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# **Scientific Computing - Supporting Experiments in their Scientific Endeavors**

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47th Annual Fermilab Users Meeting

12. June 2014

# Fermilab's Computing Landscape

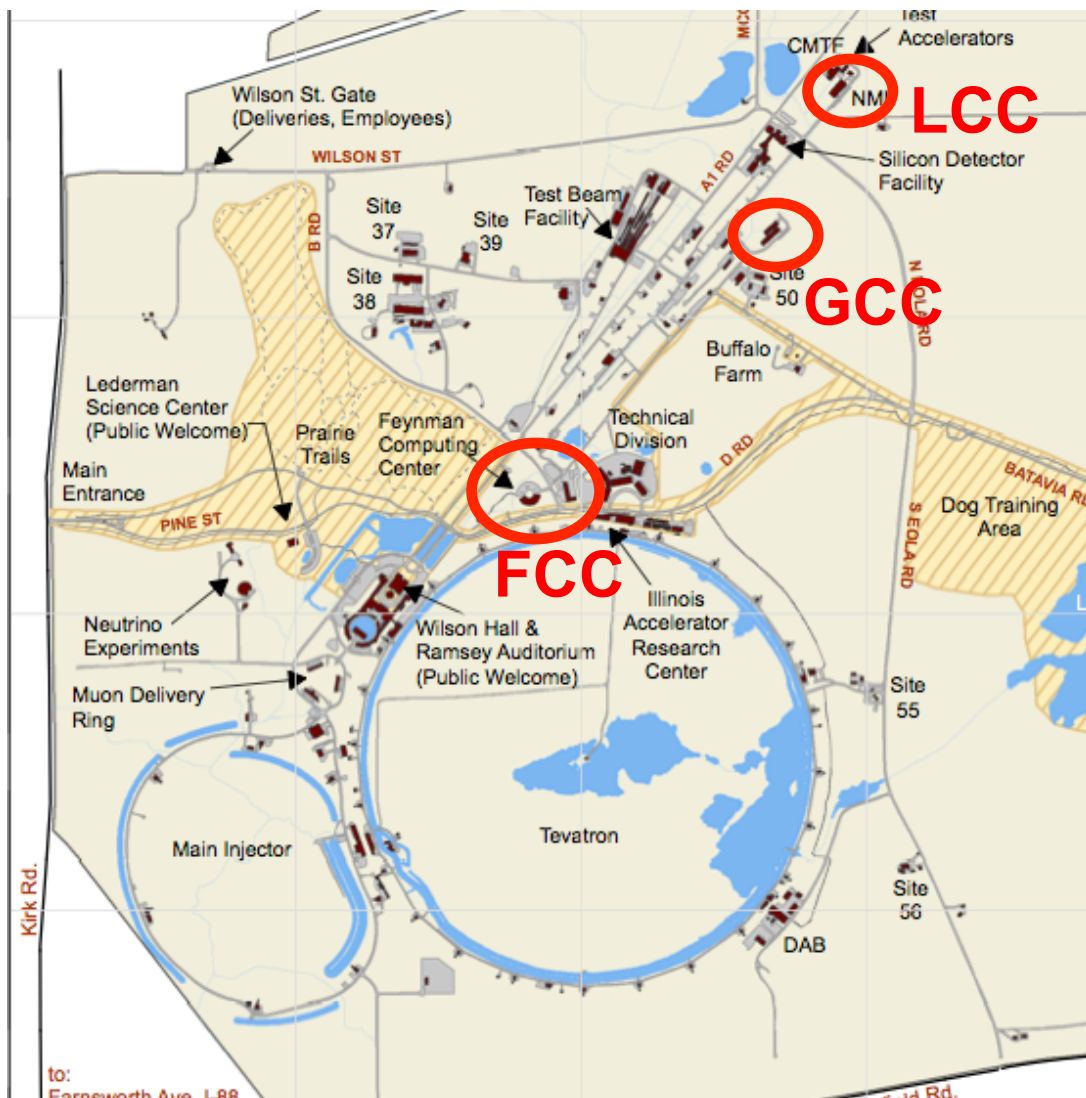
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- Fermilab is a great place!
- We have an interesting and diverse science program:
  - Many different experiments from collider physics, neutrino physics, astro-particle physics, ...
  - Vibrant theory community
  - Advanced accelerator science
- Everyone is using computing!
  - And scientific software, workflow tools, data handling, databases, ...
  - We are supporting all experiments
    - With a diverse scientific computing services catalog
    - With direct or indirect support of a variety of software packages
- Fermilab's Scientific Computing is a big part of everybody's daily scientific life!



