Scientific Computing Division – FY15

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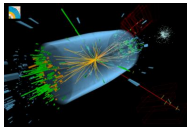
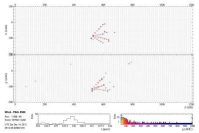
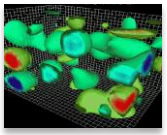
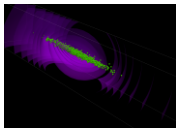




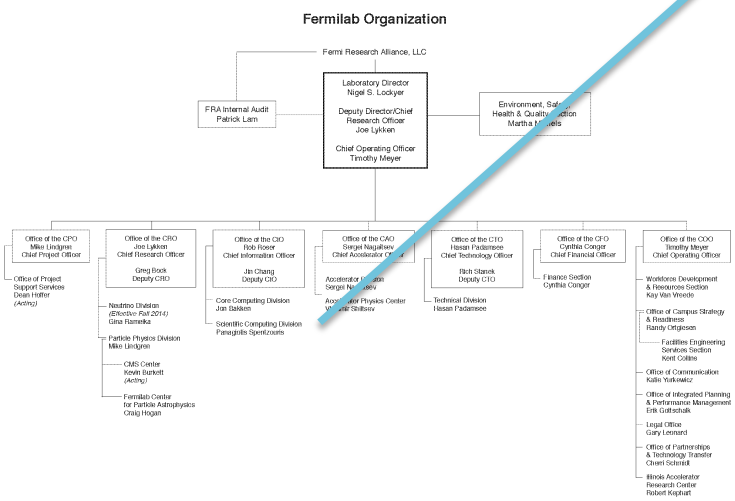


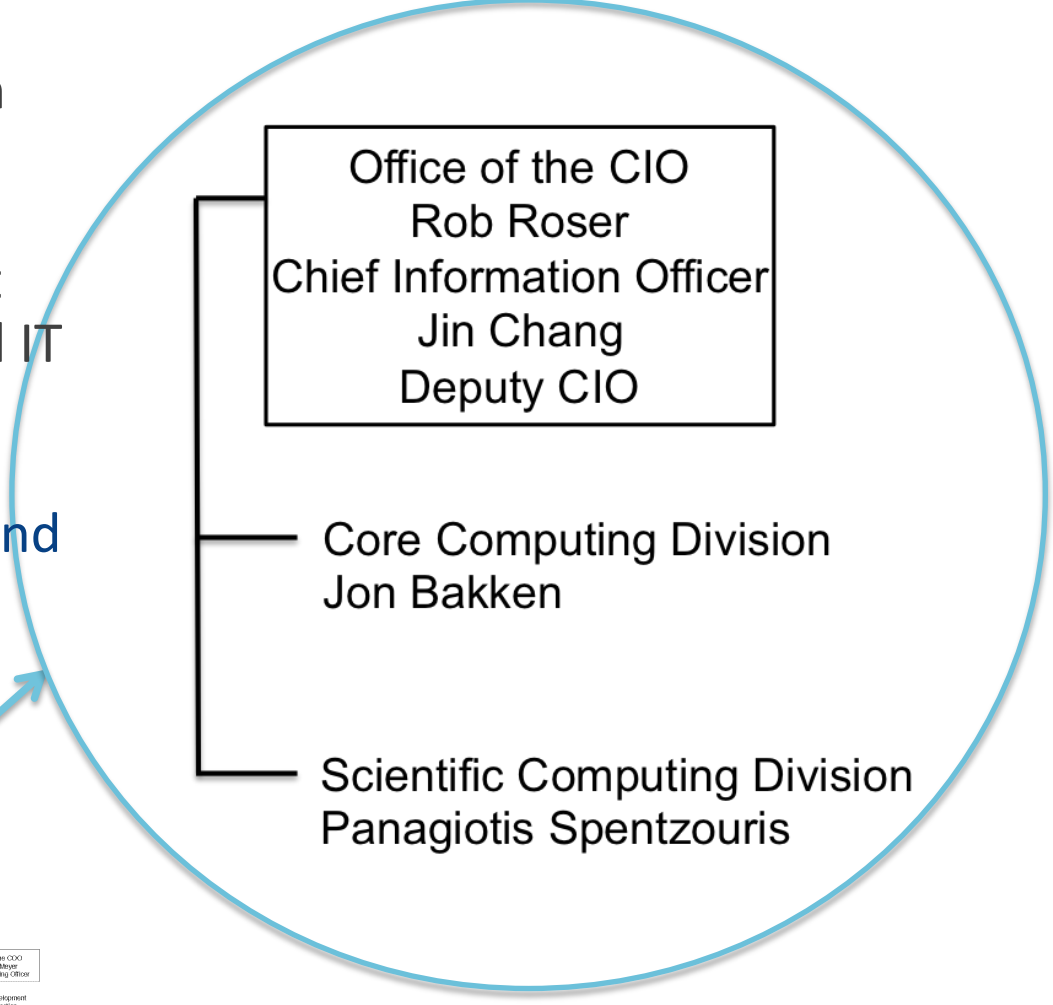


SCD part of Computing, with the Office of CIO providing

- admin, ES&H, QA, and financial services support
- Service Management and IT governance

Work closely with, and depend on, CCD (facility operation & infrastructure)





- Work closely with all other divisions at Fermilab
- Collaborate with HEP and ASCR groups at other labs

Drivers for FY15 (1/2)

- Support the **CMS science program.** Continue
  - hosting and operating the top performing CMS Tier-1 facility and the LPC computing facility,
  - providing storage and data management services for raw, reconstructed and simulation data (over 40 petabytes to date),
  - developing and supporting the analysis framework.
- Support the diverse FNAL **IF experimental program,** in all aspects of its computing needs, by providing
  - facility with performance at the same high level as the Tier-1,
  - common tools, services, and operations for physics analysis,
  - detector and physics simulation expertise.
- Support selected CF experiments as per P5 and FNAL priorities, with
  - Emphasis on workflow, workflow management, data storage, DAQ
  - Focus on DES, LSST (standby mode), begin DESI involvement
  - Ramping down on DS50, holometer, DAMIC; low level R&D on CCD/MKIDS
- Maintain and upgrade our facilities to the capacity and capability necessary for CMS Run2 and the IF Fermilab program

Drivers for FY15 (2/2)

- Maximize **impact of our scientists** on the Fermilab program
- Enhance understanding for and optimize performance of **current and future FNAL accelerators**
  - Leverage HPC modeling competencies, focus on PIP and PIP-II
- Participate in high-priority projects where our competencies match or there is opportunity to grow
  - LCLS-II engineering (not in budget, under discussion, but good example), CF analysis frameworks, CMS upgrade trigger
