



Scientific Computing at Fermilab

Tammy Walton

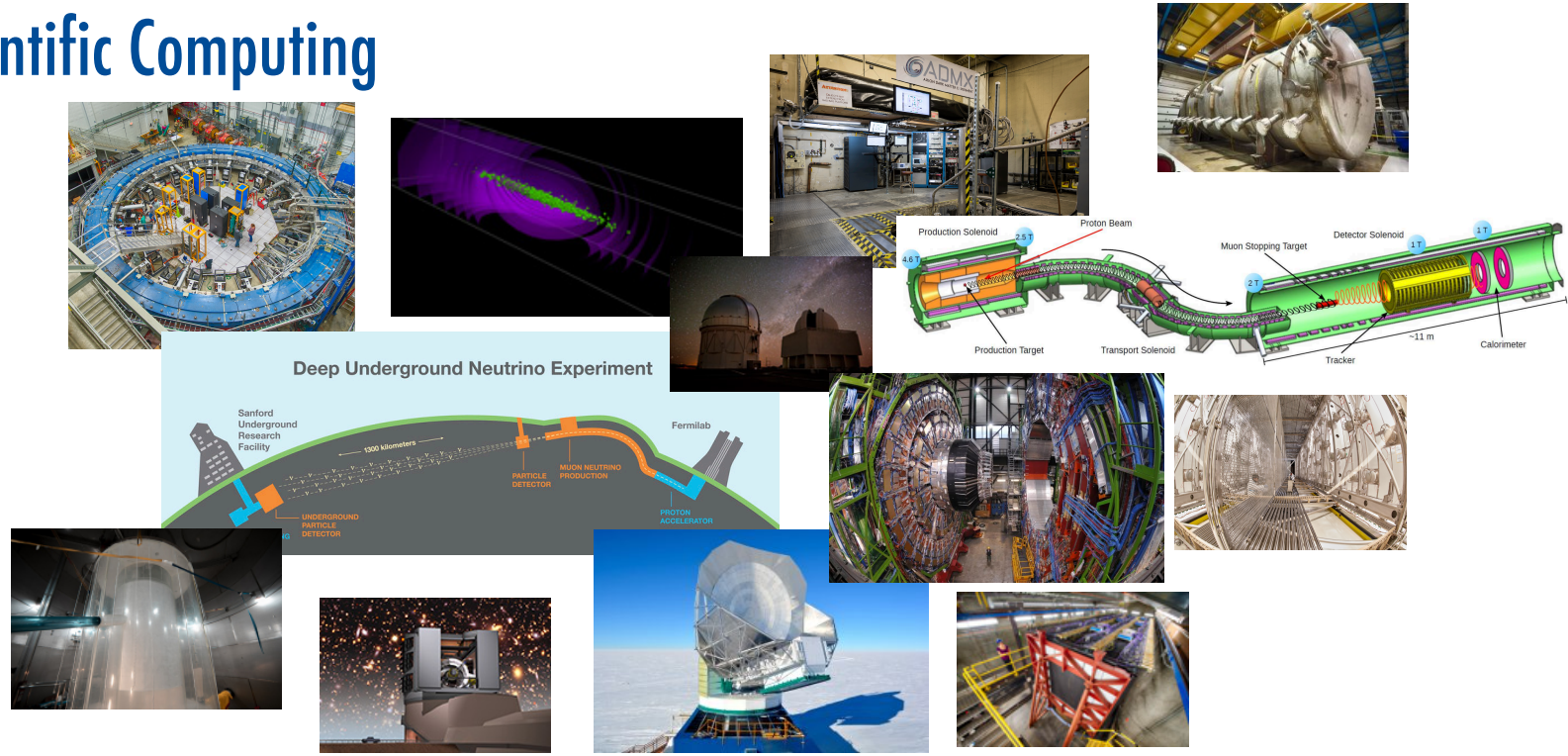
54th Fermilab Annual (Virtual) Users Meeting

August 4, 2021

Outline

- Introduction
- Scientific Computing Services
- Scientific Computing Projects and Facilities
- Summary

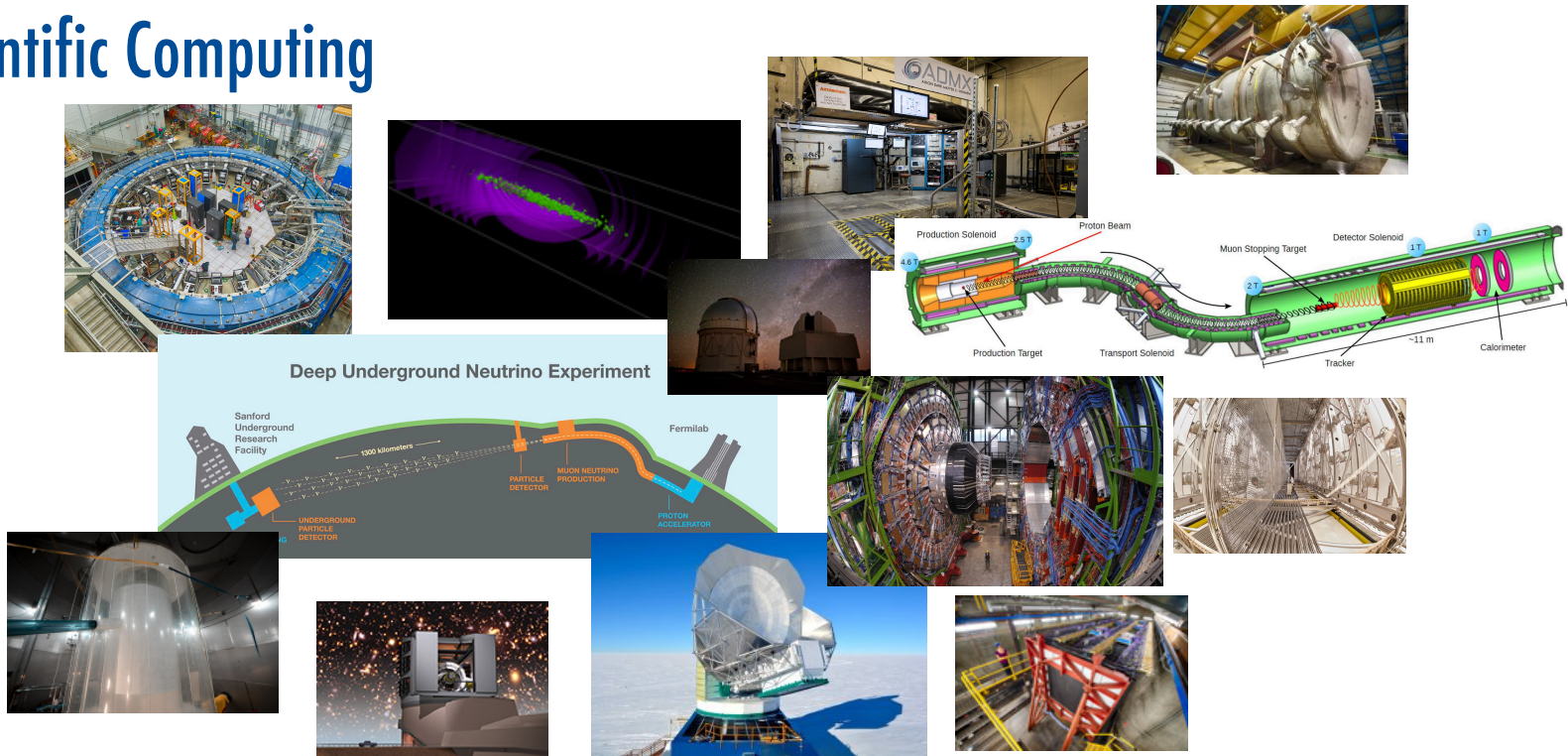
Scientific Computing



Fermilab hosts and participates in a variety of scientific physics programs

- Neutrino physics
- Muon physics
- CMS physics
- Dark matter and energy physics
- Accelerator physics