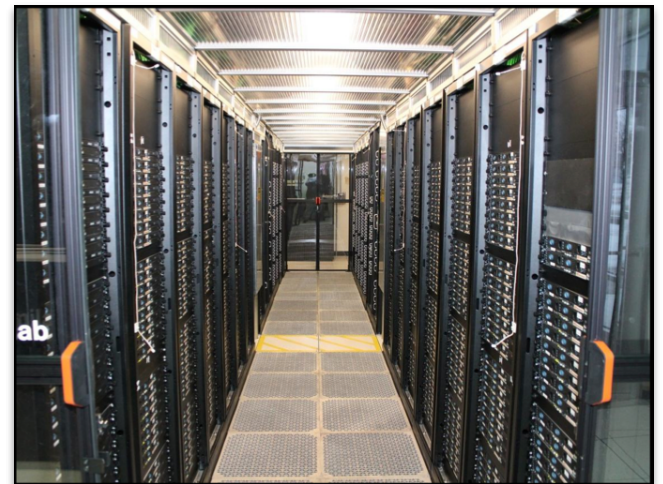
# Supporting Experiments in their Scientific Endeavors

- Facilities
  - People
  - Services
  - Software
  - Experiments
- Enabling the Future
    - Offline Processing Operations Group
    - Data Archival Facility
    - New hardware platforms



# Fermilab's Computing Facilities: Large Numbers

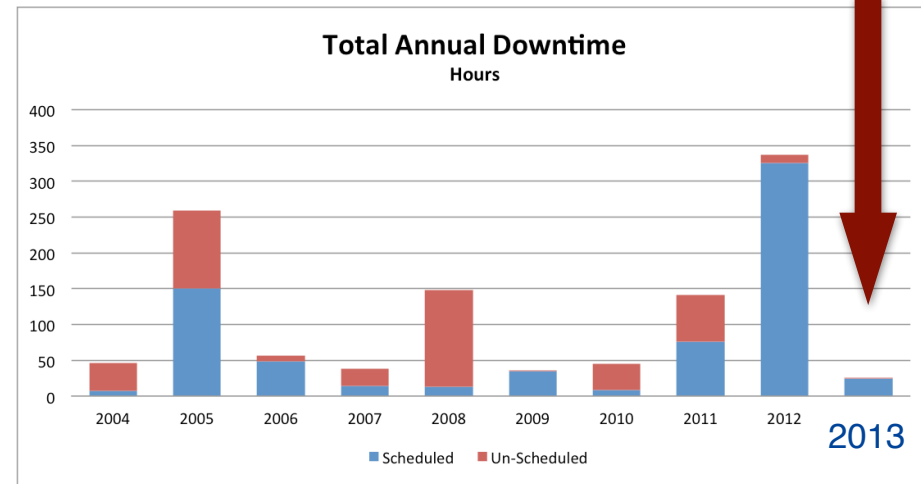
- CPU: 65,000 cores
  - ½ experiments - ½ lattice QCD (numerical theoretical calculations)
- Disk: 25 PetaBytes
  - Technologies: dCache, EOS, BlueArc, Lustre
- Tapes: 375 PetaBytes capacity
  - 70,000 tape slots in robots (not all used)
  - Current usage: 88 PetaBytes
- Network:
  - Internal: ~32,000 network ports
    - connected through network fabric from copper and fiber links
  - External: 130 Gb/s
    - 1 x 100 Gbps and 3x 10 Gbps fiber links