- **R&D for new tools and services**: evolution of computing architectures and technologies calls for major software re-engineering to maintain capabilities as we move in the future
  - multicore/many-core, co-processors, reduced memory/core footprint
  - the emergence of the cloud concept as a scientific computing tool
  - Focus on selected high impact/relevance areas: analysis frameworks, Geant4, accelerator modeling

SCD Tactical Approach

- Supporting the current program and preparing for the future requires significant investment. Leveraging resources and expertise essential
  - Work closely with the other lab organizations to support the entirety of the lab's program
  - Build stronger ties and initiate collaborative efforts with other labs
    - Building infrastructure and support for projects and experiments
    - R&D on new architectures to transform major HEP toolkits
    - This, after all, is a P5 recommendation
- Continue to provide state of the art, reliable facilities and computing services to the community
  - Leverage expertise and tools from our very successful CMS program and integrate tools and services we have developed for the IF program
  - Rely on the Scientific Project Portfolio Management Process and the SCD Liaisons for up-to-date information on experiment goals and needs
    - continuous feedback both for planning and operations
- Maintain competencies and infrastructure capabilities to help the lab position itself to play a significant role in next-generation experiments, upgrades, and develop future programs
- Continuously work on improving all aspects of the organization

Organization agility and efficiency: re-org for FY15

- Take the next step in better aligning the organization along functional areas of the division
  - Eliminate any leftover “stovepiping” for specific applications or experiments, increase resource utilization effectiveness
- Tighter coordination across activity areas, defined by overall service deliverables
  - Increase efficiency and quality of service
- Organization evolution
  - Established high-level, cross-cutting, activity areas across SCD
  - Introduced area coordinators to complement, augment, and (in a healthy way) challenge the line organization
  - Line organization changes
    - *To be finalized soon*