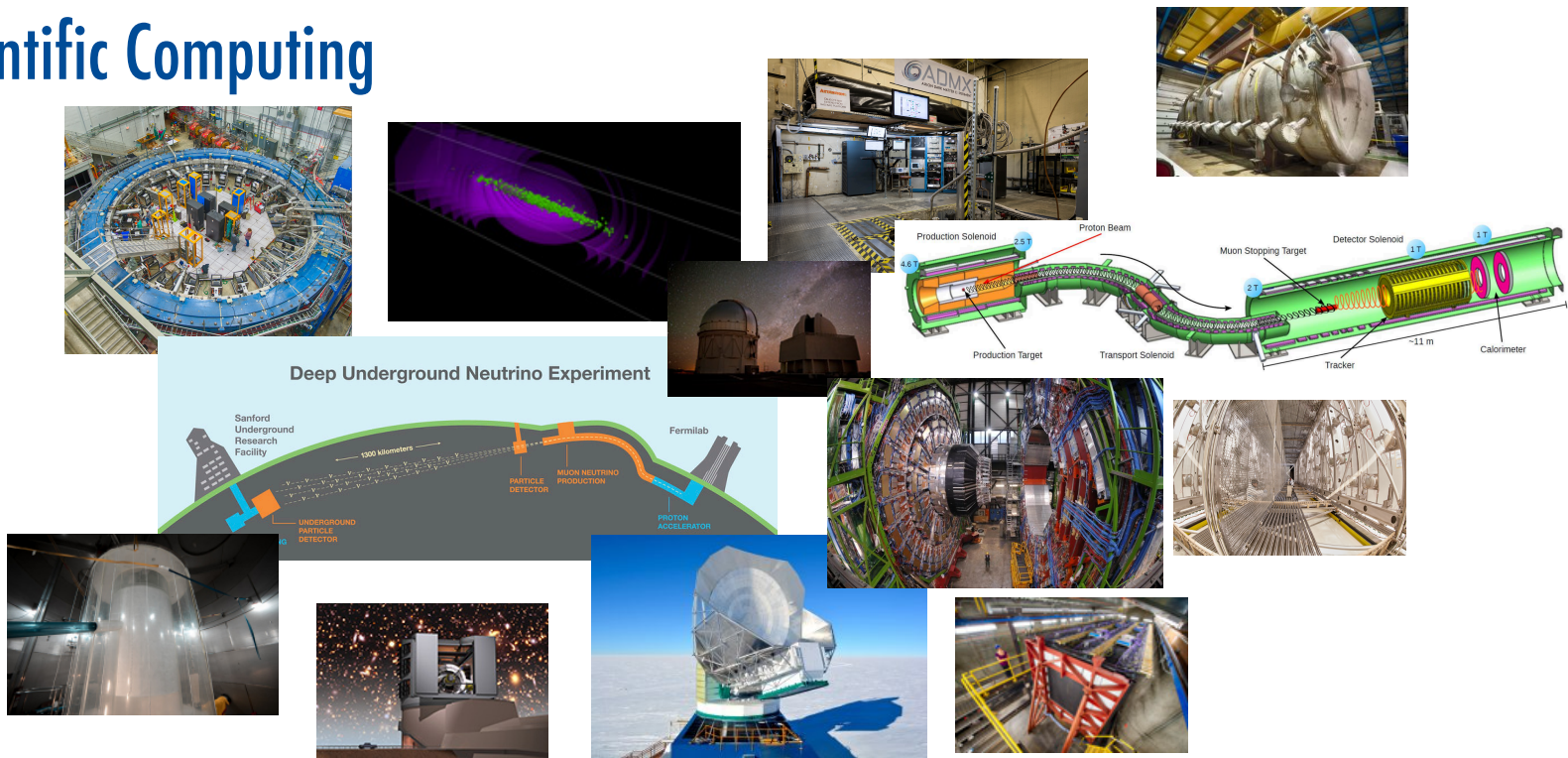
Scientific Computing



Fermilab hosts and participates in a variety of scientific physics programs

- Some experiments are projected to produce big data events.
 - DUNE supernova event : 185 terabytes
 - HL-LHC total data collection : ~20 exabytes = 20,000,000 terabytes

Scientific Computing

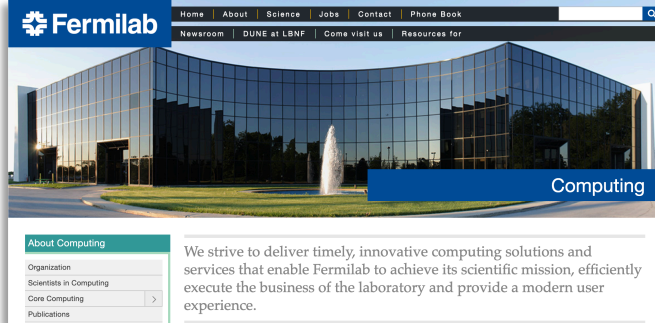


Fermilab hosts and participates in a variety of scientific physics programs

- Scientific computing supports and develops the leading-edge computational tools and facilities that experiments need for a successful physics program.

Scientific Computing

<https://computing.fnal.gov/>



<https://indico.fnal.gov/event/47936/>



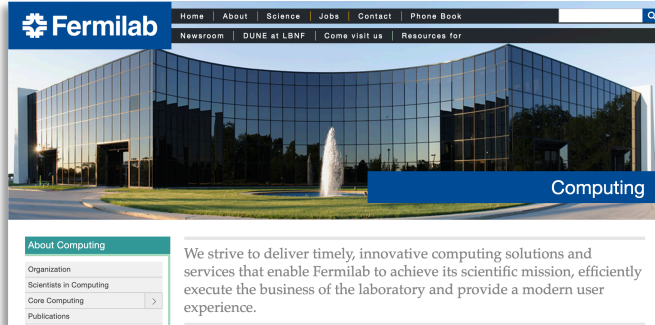
James Amundson
*Head of Scientific Computing
Division*

Fermilab hosts and participates in a variety of scientific physics programs

- Scientific computing supports and develops the leading-edge computational tools and facilities that experiments need for a successful physics program.
- Scientific computing division consists of computing professionals, scientists and researchers; experimental, theoretical, and accelerator physicists; engineers, research associates