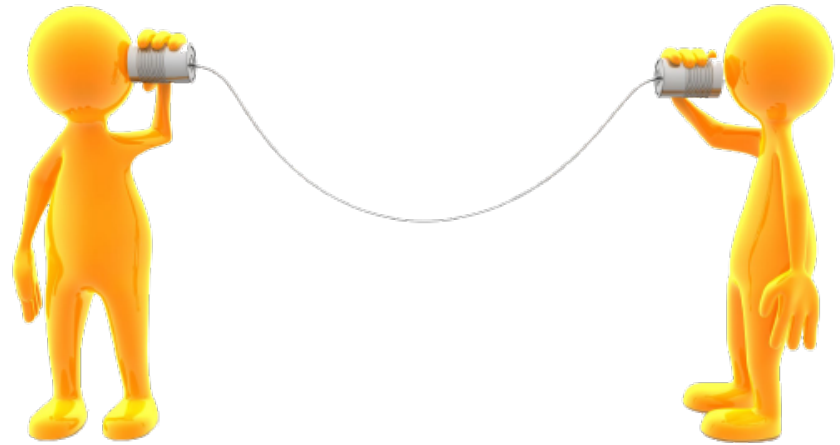
# Fermilab's Computing Facilities: Saving money for the Future

- Top facilities → Top science
  - Phenomenal availability in 2013:
    - Less downtime → less hassle for everyone doing science
- Continuously improving to save energy
  - Latest: cold aisle containment in computing rooms → reduces cooling costs
  - Cost will be recovered in 21 months
    - After 21 months, we are saving money → can be used for science



# Scientific Computing Division (SCD): People & Communication

- SCD is working closely with the scientific community and all other laboratory functions to support the scientific mission
- Good communication is the key to efficient use of facilities and services and to help everyone succeed
  - Approach: Liaisons and Portfolio Management
  - Liaisons: communication between experiments and SCD
    - Every experiment, scientific project and collaboration has SCD liaison
    - Liaisons are embedded in Scientific Computing and vice versa → ensuring smooth operation and communication
    - Bi-weekly liaison meetings → Experiments included in management of scientific services
    - Works well!
      - Important: FIFE workshop 16. - 17. June 2014
  - Portfolio Management
    - Annual review of computing plans, requirements and concerns of experiments
      - Last review was 1. - 2. May 2014
      - Successful model: most problems from 2013 review solved, solutions are available



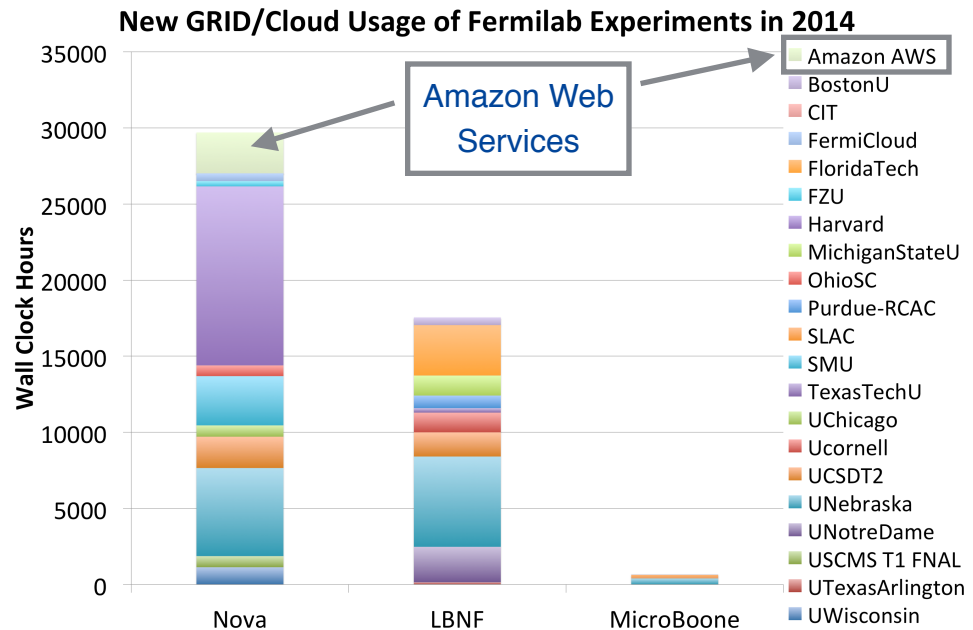
# Scientific Services Catalog available to Experiments

