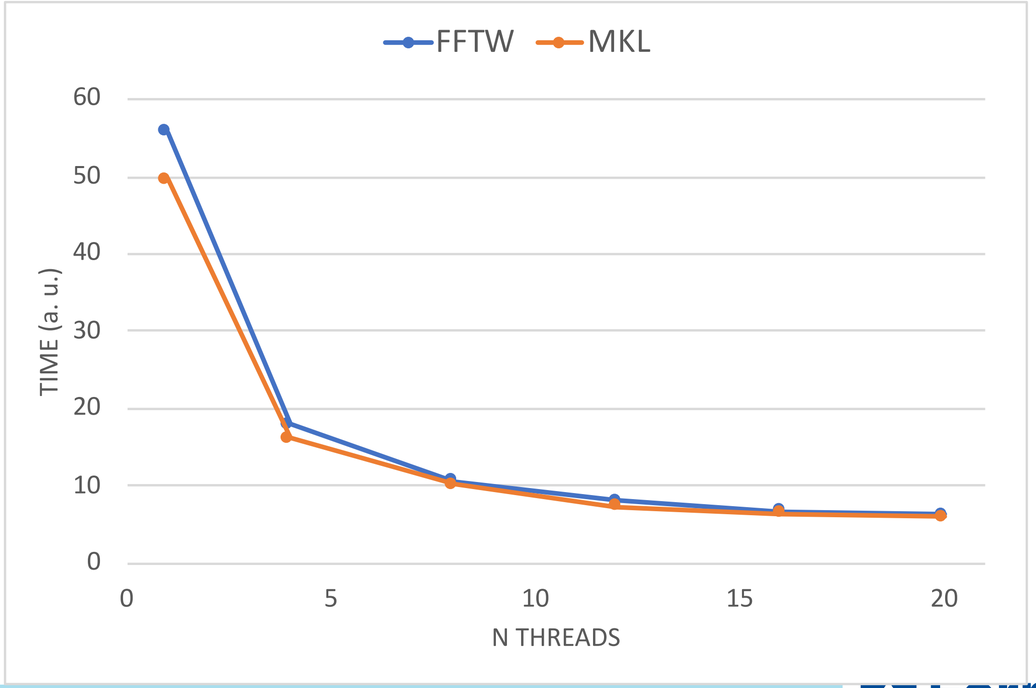




Studies of FFT libraries

- Fast Fourier Transform (FFT) is a core component of signal processing algorithms for LArTPC
- Comparing state of the art **FFT libraries**: FFTW and MKL
  - **MKL** is precompiled with AVX-512; **FFTW** compiled with gcc and different vector extensions
- Test **single fwd+inverse FFT** on wire waveform data:
  - Up to **~3.5x speedup** for FFTW with AVX2 and **AVX-512**; **MKL ~10% faster** than FFTW
- Also starting to look into FFT implementations for GPU





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LArTPC Reconstruction on HPC

- Work is ongoing to develop a **reconstruction workflow for HPC** centers. Initial target experiment and center are **ICARUS** and **Theta**@ALCF, respectively.
- Goal is an **efficient** utilization of parallel resources of HPC centers, which requires building algorithm code with **custom compilers and vector extensions**
  - the workflow is designed to be part of a central campaign
- Building experiment's software with **Spack** would allow us to use custom compilation options
  - icc and AVX-512 are needed for optimal vectorization speedups
  - initial tests of Spack build are complete
  - next steps: customization for specific packages, building on Theta

Spack

- Workflow being defined in collaboration with HEP-on-HPC SciDAC project
  - https://computing.fnal.gov/hep-on-hpc/
  - use HDF5+HEPnOS to organize the data: https://xgitlab.cels.anl.gov/sds/hep/HEPnOS
  - framework uses DIY to distribute the workload across nodes: https://www.anl.gov/mcs/diy-doityourself-analysis

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Snowmass advertisement

- Join the Snowmass process to plan for the next years and prioritize possible future directions and projects: https://snowmass21.org/

- Modernizing the reconstruction software is crucial for the future of HEP experiments. Join the Computational Frontier and the “Experimental Algorithm Parallelization” Working Group, which is particularly relevant for the topics of this talk
  - Computational Frontier Workshop: https://indico.fnal.gov/event/43829/
  - Experimental Algorithm Parallelization WG: https://snowmass21.org/computational/algorithms

Summary

- Projects are actively working to exploit new computing architectures to speed up reconstruction of current and future HEP experiments

- mkFit: Kalman filter track building with large speedups from parallelization. Integrated in CMSSW, 6x faster single thread application. Work ongoing towards deployment in workflows and exploring GPU applications.

- LArTPC reconstruction: vectorized and multi-threaded hit finder O(10)x faster and adopted by experiments. Work in progress to define workflow for efficient usage of HPC centers

Acknowledgments

- Project websites:
  - https://trackreco.github.io/
  - https://computing.fnal.gov/hepreco-scidac4/

- Funding agencies and collaborating institutions:

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