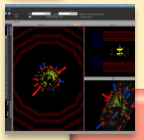
Increasing organization agility: 3 major activity areas

- **Development, Integration and Research**
  - for offline, simulation, and real-time software and engineering tools
    - Complete stack: workflow, workflow-management, data management, build, computational physics algorithms, simulation algorithms, …
  - Develop the **software *"products"*** and ***architecture*** for the Scientific Facility.
- **Scientific Facility**
  - An "über"Tier-1 center-like function for ALL of our users
    - Providing and managing the resources and services for data storage and bulk data processing and analysis (and DAQ for FNAL based experiments)
  - Tier-0 center function for users with such needs (recording & archiving data, …)
- **Science Operations and Workflows**
  - Developing, configuring, and operating the actual applications for projects and experiments, utilizing the services provided by the facility
- Each of these areas has a coordinator that reports to the division.

Science Operations and Workflows

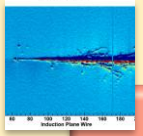
Develop workflows for experiment/project to execute on the facility and provide operations support

Facility



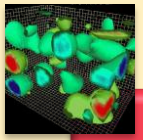
CMS T1

- Compute and storage resources
- Services stack



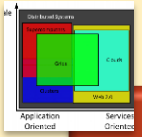
IF and CF

- Compute and storage resources
- Services stack



HPC

- LQCD, accelerator modeling, and cosmology compute and storage resources
- HPC services
- New computing architectures



Virtual Facility

- Cloud, on demand resources
  - Commercial & local
- Virtualization services stack

Facility hardware housed in CCD operated computing centers

Development, Integration, and Research

R&D for creating, research for adapting, and architecture work for delivering “products” for the scientific software stack of the facility

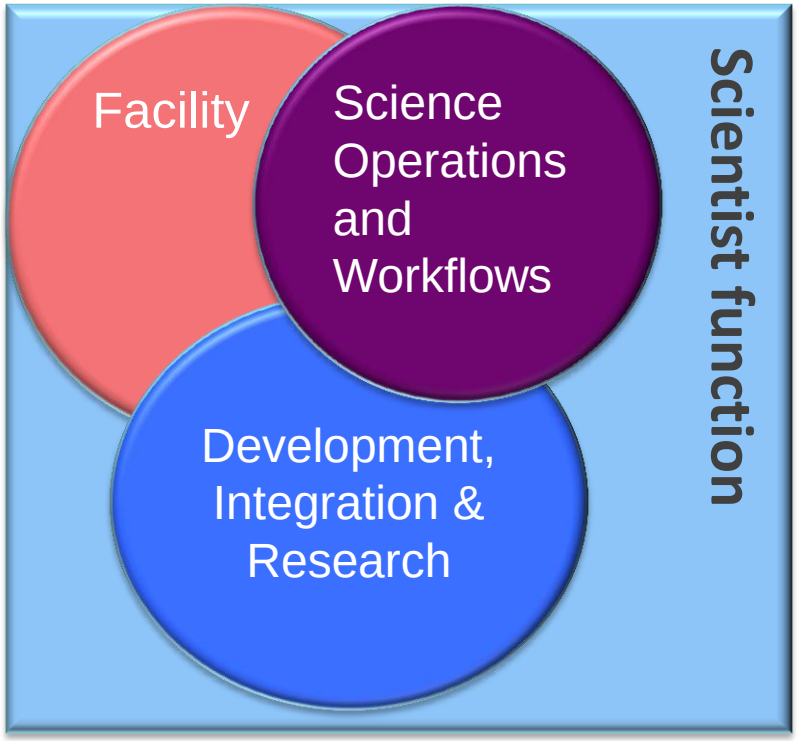
Already broad buy-in for cross-cutting development and services across research areas