	DAQ	Fermilab	Jobsub	Fifemon	Redmine	CVS/Subversion/ Git	ECL	ups/psd	CVMFS	Interactive machine in GPCF	Continuous Integration - middleware	sam/ftsh	file transfer service (FTS)	J/Beam	custom databases
	DAQ and Controls	Grid and Cloud			scientific collaboration tools			scientific computing systems			scientific data management		scientific databases		
<b>CDF</b>	N/A	plan	plan	plan		yes		yes				SAM			
<b>D0</b>	N/A	test	test	test		yes	yes	yes	test		plan	SAM			
<b>ArgoNeut</b>		yes	yes	yes	yes	yes		yes	no	yes		no			
<b>Lariat</b>	artdaq?	yes	yes	yes	yes	yes	yes	yes	In Design	yes	yes	SAMweb	plan	yes	plan
<b>LBNF</b>	artdaq	yes	g-wms	yes	yes	yes		yes	progress	yes	yes	SAMweb	plan		progress
<b>LBNF 35T</b>	artdaq	yes	yes	yes	yes	yes	yes	yes	yes		yes	plan	plan		plan
<b>uBoone</b>	custom	yes	yes	yes	yes	yes	yes	yes	progress	yes	yes	SAM	yes	yes	
<b>Minerva</b>	Custom	yes	yes	yes	yes	yes	yes	yes		yes	buildbot	SAMweb	yes	yes	yes
<b>MiniBoone</b>	custom	yes	?	yes	yes	yes	yes	yes	no	yes	no	no			
<b>Minos+</b>	Custom/artdaq?	yes	yes	yes	yes	yes	yes	yes	yes	yes		SAMweb		yes	
<b>Mu2e</b>	artdaq	yes	yes	yes	yes	yes	plan	yes	plan	yes	yes				
<b>Muon g-2</b>	midas	yes	yes	yes	yes	yes		yes	yes	yes	yes	SAMweb	yes		progress
<b>NoVA</b>	novadaq	yes	yes	yes	yes	yes	yes	yes	yes	yes	yes	SAMweb	yes	yes	yes
<b>Darkside</b>	artdaq	yes	yes	yes	yes	yes		yes	plan	yes		SAMweb	yes		
<b>seaqwest</b>	PREP HW	yes	yes	plan	yes	yes	shift cal	plan	plan	yes	no	no	no		
<b>coupp</b>	custom	yes	yes	interested	no	interested	yes	yes	no	yes	no	yes	yes	no	

- In the past, fewer experiments were competing for resources → SCD was able to work with individual experiments and help them succeed
- Now, even more experiments are competing for resources → Necessary to look for communality and leverage sharing wherever possible
- We are now providing a Catalog of Scientific Services that experiments can choose from
  - Same services can be used by different experiments
- Big success!
  - We are providing solutions that experiments find useful!
- New: Effort to be more transparent to Experiments' needs
  - Running many services for many experiments needs higher level of organization that ensures success → working on service level agreements

# Fermilab and the OSG: Enabling GRID/Cloud usage

- Fermilab's facilities well used, utilization in the last year was around 80%
  - But peak demand is  $> 100\%$  (everybody wants to produce results for the same conferences)

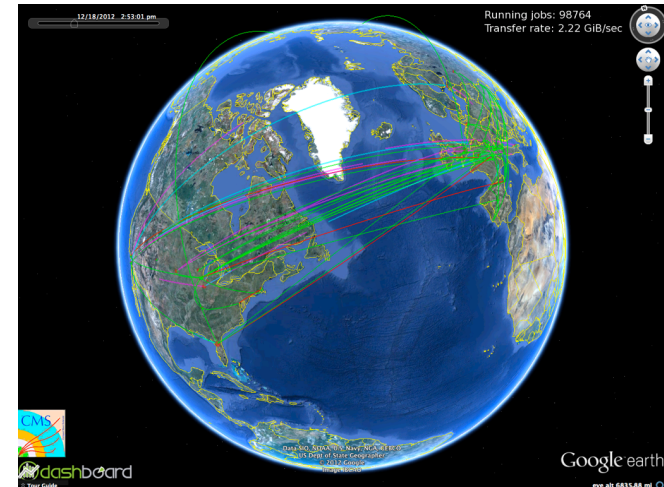


- SCD is enabling experiments and users to use the OSG for peak demands
  - Easier for the experiments if they are already setup to run on FermiGrid
- CMS, OSG and FNAL experiments are working together more closely
  - NOvA is now first class citizen on the GRID, MicroBoone is on its way, Muon g-2 is coming soon too