Scientific Computing

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James Amundson
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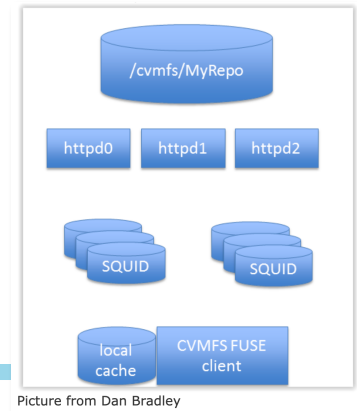
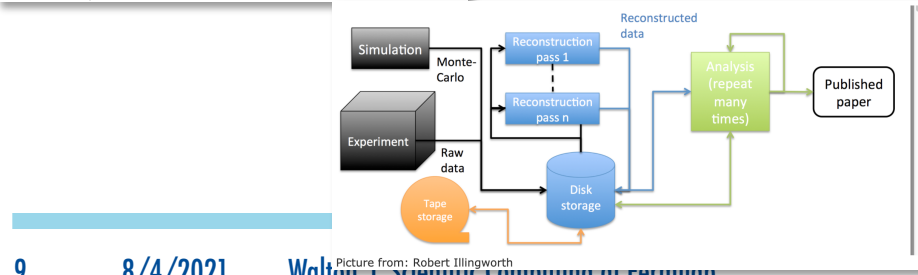
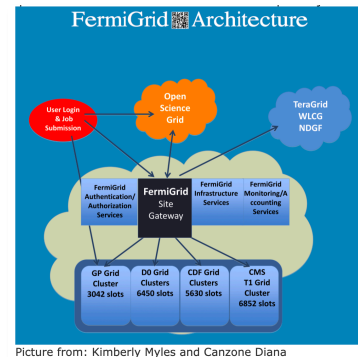
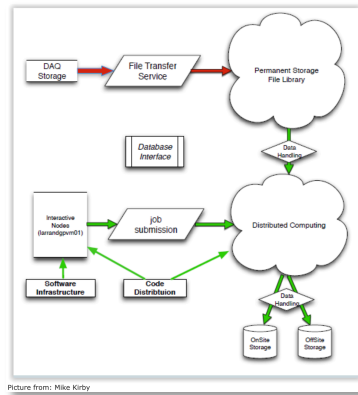
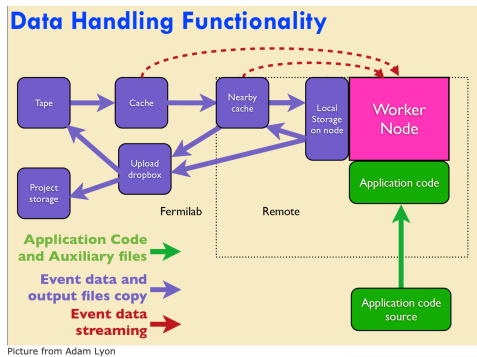
This presentation provides an overview of contributions from some of the available services, projects, and facilities

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- Scientific Computing Services
- Scientific Computing Projects and Facilities
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Scientific Computing Services

- Support and develop common computing tools for all experiments
 - Data management and submission
 - Software distribution and build systems
 - Source code version control systems and repositories
 - Access to Open Science Grid and High-Performance Computing centers
 - Interactive computing machines
 - Online and Offline software frameworks
 - Interactive Analysis Tools



Scientific Computing Services

- Support and develop common computing tools for all experiments
- Provide services to answer questions from experiments about computing

<https://fermi.servicenowservices.com>

| | | |
|--|----------------------------|---|
| DAQ and Scientific Hardware | Data Acquisition (DAQ) | ▼ |
| | Scientific Hardware | ▼ |
| | Test Stand | ▼ |
| Physics and Detector Simulation | Event Generators | ▼ |
| | Simulation Toolkits | ▼ |
| Scientific Collaboration Tools and Database Applications | Collaboration Tools | ▼ |
| | Database Applications | ▼ |
| Scientific Data, Development and Storage | Scientific Data Management | ▼ |
| | Scientific Development | ▼ |
| | Scientific Storage | ▼ |


| | | |
|--|----------------------------|---|
| Scientific Data, Development and Storage | Scientific Data Management | ▼ |
| | Scientific Development | ▼ |
| | Scientific Storage | ▼ |
| Scientific Job Management | Job Management | ▼ |
| | Job Monitoring | ▼ |
| Scientific Servers and Facilities | Scientific Facilities | ▼ |
| | Scientific Servers | ▼ |
| Scientific Workstations and OS | Scientific Linux | ▼ |
| | Scientific Workstations | ▼ |


Scientific Computing Services

- Support and develop common computing tools for all experiments
- Provide services to answer questions from experiments about computing
- Provide tutorials and workshops to learn about the various computing tools

<https://indico.fnal.gov/event/49414/>

2021 Intensity Frontier Computing Summer School



 Jun 17, 2021, 9:00 AM → Jun 22, 2021, 12:00 PM US/Central


 Lisa Goodenough (Fermilab) , Kenneth Herner (Fermilab)


Description **A virtual school covering the computing skills needed by Intensity Frontier experimentalists at Fermilab to do data processing and analysis. Activities include videos, lectures and hands-on exercises.**

The school consists of a self-paced portion, in which students go through various training modules from MIT and HSF, a live 6-hour virtual portion run over three days taught by Fermilab Computing Division staff and experiment scientists, and a 2-hour ‘Office Hours’ session where students can get help with the tutorials introduced in the live session.

Students should read the attached Google doc for more information about prerequisite training modules.

 [Information for Stu...](#) **Homework** 

Surveys  [Post-school Survey](#) [Fill out](#)