	Minos	Minerva	NoVA	uBoone	LBNE	Gm2	Mu2e	35T proto
DAQ	Custom	Custom[4]	novadaq[6]	Custom	artdaq	midas	artdaq	artdaq
Software Framework		gaudi	art	Larsoft	Larsoft	art	art	Larsoft
Generators	Genie	Genie			Genie			
Data Management	SAM	SAM	SAM	SAM	SAM	SAM	SAM	SAM
Job Submission	Jobsub/ glideinwms	Jobsub/ glideinwms	Jobsub/ glideinwms	Jobsub/ glideinwms	glideinwms	Jobsub/ glideinwms	Jobsub/ glideinwms	
Onsite Grid Enabled	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
CVMFS	Yes	Yes	Yes	Yes	Yes	Yes	Yes	
OSG Enabled		No	Partially	No	In Progress	In Progres	No	not yet
ECL	Yes	Yes	Yes	Yes				
IFBeam	Yes	Yes	Yes	Yes				
tape storage	enstore	enstore	enstore	enstore	enstore	enstore	enstore	enstore
data cache	dcache	dcache	dcache	dcache	dcache	dcache	dcache	dcache

- Scientific framework/workflow for IF experiments (art), leveraged for LAr experiments (LArSoft) as well as DAQ systems (artdaq)
- FIFE – an integration project for common data management, distribution, processing and analysis integration and operations
- Leveraging tools and expertise from CMS computing and OSG (job submission & workflow management tools)

SCD scientists

- **Science** – SCD scientists continue to excel on their scientific responsibilities and aim to be leading members of the Fermilab program and the community.
- **Service** – in addition to their individual technical responsibilities within the organization, scientists contribute by providing feedback on user requirements and communicating functionality of the services to users through their involvement to the lab's science program



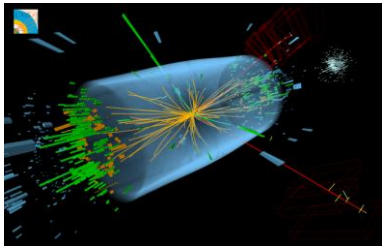
SCD scientists work together with computer science staff and computing professionals in all division activities, providing essential domain expertise and scientific judgment.

USCMS Tier-1 Facility
Resources to (re)process data and MC, custodial storage of RAW data and other samples on tape, local and remote access to samples on large disk pools

A very successful approach!

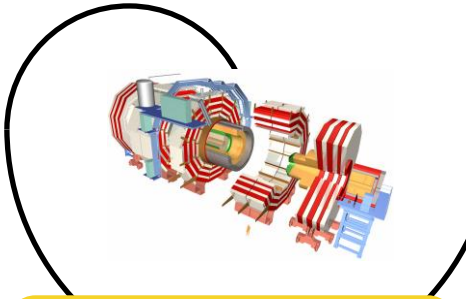
CMS Software Framework
Core framework for all CMS software applications from processing to analysis

Higgs!
SUSY?
DM?



Processing Infrastructure
MC production and Data/MC processing

Tier-0
Prompt reconstruction and calibration, express processing



Transfer system
Moving 1 PB per week between > 60 CMS sites

Data Acquisition (PPD)
Data quality and trigger and detector operation monitoring

Metadata Book keeping
Dataset Book keeping System to catalog all CMS data and MC

USCMS Analysis Facility
dedicated batch farm with access to all data at FNAL

Legend:

Lead by SCD

Lead by PPD

A very successful approach!

"Tier-0" Facility

Resources to (re)process data and MC, storage of samples on tape, local and remote access on large disk pools

artdaq and art frameworks

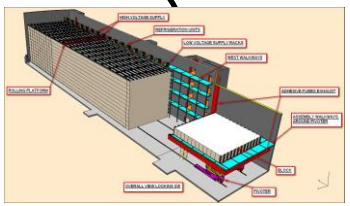
core frameworks for IF experiments. NOvA specific application for DAQ, triggering and offline

Processing Infrastructure

MC production and Data/MC processing

Buffering and data driven triggering

3200 core farm for asynchronous triggering and correlation with beam



Data Acquisition

Design, fabrication, firmware, software, commissioning

Data Catalog and archival

SAM, dCache and Enstore

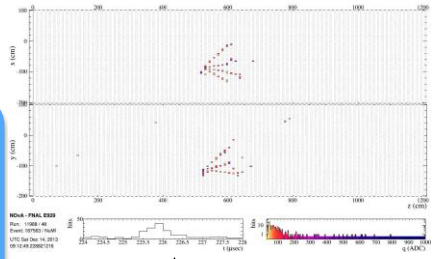
Data transfer

Fermilab File Transfer system, 10k physics files/day from Ash River to Fermilab

Analysis Facility

Fermigrid and OSG access through Fermilab batch tools

Neutrino oscillations with NOvA



Legend:

Lead by SCD

Scientific Computing funding

- Computing is essential to experiments through their entire life-cycle
  - Experiments require tools, facilities to run them and store the data, and consulting expertise
- Projects may pay for some development effort – but effort for services and expertise needed go well beyond
- With the exception of CMS, computing is not part of the project/experiment in a programmatic way
  - Operations funding has to track these needs for SCD to be able to deliver the necessary support to our program
- Our vision for SCD moving forward involves new services, utilization of new technologies, and partnership with other labs
  - For its success we need to transform the SCD workforce with strategic hires and execute a succession plan

Collaborations to meet Strategic and Tactical Goals

- Shared distributed Computing Facility LHC, IF and Multiple Disciplines – **(OSG)**
  - Labs: BNL, FNAL, PNNL, SLAC; Universities: U Wisconsin, UCSD, Nebraska, U Chicago, IU…
- Shared Analysis Code for LArTPC based Neutrino Experiments **(LArSoft)**
  - Labs: FNAL, BNL, SLAC, LBNL, LANL; Universities: Cambridge, MIT, Yale, Columbia…
- Accelerator Modeling across multi-scale accelerator technologies **(ComPASS**)
  - Labs: FNAL, ANL, LBNL, SLAC; Universities: UCLA, UTA; SBIR Company: Tech-X
- Worldwide HEP and other sciences modern detector simulation project **(Geant4)**
  - CERN, Japan + In US: ANL, FNAL, SLAC
- US Lattice QCD – BNL, JLab, FNAL
- Cosmology Worklows for Simulation and Experment (PDAC's)
  - In early stages of full development, ANL, BNL, Fermilab
- Enabling LHC on the Nation's High Performance Computers (HPC for CMS)
  - Labs: FNAL, LBNL(NERSC); Universities: Brown, Princeton, Nebraska

Working to extend partnerships with local universities (e.g. U of Chicago (some support for SNO+), U Wisconsin (some support for ICECUBE), Northern Il. U.)

Such collaborations - leveraging resources and expertise – are win-win and **an important part of our strategy**

Deliverables -summary

- High availability operations of Tier-1
  - LHC startup in March, 25 ns running in August; expect to receive data at ~2x rate of prior running
  - Upgrade computing infrastructure: disk and tape storage, worker nodes, networking
- High availability operations of IF compute farms and servers
  - Upgrade computing infrastructure
- Available, secure, high capacity disk and tape storage operations
  - Move to higher-density drives for some users; migrate some less dense media
- Support ROC-West commissioning and operations
- Operate LQCD HPC clusters at high efficiency, operate Accelerator modeling and Cosmology HPC clusters, and GPU and Intel Phi development clusters
- Enhance dynamic resource provisioning services for high availability
  - Commissioning / operation of GPCF2 for virtual resources
  - Commission virtual machine file system (OASIS distributed CVMFS repository)
- Provide a stable Linux computing platform, Scientific Linux (SL) and Scientific Linux Fermi (SLF), for Fermilab and its collaborators.

Deliverables -summary

- Continue software integration (FIFE) for the intensity frontier program, and enabling experiments to use OSG resources.
  - Migrate users still only utilizing Fermigrid
- Incorporate cloud resources in our facility operations
  - Better services and accessibility to the end users including negotiating sizable hours on Amazon.
- Increase responsibilities and continue to improve function of the production operations group.
  - Adding experiments (uBoone)
  - Improved services such as monitoring for end users and an automated request system for experiments.
- Finalize the effort from LHC shutdown to optimize resource utilization on grids, clouds, and leadership class facilities, to enable quick physics harvest of LHC collisions in 2015.