# Fermilab's biggest experiment: CMS

- Fermilab is CMS' largest Tier-1 center
  - Half of the CPU, disk and tape available to experiments at FNAL is for CMS
- CMS is preparing for LHC Run 2
  - Higher center-of-mass energy and higher inst. luminosity leads to significantly higher event complexity
    - Re-engineering of software and computing components is nearing completion
    - Capacity of facilities will be ramped up by a factor of two
- Re-engineering done during shutdown:
  - Software CMSSW was optimized for higher number of PileUp events
  - Computing model was adapted to increase efficiency and flexibility
    - Dynamic and automated data placement on GRID sites
    - Increased usage of access to files through the wide area network (xrootd, AAA)
    - Opportunistic resource usage on non-CMS GRIDs/Clouds/etc. based on glideinWMS
      - Mutually beneficial for CMS and other Fermilab experiments
  - Data challenge starting in a few weeks

CMS worldwide:  
62 computing centers



Level	US	Non-US	Total
Tier-0		1	1
Tier-1	1	7	8
Tier-2	8	45	53







# SCD Software Support: Experiment Software

	Software Framework software processing	
	scientific frameworks	
<b>CDF</b>		
<b>D0</b>		
<b>ArgoNeut</b>	art	larsoft
<b>Lariat</b>	art	larsoft
<b>LBNF</b>	art	larsoft
<b>LBNF 35T</b>	art	larsoft
<b>uBoone</b>	art	larsoft
<b>Minerva</b>	gaudi	
<b>MiniBoone</b>		
<b>Minos+</b>	root/SRT	
<b>Mu2e</b>	art	
<b>Muon g-2</b>	art	
<b>NoVA</b>	art	
<b>Darkside</b>	art	
<b>sequest</b>	custom	custom
<b>coupp</b>	custom	custom

- SCD supports the core software frameworks for the Fermilab experiments: CMS and Intensity Frontier
  - CMSSW and Art are key ingredients for the success of the Fermilab experiments and continue to be very successful
  - Reason for success of both:
    - Quality of the framework code (advanced C++ that physicists use - not write)
    - In-house expertise
    - Truly collaborative effort between the framework authors and the stakeholder experiment(s)
  - Art was forked from CMSSW → common concepts and base ideas
- New:
  - Multi-threading: one executable uses several cores in parallel to speed up processing and reduce memory requirements per core
  - Concrete help for the experiments:
    - ART workbook (documentation)
    - C++ courses (also see next slide about training)
- On top of ART: LarSoft
  - Specialized on reconstructing data from Liquid Argon detectors
  - Developed in international collaboration with contributors from many universities/labs, amongst those Fermilab

# Training - FNAL Software School - C++

- Quote from OHEP task force on workforce development, “Lab-university partnerships can provide necessary research infrastructure, expert support, and direct training...”



## FNAL Software School

4-8 August 2014  
*Fermilab, LPC*  
US/Central timezone

### Overview


- Scientific Programme
- Timetable
- Contribution List
- Author index
- Registration
  - Registration Form
- List of registrants
- Organising Committee

The course is intended for graduate students and starting postdocs who have programming experience but have not developed software within the framework of a large computing project. The course focuses on programming reconstruction software using tracking reconstruction in C++ as an example. The course is otherwise general and applies to programming problems in any large experimental particle physics project.

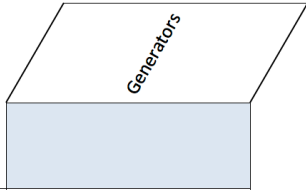
Course prerequisites:

- Students should have introductory level experience in C++ programming.
- Students should have familiarity with the process of compiling, linking and running programs in a UNIX environment
- Students should have familiarity with the physics of charged particle trajectories in magnetic fields
- For students who need to learn C++ programming before the course an excellent book is [Accelerated C++ by Andrew Koenig and Barbara Moo](#)

**Dates:** from August 4, 2014 08:00 to August 8, 2014 18:00  
**Timezone:** US/Central  
**Location:** *Fermilab, LPC*

 Powered by [Indico](#)