Lisa Goodenough  goodenou@fnal.gov

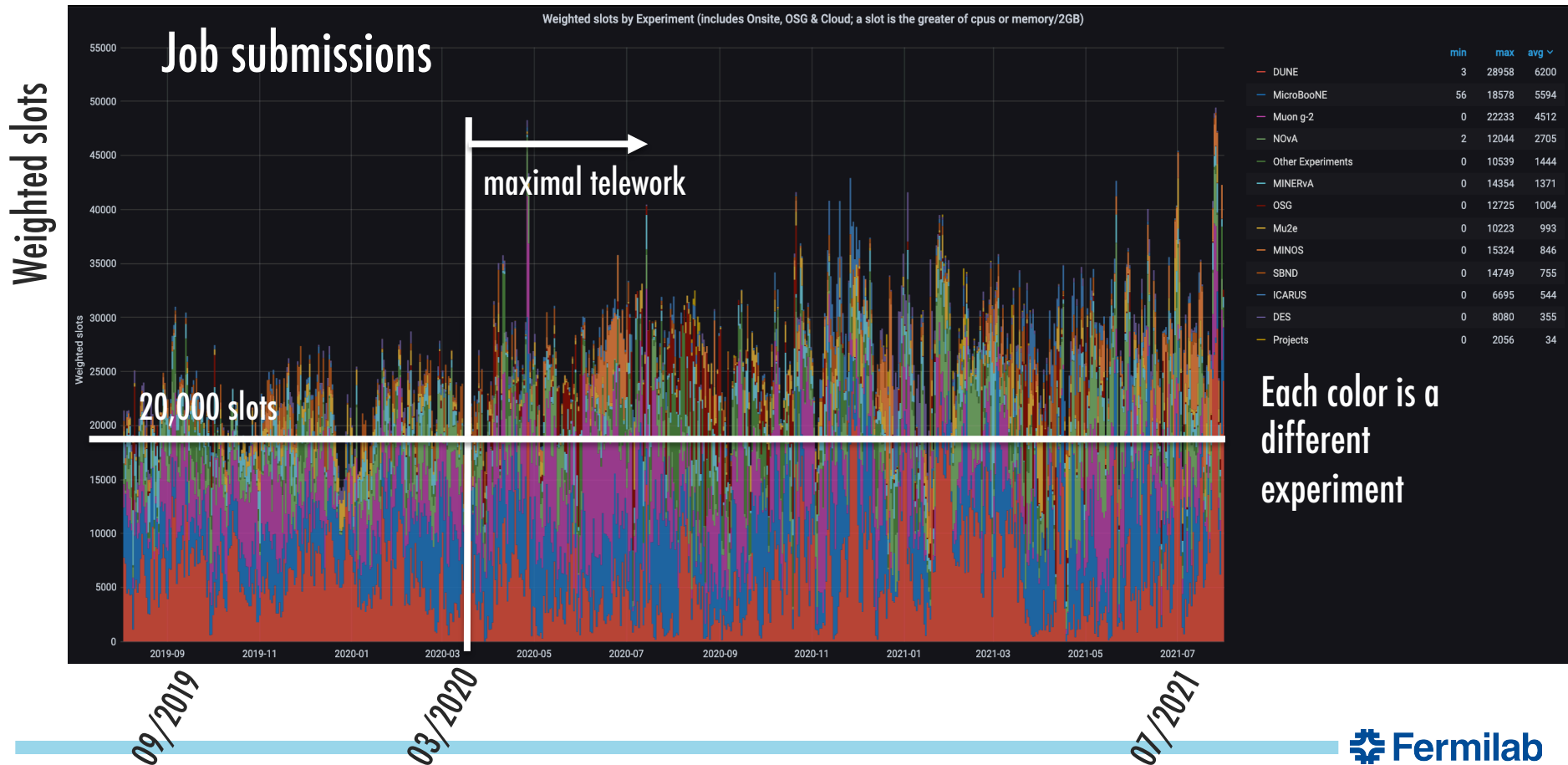
Scientific Computing Services

- Support and develop common computing tools for all experiments
- Provide services to answer questions from experiments about computing
- Provide tutorials and workshops to learn about the various computing tools
- Support and develop data monitoring tools for experiments

The screenshot displays the FIFEMON web interface for FIFE Batch Monitoring. The top navigation bar includes 'Fifemon Home', a search icon, and a 'Last 6 hours' filter. The main header features the Fermilab logo and the title 'FIFE Batch Monitoring' with a 'Landscape' sub-header. A secondary navigation bar contains links for 'Help', 'About Fifemon', 'FIFE Summary', 'CMS Summary', 'GPGrid Summary', and 'Experiment Summary'. The main content area is divided into several sections: 'Experiments' with buttons for DES, DUNE, protoDUNE, ICARUS, LAIAT, MicroBoONE, MINERVA, MINOS, Muon g-2, Mu2e, NOvA, SBND, and Other; 'Campaign Data' with links for Campaigns, Campaign Stages, and Sample Campaigns; 'Configure Work' with links for Campaigns, Login/Setup, Compose Job Type, Config File Templates, and Jobs; and 'News'. A 'POMS' sidebar is visible on the left. The central 'Job Launches: allowed' section shows a 'gm2' dropdown and a 'production' dropdown. Below this are several informational cards: 'Obtaining a POMS Account', 'Creating a Campaign', 'Monitoring', 'Debugging', 'POMS Statistical Overview' (with a pie chart), 'Fife Utils', 'FifeMon', 'SAM', 'Jobsub', and 'dCache'. The bottom of the page features a footer with '12', '8/4/2021', 'Walton | Scientific Computing at', and a 'Release Notes: v4.2.0' link.

Scientific Computing Services

- Support and develop common computing tools for all experiments
- Provide services to answer questions from experiments about computing



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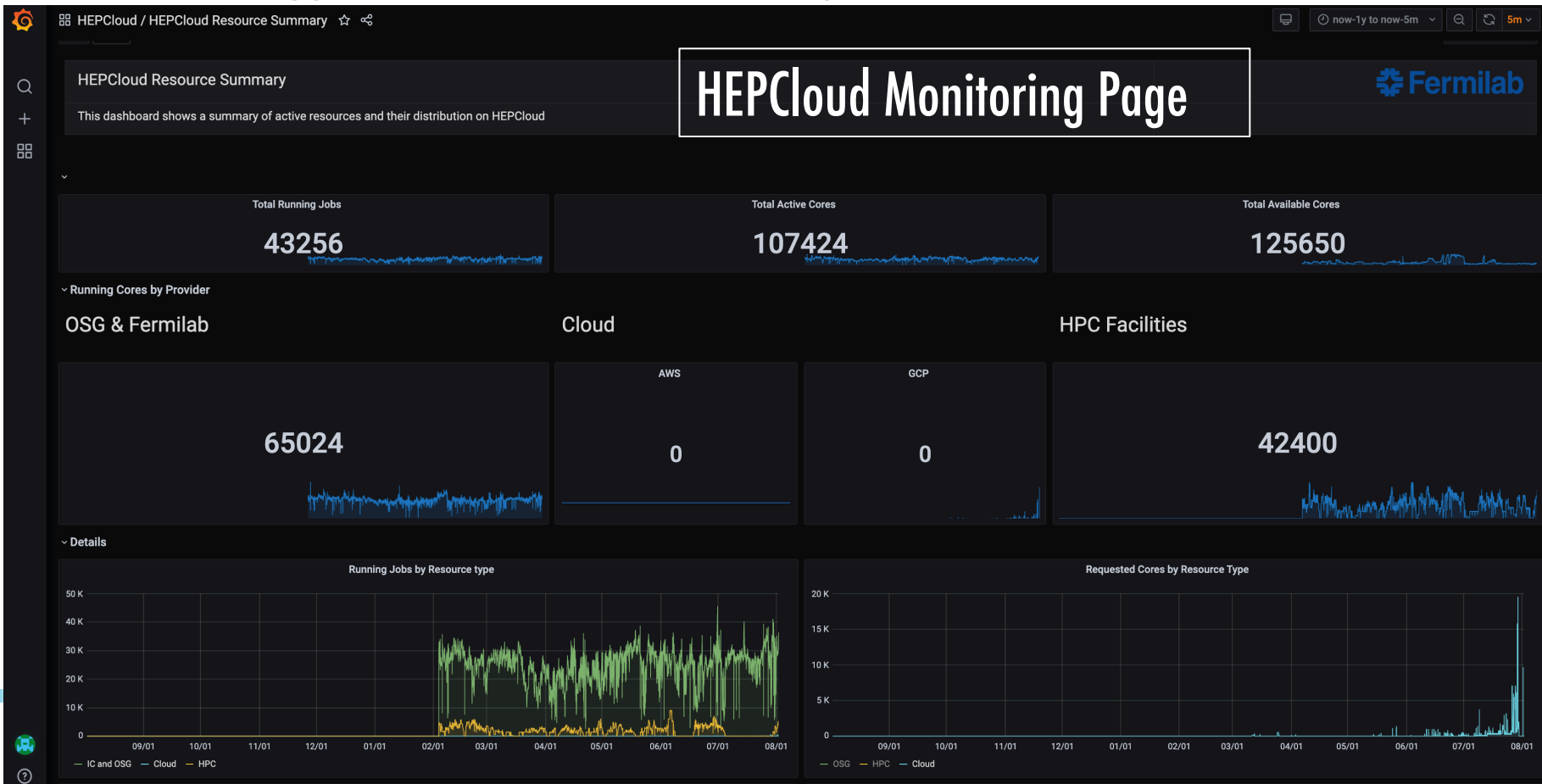
Scientific Computing Projects and Facilities