Deliverables -summary

- Continue support and development of the art (IF experiments) and CMSSW analysis frameworks
- Continue support and development of LArSoft
- Continue development and support of collaborative workflow projects for CF experiments (CosmoSIS and PDACS)
- Develop and commission build and release system needed for LArSoft and art users
- Continue support and development of Synergia, contribute to PIP and PIP-II with HPC accelerator simulations
- Advance physics models in Geant4 (muon and neutrino experiments) and Genie (neutrinos)
- Develop and commission validation suites for Geant and Genie and continue participation in development of the Pythia event generator.
- Increased coordination of post-docs and IF scientists for coherent contributions to neutrino and muon program analysis
  - First steps toward an “Analysis Center”

Deliverables -summary

- Continue support for DAQ engineering and software for CMS upgrades and NOvA
  - including FPGA, adoption of commodity components, optical links,…
- Provide second-level support for the uBooNE DAQ software applications, infrastructure, and system features in our areas of responsibility. Contribute to the commissioning of the DAQ system.
- Develop software and perform project management functions for Mu2e DAQ.
- Support 35 ton operations, provide software and system integration for full LBNF detector
- Continue development and support of the artdaq framework
- Operate the PREP pool effectively for the Fermilab program and NOvA electronics support into PREP processes.
- Provide expertise and support for real-time systems for operating FNAL experiment data acquisition and control systems.

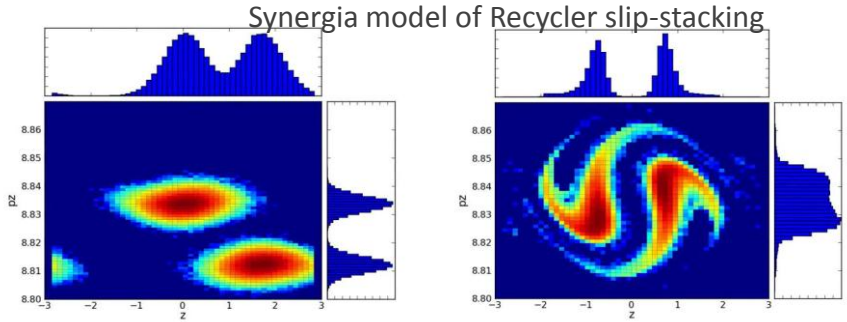
Risks, gaps

- Facility infrastructure: USCMS running significant amount of equipment past warranty; funding profile not smooth enough to replace promptly
- Facility services: in the medium term will have to rely more on dynamic resource provisioning, including non-owned Fermilab resources.
  - ongoing pressure to trade highest availability of facilities with more cost-effective and flexible operations approaches. Will need to develop operation and costing models for such approach
- Data Storage:
  - contamination issues on tapes at GCC not fully understood. Observed issues on ~0.1% of tapes, affecting ~0.1% of files on these tapes (10^{-6} error rate)
  - BlueArc (CCD managed), provides high performance storage, but at ~10x the cost for dCache. Need to examine options for BlueArc replacement at better cost.
- Overall effort sub-critical for most of our R&D and forward looking projects
  - Ability to keep necessary pace to provide tools and services required for LBNF and LHC upgrade era in jeopardy
- Path for evolving PREP not well defined
  - Existing recommendations too costly and difficult to implement

Risks, gaps

- Not able to execute succession plan significant risk in important areas
  - Accelerator Modeling: applied scientist II in phased retirement, scientist II (the speaker) with reduced participation
    - Mature tools and expertise very relevant to PIP and PIP-II
    - BTW, activity provides an excellent example of the success that small initial investment on new competencies could provide (and the benefits of leveraging collaborative efforts)
  - HPC facility (lattice QCD,…): principal system architect ramping down
    - A very successful facility that has enabled excellent scientific work in this domain
    - At the cross-roads of hardware architecture evolution

Synergia model of Recycler slip-stacking



Unfunded Needs and Strategies – how we aim to fill the gaps:

- **LDRDs:** R&D at Fermilab into software and computing are critical to allowing us to be successful in the rapidly changing computing environments and scaling experiment needs. Working to more successfully persuade our peers at the Lab of this for FY15!
- **DOE solicitations:** HEP and ASCR program officers continue to work together to co-fund R&D projects
- **Stimulate University NSF proposals:** e.g. Data Preservation Project (DASPOS) well regarded by multi-disciplinary offices in NSF; OSG co-funded by DOE and NSF; Proposals for advanced network middleware, use of new compute hardware etc.