# SCD Software Support: Simulation & Modeling



<b>CDF</b>	
<b>D0</b>	Pythia, Geant, Alpgen
<b>ArgoNeut</b>	Genie, Fluka
<b>Lariat</b>	Genie, Cry
<b>LBNF</b>	Genie, geant4
<b>LBNF 35T</b>	Genie, Cry
<b>uBoone</b>	Genie
<b>Minerva</b>	Genie
<b>MiniBoone</b>	
<b>Minos+</b>	Genie
<b>Mu2e</b>	
<b>Muon g-2</b>	
<b>NoVA</b>	Genie, Flugg, Cry and Coriska
<b>Darkside</b>	g4ds
<b>seaqwest</b>	pythia 8, g4, custom
<b>coupp</b>	srin, geant4, mcnp

- **Generators:**

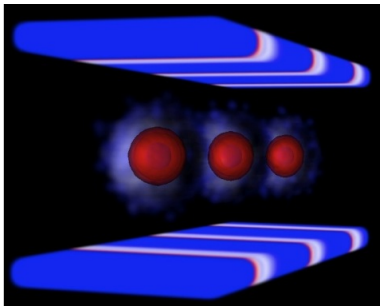
- Strong involvement in Pythia
- Genie (neutrino generator) → began participation in the development team

- **Simulation:**

- Strong Geant4 team working with experimenters and experiments
- Working on the evolution of Geant4 to enable multi-threading

- **Accelerator modeling tools:**

- Development and support of:
  - single-particle beam dynamics code CHEF
  - multi-particle beam dynamics framework Synergia



Wakefield simulation

# New: Fermilab's Offline Processing Operations Group

- Large scale workflow execution on GRIDs/ Clouds and other opportunistic resources is not easy!
  - Not every experiment has the required people and skills
- SCD is planning to support Fermilab's experiments also in executing workflows
  - Help the experiments execute their workflows on GRIDs/Clouds/etc.
  - Modeled after the CMS operations group
- Effort is ramping up, Fermilab Application Physicist position was opened to lead effort

Fermilab ROC



## Coming soon

A new remote operations center



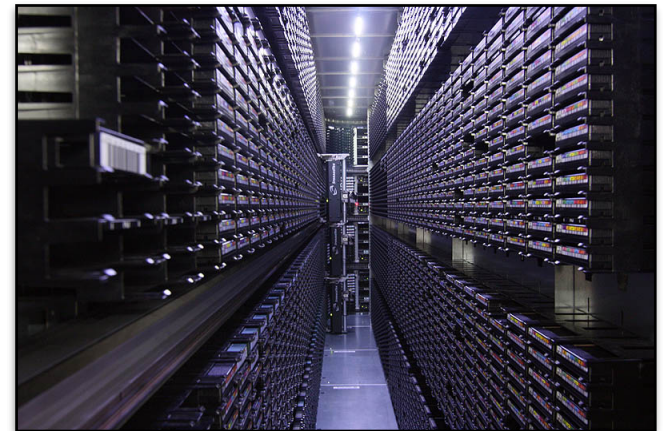
Behind this temporary wall is the future home of the new remote operations center.

The remote operations center will serve as a hub for scientists on Fermilab's neutrino and muon experiments.

When completed this fall, the scientists will use the new facility for experiment operations, similar to scientists using the LHC Remote Operations Center on the east side of the atrium for the CMS experiment.

# New: Scientific Data Archival Facility

- Develop and provide service to store data of DOE Office of Science experiments
  - Based on large experience on storing data on tape at Fermilab
- Designed as a pay for service model
- Pilot project with the University of Nebraska and their Biology department
  - Several other experiments/ Universities have expressed interest