- Computing resources
 - Spring 2019: rollout of HEPCloud (<https://hepcloud.fnal.gov/>)
 - Unified portal to access many computing resources
 - Local (FermiGrid) and Offsite (Open Science Grid) resources
 - High Performance Computing (HPC) sites (commercial cloud and scientific centers)
 - Supercomputers that use parallel processing for running advanced applications fast and efficient
 - Performance is measured in floating-point operations per second



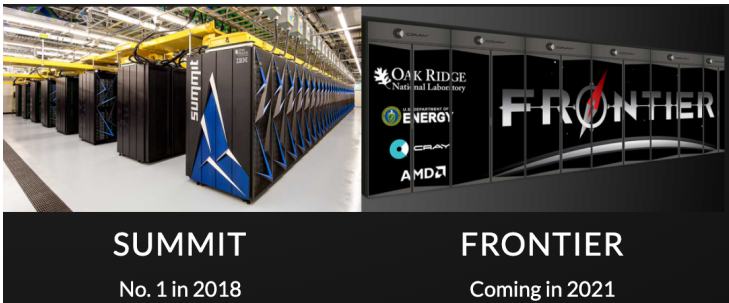
Scientific Computing Projects and Facilities

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 - FIFE support is the interface between experiments and facilities



Scientific Computing Projects and Facilities

- Computing resources
 - Spring 2019: rollout of HEPCloud (<https://computing.fnal.gov/hep-cloud/>)
 - Unified portal to access many computing resources
 - FIFE support is the interface between experiments and facilities
 - Plans include to integrate facilities that will support exascale computing resources
 - Oak Ridge National Laboratory 200-petaflop supercomputer, Summit, is on the road to an exascale upgrade



Scientific Computing Projects and Facilities

- Computing resources
- Advanced applications and algorithm techniques; large-scale data analytics
 - HPCs are required for success in HEP
 - Fermilab has hosted the Institutional Cluster for over a decade, and is used largely by the US Lattice QCD collaboration
 - Experiments (CMS, NOvA, DUNE, mu2e, g-2, etc) are actively running production jobs on HPC sites via HEPCloud

A very nice overview update on HPCs presented by Lisa Goodenough at 2020 Users Meeting

The Future of HEP Computing: HPCs

DOE Leadership Computing Facilities: Argonne (ALCF) and Oakridge (OLCF)

ALCF: Theta (current)

- 11.60 Petaflops (10^{15} floating point ops/sec)
- 4392 nodes, each with one Intel KNL CPU (64 cores/node w/4x hardware threads)
- 192 GB DDR4 + 16 GB MCDRAM/node
- vectorization



ALCF: Aurora (2021)

- >1 Exaflops (10^{18} floating point ops/sec) EXA
- hybrid architecture, no vectorization
- nodes: two Intel Sapphire Rapids CPUs with six

6 11 Aug '20 Lisa Goodenough | Users Meeting 2020: S

OLCF: Summit (current)

- 193 Petaflops
- 4608 nodes, each with two IBM Power9 CPUs

The Future of HEP Computing: HPCs

National Energy Research Scientific Computing Center: NERSC

NERSC: Cori (current)

- ~30 Petaflops
- 2388 Intel Haswell nodes (32 cores/node w/2x hyper-threading), 112 GB DDR4 + eight 16 GB DIMMS/node
- 9668 Intel KNL nodes (68 cores/node w/4x hardware threads), 96 GB DDR4 + six 16 GB DIMMS/node
- vectorization



NERSC: Perlmutter (2020-2021)

- ~100 Petaflops
- hybrid CPU/GPU architecture

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Scientific Computing Projects and Facilities

- Computing resources
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 - Experiments (CMS, NOvA, DUNE, mu2e, g-2, etc) are actively running production jobs on HPC sites via HEPCloud
 - DOE is funding tools for the community to use HPCs

User Facilities

The [Advanced Scientific Computer Research](#) program supports the following national scientific computing facilities:



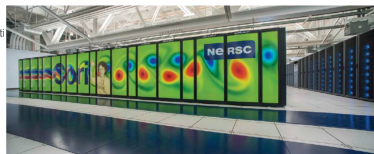
Argonne Leadership Computing Facility (ALCF)

The ALCF provides the computational science community with a world-class computing capability for breakthrough science and engineering.



Energy Sciences Network (ESnet)

The ESnet is a high-speed network serving thousands of Department of Energy researchers worldwide.



National Energy Research Scientific Computing Center (NERSC)

The NERSC is the mission high performance computing facility for the Department of Energy, and is a world leader in accelerating scientific discovery through computing.



Oak Ridge Leadership Computing Facility (OLCF)

The OLCF provides the computational science community with world-class computing capability dedicated to breakthrough science and engineering.



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ENERGY

Office of
Science

<https://science.osti.gov/ascr>

About

The mission of the Advanced Scientific Computing Research (ASCR) program is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy (DOE). A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous significant modifications to today's tools and techniques to deliver on the promise of exascale science.

Scientific Computing Projects and Facilities

- Computing resources
- Advanced applications and algorithm techniques; large-scale data analytics
 - HPCs are required for success in HEP
 - Fermilab has hosted the Institutional Cluster for over a decade, and is used largely by the US Lattice QCD collaboration
 - Experiments (CMS, NOvA, DUNE, mu2e, g-2, etc) are actively running production jobs on HPC sites via HEPCloud
 - DOE is funding tools for the community to use HPCs
 - **Develop and quantify performance on various HPC architectures [CPU, GPU, and CPU/GPU architectures]**

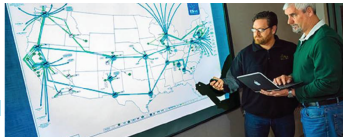
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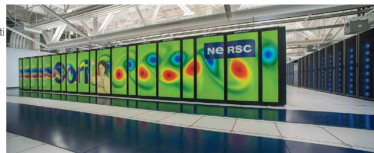
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Scientific Computing Projects and Facilities

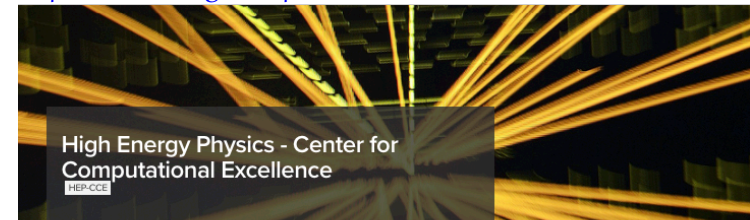
- Computing resources
- Advanced applications and algorithm techniques; large-scale data analytics
- Developed applications to run HPC platforms
 - HEP-Center for Computational Excellence (HEP-CCE)
 - Fermilab institutional lead, Liz Sexton-Kennedy
 - Focuses on HPC I/O systems and storage
 - Order of magnitude increase in data rates



Elizabeth Sexton-Kennedy
Chief Information Officer



<https://www.anl.gov/hep-cce>



Helping members of the community connect to one another to share or engineer experiment-independent solutions.

The High-Energy Physics Center for Computational Excellence (HEP-CCE) is a DOE CompHEP project that develops common strategies to efficiently run HEP software applications on the next generation of DOE's exascale high-performance computers (HPCs). HEP-CCE is a 3-year project that began in January 2020.