Strategic Initiatives for the Future – currently unfunded

- **Internet of Things (IoT) DAQ**
  - DAQ based on off-the-shelf programmable hardware connected through ethernet IoT. The evolution of the Mu2e DAQ principle. (LDRD, did not make the cut last year)

- **Advances in Neutrino Physics Generators -**
  - Develop and support GENIE validation facility for the community.
  - Neutrino generator fidelity essential for the success of the neutrino program. A lot of model development and validation needed.
  - Develop infrastructure for collecting and cataloging cross-section data, tools to analyze, perform multi-parameter fits to optimize MC models. If successful, extend to Geant4

- **Big Data Systems**
  - Supports Lab Agenda item of Big Data Collaboration reaching beyond HEP community. (Will also try LDRD, for the facility)
  - Leverage key expertise in PetaByte-scale (soon Exabyte-scale) data management, storage and analysis in HEP to investigate, implement and support Big Data archiving, handling technologies.
  - Extend our storage systems to support others as a paid service.
  - Led by Deputy-CIO Jin Chang develop opportunities for collaboration on and funding of Cloud Event Monitoring and Archive System (CEMAS) to marry DAQ for IOT with Active Archive and high-performance Physics Analysis tools.

Smaller/Shorter term Strategic Initiatives ..

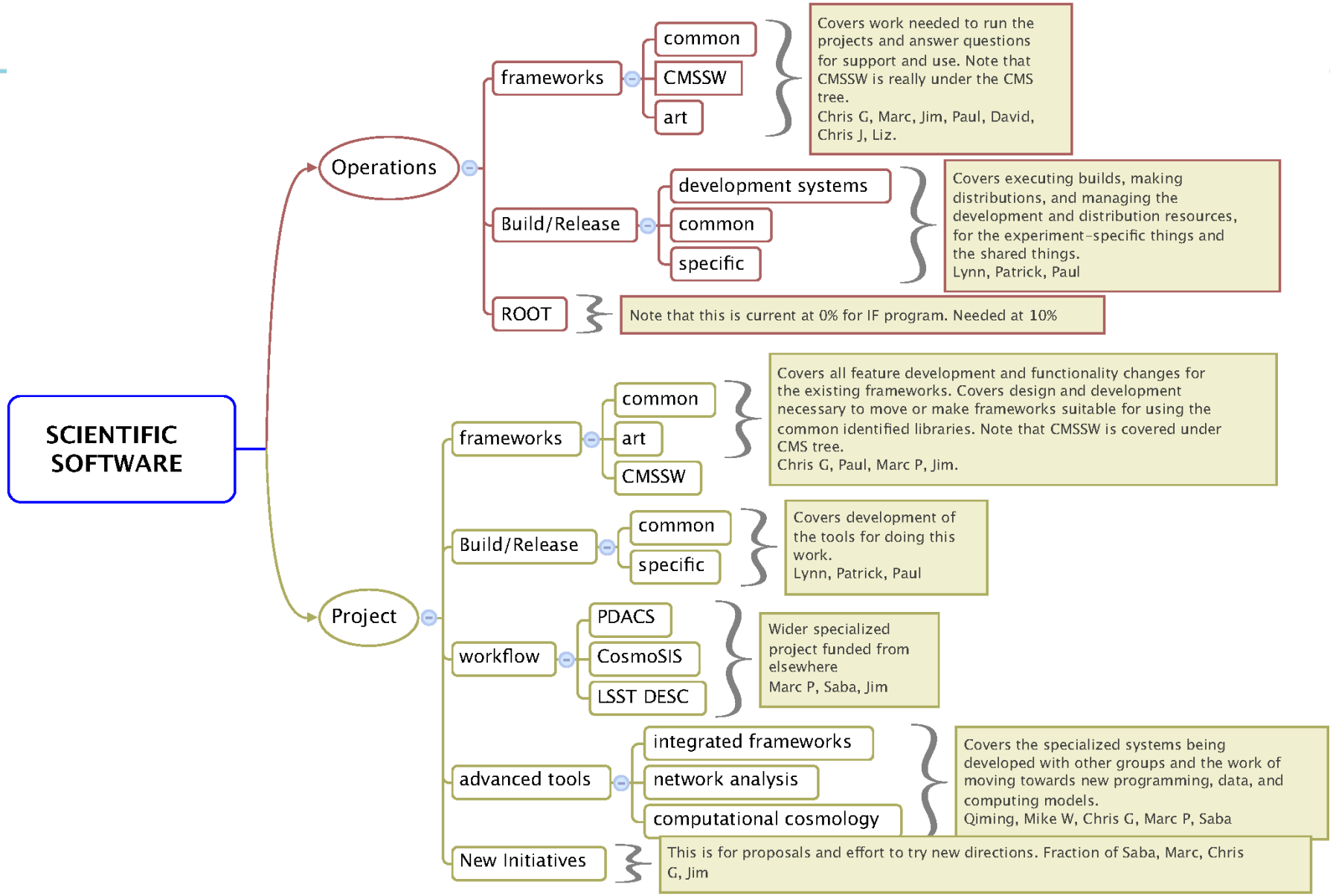
- ***More-Usable Security and Trust for the International Physics Community***
  US CMS and OSG have demonstrated our value here. Community of one voice that current challenges are significant. We have expertise in a small but crucial field.
  - *Opportunity to significantly improve the authentication/authorization experience for our end users.*
- ***Improving Operational Efficiencies***
  - *Developing current system administration and facility support tools into a robust, sustainable production service*
- ***Modernize and make Common Software Lifecycle Support Solutions***
  Nightly build and then validation services across common software suites (e.g. LArSoft, art, GENIE).
  - *Leverage expertise from US CMS, Run II etc.*
  - *If made generic, we could offer to experiments for their production code*