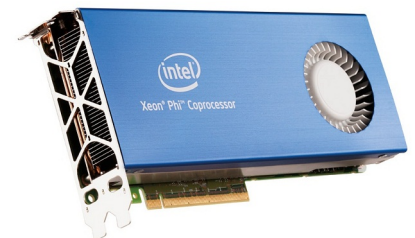




# New: Preparing for the future: new hardware architectures

- Traditionally we are using Intel compatible hardware for processing, production and analysis of data
- New hardware architectures are emerging
  - Significantly increasing the speed of specific calculations
    - Systems with Graphics Processor Units (GPGPU)
    - Intel Phi coprocessors
  - Reducing the power consumption and getting more cycles per watt
    - ARM architectures
  - All the new architectures will have significantly less memory per core → need to prepare software and hardware for transition
- Fermilab provides access to these new hardware architectures to experiments for evaluation and tests:
  - Intel Phi systems
  - GPU systems with the latest cards
  - Setting an ARM system now

Fermilab's Phi Cluster



# Summary & Conclusions

- Fermilab's Scientific Computing is supporting all its experiments' computing needs:
  - The Catalog of Scientific Services is well received and used throughout the experiments
  - The core and simulation/modeling software efforts are integral parts of the experiments' strategies
- Looking into the future, Fermilab's Scientific Computing is planning to
  - Help experiments execute their workflows at large scales on GRIDs/Clouds and other resources
  - Enable other DOE experiments to store data on tape, building on the large experience of Fermilab
  - Help experiments evaluate and test new hardware architectures to prepare for the future



# Glossary

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- **GPGPU**: General-Purpose computing on Graphics Processing Unit
- **Intel Phi**: Brand name for Intel's Many Integrated Core Architecture or Intel MIC (pronounced Mike): multiprocessor coprocessor architecture developed by Intel
- **LT04**: Linear Tape-Open (or LTO) is a magnetic tape data storage technology, LT04 capacity: 800 GB
- **T10k**: Magnetic tape data storage format developed by the Storage Technology Corporation owned by Oracle; T10kc capacity: 5 TB
- **dCache**: is a system for storing and retrieving huge amounts of data, distributed among a large number of heterogeneous server nodes, under a single virtual file system tree with a variety of standard access methods.
- **EOS**: is a Xroot-managed disk pool for analysis-style data access
- **Xrootd**: is a fully generic suite for fast, low latency and scalable data access, which can serve natively any kind of data, organized as a hierarchical file system-like namespace, based on the concept of directory
- **BlueArc**: network-attached storage (NAS) systems that are sold either as appliances bundled with storage, or as "NAS heads" supporting third-party storage area network connected storage
- **Lustre**: is a type of parallel distributed file system, generally used for large-scale cluster computing
- **Gbps**: giga bits per second
- **Cold aisle containment**: Workernodes are arranged in rows. The aisles between the rows are alternating hot and cold, where the workernodes fronts point to the cold aisles to suck in cold air. Cold aisle containment consists of a physical barrier that allows the cold air to pool inside the aisle between the worker node racks.
- **ISO20k**: first international standard for IT service management to reflect best practice guidance contained within the ITIL framework
- **ITIL**: The Information Technology Infrastructure Library (ITIL) is a set of practices for IT service management (ITSM) that focuses on aligning IT services with the needs of business.
- **GENIE**: (Generates Events for Neutrino Interaction Experiments) is a universal object-oriented neutrino MC generator supported and developed by an international collaboration of scientists whose expertise covers a very broad range of neutrino physics aspects, both phenomenological and experimental.
- **CRY**: cosmic ray generator used by neutrino experiments to study backgrounds
- **GEANT4**: (for GEometry ANd Tracking) is a platform for "the simulation of the passage of particles through matter," using Monte Carlo methods.
- **SAM**: SAM is a data handling system organized as a set of servers which work together to store and retrieve files and associated metadata, including a complete record of the processing which has used the files.
- **SVN**: Apache Subversion (often abbreviated SVN, after the command name svn) is a software versioning and revision control system distributed as free software under the Apache License.
- **GIT**: is a distributed revision control and source code management (SCM) system with an emphasis on speed.
- **docDB**: is a powerful and flexible collaborative document server.
- **redmine**: Redmine is a free and open source, web-based project management and bug-tracking tool.
- **daq**: Data Acquisition
- **FIFE**: FabrIc for Frontier Experiments, provides collaborative scientific-data processing solutions for Frontier Experiments
- **OSG**: Open Science Grid: provides common service and support for resource providers and scientific institutions using a distributed fabric of high throughput computational services.
- **AAA**: "Any data, anywhere, any time": CMS global data federation based on Xrootd