EXPERIMENTS



| |
|---------------|
| HEP-CCE |
| About Us |
| Participants |
| Activities |
| Results |
| Events |
| Opportunities |



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CONTACT US
Email the HEP-CCE Team
hep-cce@anl.gov
[Join HEP-CCE Mailing List](#)

HEP-CCE COLLABORATION TOOLS
[FPS Internal github \(invitation only\)](#)
[ICS Internal github \(invitation only\)](#)
[HEP-CCE Slack Workspace \(invitation only\)](#)

Scientific Computing Projects and Facilities

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 - Fermilab institutional lead, Liz Sexton-Kennedy
 - Focuses on HPC I/O systems and storage
 - Fermilab involvement
 - Measuring the performance of ROOT I/O on HPC (using the profiling tool Darshan)
 - Important because ROOT is the primary toolkit used in HEP
 - Must efficiently manage workflows for big and complex data

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 - Measuring the performance of ROOT I/O on HPC (using the profiling tool Darshan)
 - Investigating Hierarchical Data Format (HDF5) as an intermediate event storage for processing data on HPC
 - Design to handle large amount of data
 - Organize the data in many different structures
 - Runs on a variety of computing platforms

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 - Measuring the performance of ROOT I/O on HPC
 - Investigating Hierarchical Data Format (HDF5) as an intermediate event storage for processing data on HPC
 - Quantifying the disadvantages and advantages of running different data structures on GPUs

Scientific Computing Projects and Facilities

- Computing resources
- Advanced applications and algorithm techniques; large-scale data analytics
- Developed applications to run HPC platforms
- End user analysis toolkits beyond ROOT
 - Tools such as python, jupyter, julia, etc are becoming more popular
 - Well-maintained
 - Easy to use

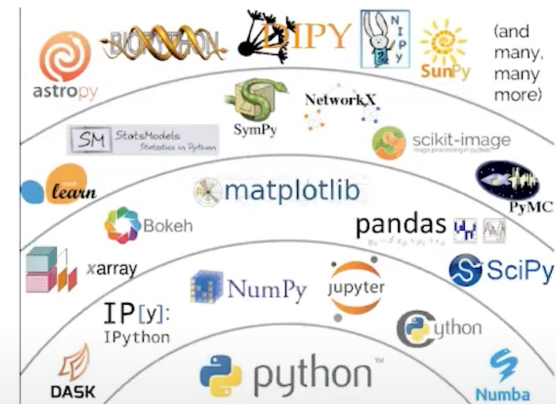


<https://root.cern.ch/>

paradigm shift

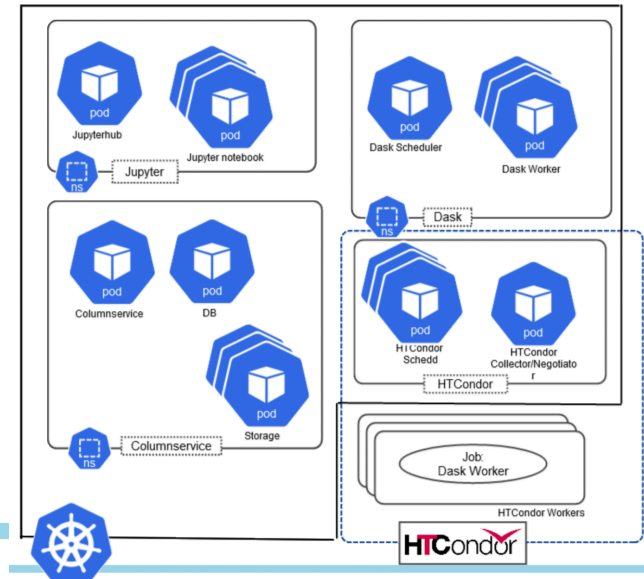
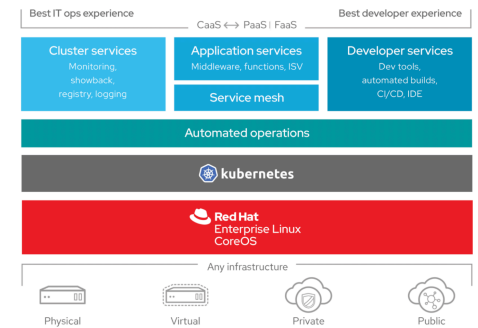


CMS columnar-based python ecosystem



Scientific Computing Projects and Facilities

- Computing resources
- Advanced applications and algorithm techniques; large-scale data analytics
- Developed applications to run HPC platforms
- End user analysis toolkits beyond ROOT
 - CMS Elastic Analysis Facility (R&D project)
 - Column-wise analysis and supports row-wise analysis
 - Low-latency access to CPU resources
 - Fast access to large amount of disk
 - Containerized infrastructure (Kubernetes-based)
 - Jupyterhub deployment



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“Computing is a catalyst for building bridges to other areas of science and society at large.” – Snowmass Computation Frontier Conveners

Summary

- Fermilab offers a variety of services for experiments.
 - If you are unsure, please contact your Fermilab scientific computing liason for questions regarding SCD services.
- The next generation of HEP experiments are projected to produced big data.
 - High-Performance Computing will play a major role in data production and algorithm development.
- The community is adapting tools beyond ROOT.
 - Expect many analysis facilities to integrate tools (python, Julia,...) that are supported and developed by many fields within the scientific community.
- There are many ongoing computational R&D activities.
- HEP is not alone in facing the challenges of big data.

For more information on the future of scientific computing at Fermilab, please feel free to contact members within the SCD community

Thank you!

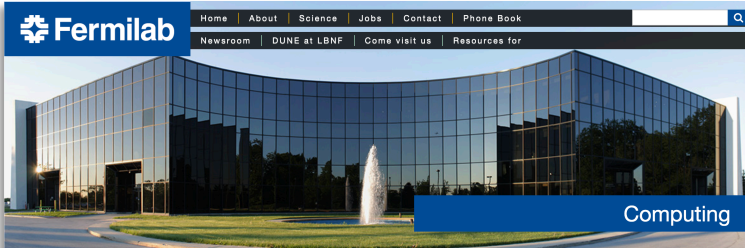
Special thanks to everyone who help with the contents of the talk

- Adam Lyon, Oliver Gutshe, Phil Demar, Andrey Bobyshev, Bo Jayatilaka, Burt Holzman, Lindsey Gray, Nick Smith, Lisa Goodenough, Kyle Knoepfel, Ken Herner

Back up Slides

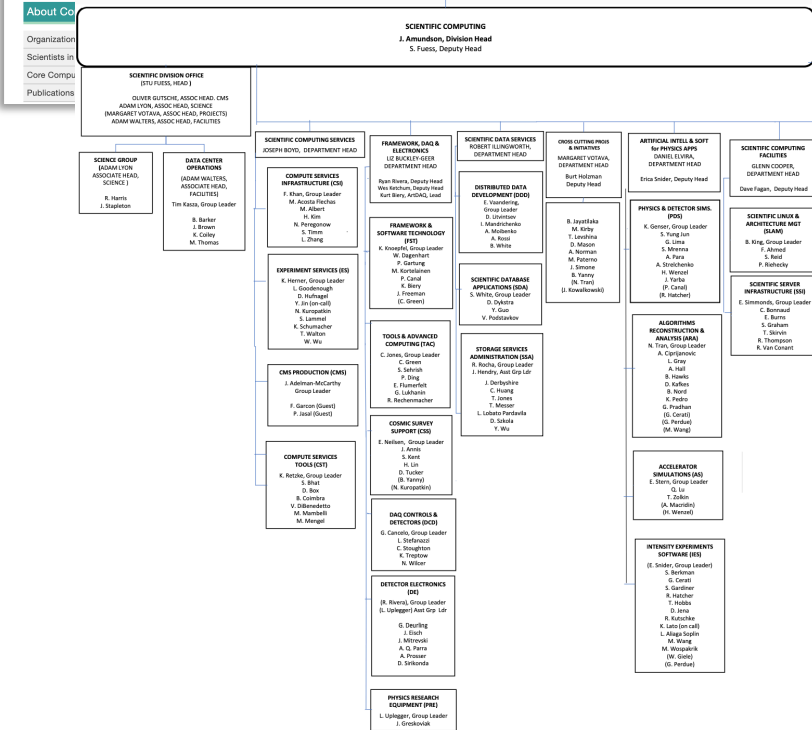
Scientific Computing

<https://computing.fnal.gov/>



Scientific Computing Division consists of :