Summary

- SCD has a very successful program in providing services and enabling and contributing to the scientific program, which we are continuing and improving in FY15
- We have transitioned SCD to align better with the new FNAL (and US-HEP) priorities, and are continuing to work on improving all aspects of the organization
- To maintain essential competencies and evolve to meet future needs, we need to transform our workforce with strategic hiring and execute a succession plan.
- We are working on strategies to fill the gap, including exploring new funding sources and leveraging collaborations

Scientific Project Portfolio Management

- Programmatic SCD resource allocation based on global scientific needs (hardware and effort)
  - Process is Science driven – ask each experiment to present their goals for the coming two years – power point template given to help frame discussion
  - Well aligned with OCIO IT governance process
- External committee present to offer advice
- SCD puts together a spreadsheet of proposed allocations (M&S and FTE) based on presentations and iterations with committee
- Presents findings to experiments in case fine tuning needed
  - https://sharepoint.fnal.gov/project/sppm/SitePages/Home.aspx


SCIENTIFIC SOFTWARE
Operations
frameworks
common
CMSSW
art
Covers work needed to run the projects and answer questions for support and use. Note that CMSSW is really under the CMS tree.
Chris G, Marc, Jim, Paul, David, Chris J, Liz.
Build/Release
development systems
common
specific
Covers executing builds, making distributions, and managing the development and distribution resources, for the experiment-specific things and the shared things.
Lynn, Patrick, Paul
ROOT
Note that this is current at 0% for IF program. Needed at 10%
Project
frameworks
common
art
CMSSW
Covers all feature development and functionality changes for the existing frameworks. Covers design and development necessary to move or make frameworks suitable for using the common identified libraries. Note that CMSSW is covered under CMS tree.
Chris G, Paul, Marc P, Jim.
Build/Release
common
specific
Covers development of the tools for doing this work.
Lynn, Patrick, Paul
workflow
PDACS
CosmoSIS
LSST DESC
Wider specialized project funded from elsewhere
Marc P, Saba, Jim
advanced tools
integrated frameworks
network analysis
computational cosmology
Covers the specialized systems being developed with other groups and the work of moving towards new programming, data, and computing models.
Qiming, Mike W, Chris G, Marc P, Saba
New Initiatives
This is for proposals and effort to try new directions. Fraction of Saba, Marc, Chris G, Jim