- computing scientists and researchers
- experimental, theoretical, and accelerator physicists
- engineers
- research associates



Scientific Computing Division contributes to:

- Accelerator simulations
- DAQ controls, detectors, and electronics
- Data storage, handling, distribution, and production
- Computing Infrastructure and architecture
- Software and frameworks
- Algorithms and reconstruction
- Physics Analysis
- And much more

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arXiv:2104.08265v1 [cs.DC] 16 Apr 2021

Evaluation of Portable Acceleration Solutions for LArTPC Simulation Using Wire-Cell Toolkit

Haiwang Yu^{1,*}, Zhihua Dong², Kyle Knoepfel³, Meifeng Lin², Brett Viren¹, and Kwangmin Yu²

¹Department of Physics, Brookhaven National Laboratory, Upton, NY 11973, USA

²Computational Science Initiative, Brookhaven National Laboratory, Upton, NY 11973, USA

³Scientific Computing Division, Fermi National Accelerator Laboratory, Batavia, IL 60510, USA

Abstract. The Liquid Argon Time Projection Chamber (LArTPC) technology plays an essential role in many current and future neutrino experiments. Accurate and fast simulation is critical to developing efficient analysis algorithms and precise physics model projections. The speed of simulation becomes more important as Deep Learning algorithms are getting more widely used in LArTPC analysis and their training requires a large simulated dataset. Heterogeneous computing is an efficient way to delegate computing-heavy tasks to specialized hardware. However, as the landscape of the compute accelerators is evolving fast, it becomes more and more difficult to manually adapt the code constantly to the latest hardware or software environments. A solution which is portable to multiple hardware architectures while not substantially compromising performance would be very beneficial, especially for long-term projects such as the LArTPC simulations. In search of a portable, scalable and maintainable software solution for LArTPC simulations, we have started to explore high-level portable programming frameworks that support several hardware backends. In this paper, we will present our experience porting the LArTPC simulation code in the Wire-Cell toolkit to NVIDIA GPUs, first with the CUDA programming model and then with a portable library called Kokkos. Preliminary performance results on NVIDIA V100 GPUs and multi-core CPUs will be presented, followed by a discussion of the factors affecting the performance and plans for future improvements.

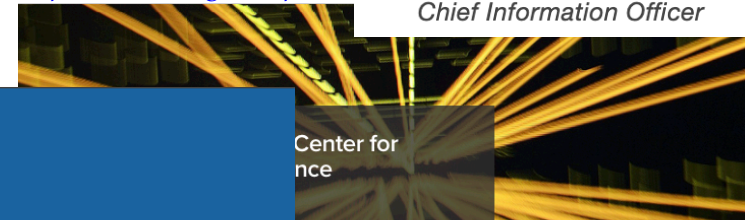
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Elizabeth Sexton-Kennedy
Chief Information Officer

<https://www.anl.gov/hep-cce>



HEP-CCE All-Hands Meeting

Nov 4, 2020, 1:45 PM → Nov 6, 2020, 4:25 PM US/Central

Description [Click Here to Join Meeting](#)

The second HEP-CCE all-hands meeting will be dedicated to reviewing Year 1 progress for our four tasks, discussing Year 2 priorities and strategizing about possible new directions for our project. The idea is to have three two-hour sessions:

- Nov 4, 2-4 PM Central - Introduction, Task 2 (I/O Strategies) status and year 2 priorities
- Nov 5, 2-4 PM - Task 1 (Portable Parallelization) status and year 2 priorities
- Nov 6, 2-4 PM - Task 3 (Generators) and 4 (Workflows) year 2 priorities, CCE outreach. Year 2+ strategy discussion.



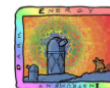
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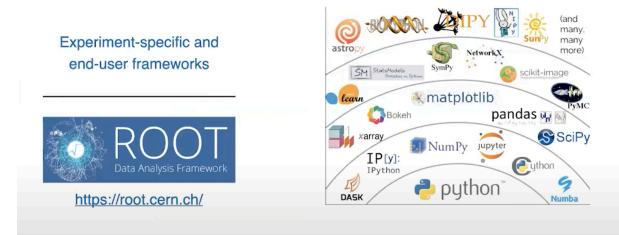


Scientific Computing Projects and Facilities

- Computing resources
- Advanced applications and algorithm techniques; large data analytics
- Developed applications to run HPC platforms
- End user analysis toolkits beyond ROOT

- CMS Coffea python toolkit

- Columnarbased analyses
- Use by 10 teams and > 20 analyses
- Backbone for many published analyses
 - <http://cms-results.web.cern.ch/cms-results/public-results/publications/EXO-20-004/index.html>
- Analyses turn-around time from 1-2 weeks to 1-2 hours
- Support a variety of computing clusters (condor, slurm,..)
- And execution engines (dask, parsl,..)
- Easy to implement data formats from others (ATLAS)
- Tutorial videos are available
 - https://www.youtube.com/results?search_query=coffea+pyhep



2008.12712v1 [cs.DC] 28 Aug 2020

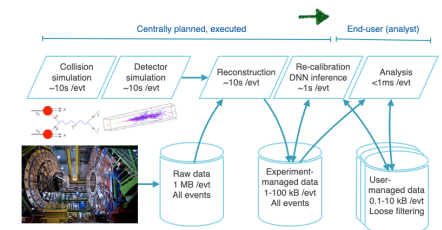
Coffea

Columnar Object Framework For Effective Analysis

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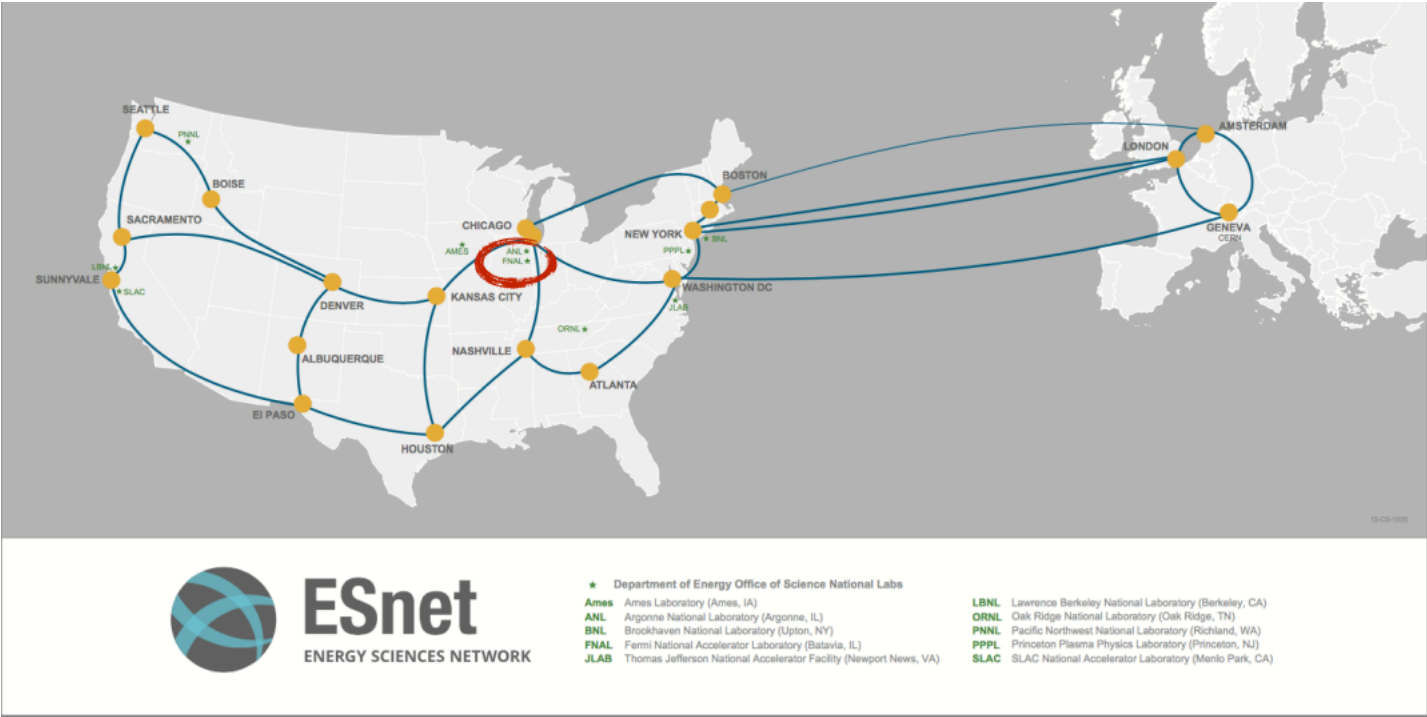
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Abstract. The coffea framework provides a new approach to High-Energy Physics analysis, via columnar operations, that improves time-to-insight, scalability, portability, and reproducibility of analysis. It is implemented with the Python programming language, the scientific python package ecosystem, and commodity big data technologies. To achieve this suite of improvements across many use cases, coffea takes a factorized approach, separating the analysis implementation and data delivery scheme. All analysis operations are implemented using the NumPy or awkward-array packages which are wrapped to yield user code whose purpose is quickly intuited. Various data delivery schemes are wrapped into a common front-end which accepts user inputs and code, and returns user defined outputs. We will discuss our experience in implementing analysis of CMS data using the coffea framework along with a discussion of the user experience and future directions.



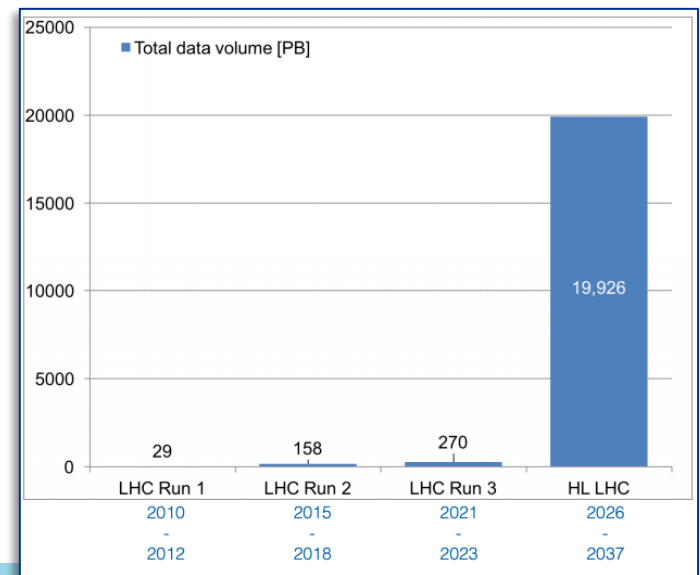
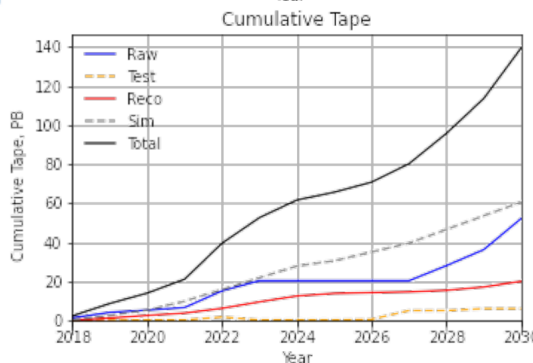
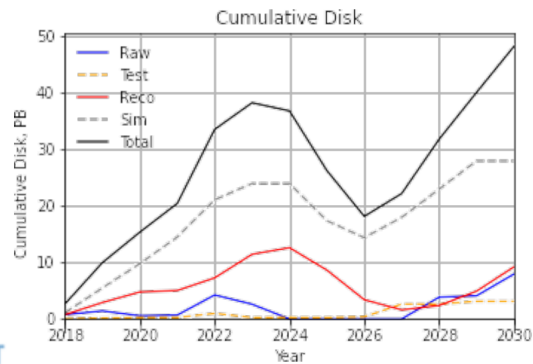
Scientific Computing Projects and Facilities

- Networking
 - Fast transportation of exascale data size around the world



Scientific Computing Projects and Facilities

- Storage
 - R&D investment in scaling storage for upcoming scientific data
 - Current tape (managed by enstore) : 269 petabytes



Scientific Computing Projects and Facilities

- Networking

- Fast transportation of exascale data size around the world

- HL LHC (~2027)

- Current Projections are for US-CMS T1 Facility to require 1Tb/s – 1.5Tb/s of off-site bandwidth at start of HL-LHC:
- Current FNAL off-site bandwidth is 3x100Gb/s for all off-site traffic
- Soon to be 4x100Gb/s
- Anticipating incremental ramp-up toward the terabit level in off-site bandwidth between now and 2027
- Step-up from 100GE network technology to 400GE technology
- US-CMST1 internal network to be correspondingly scaled up:
- 400GE network technology to become foundational basis of US-CMST1 LAN
- 100GE connectivity for server (& worker?) nodes
- LHC Data Challenges to demonstrate ramp-up of CMS data movement capabilities
 - 2021 – 10%
 - 2023 – 30%
 - 2025 – 60%
 - 2027 – 100%

Scientific Computing Projects and Facilities

- Networking
 - Fast transportation of exascale data size around the world
 - DUNE (~2026-2027)
 - Support for remote operations of Far Detector (FD) is primary network challenge
 - Will follow same model as used to support NOvA and Soudan:
 - Remote LAN logically supported as being part of FNAL internal network
 - Lies within the FNAL network security perimeter
 - Fully redundant LAN at DUNE FD:
 - Includes redundant fiber paths between cavern (detectors...) and surface
 - Based on 400GE network technology
 - Geographically-diverse WAN circuits back to FNAL:
 - 100Gb/s guaranteed bandwidth on the primary path
 - 10Gb/s guaranteed bandwidth on the secondary path