MEMORANDUM

DATE: June 20, 2017

SUBJECT: **LIGO white paper for the NSF Large Facilities Cyberinfrastructure Workshop**

- *A brief description of the facility, its science mission, and the community (including size, make up – number of individual, number of institutions, etc.). Please include a URL for more information.*

The Laser Interferometer Gravitational-wave Observatory (LIGO) comprises a distributed NSF facility with two 4 km x 4 km interferometers, separated by a baseline for 3,002 km, located on the DOE Hanford Nuclear Reservation north of Richland, WA and north of Livingston, LA. LIGO Laboratory is operated jointly by the California Institute of Technology and the Massachusetts Institute of Technology for the NSF under a cooperative agreement with Caltech and MIT as a sub-awardee. LIGO also includes major research facilities on the Caltech and MIT campuses.

The two gravitational wave detectors are operated in coincidence. LIGO detected gravitational waves from the inspiral and merger of a binary black hole system on 14 September 2015, heralding the opening of a new observational window on the Universe using gravitational waves to detect and study the most violent events in the cosmos.

LIGO serves the worldwide gravitational wave community through the LIGO Scientific Collaboration, consisting of over 40 institutions in 15 countries. This international collaboration comprises about 1,100 members. LIGO also has MOUs covering joint operations with the EU Virgo Collaboration and the Japanese KAGRA Collaboration.

More information about LIGO may be obtained at the following URL: https://www.ligo.caltech.edu

- *A description of the key products/services of the facility (data, software, services, etc.)?*

The key data product generated by LIGO is a time series recording relative changes in length between the two 4km arms of each LIGO interferometer. These strain measurements (~3 TByte/y) record audio-frequency perturbations in the local space-time metric at each Observatory at the level of 1 part in 10^{22}. This is the primary observable from the LIGO experiment, recording the signature of gravitational waves

passing through each detector. To inform data analysis efforts searching the strain data for gravitational waves, and to understand and improve the performance of the LIGO instruments, an additional ~200k channels of environmental monitors and internal instrument channels are recorded (1.5 PByte/y). The strain data are distributed in low-latency (seconds) to computing clusters running analysis pipelines to generate gravitational-wave triggers for external Astronomical observations for transient events on a timescale of 1 minute. The bulk data are locally archived at each LIGO Observatory and distributed over the Internet to a central data archive on a timescale of 30 minutes. The central data archive currently holds 7 PByte of LIGO observations in perpetuity.

LIGO data analysis software is released using native Linux packaging (.rpm and .deb) and pre-installed on dedicated computing resources via standard Linux software repositories. For computing on shared resources the software is distributed via the CERN Virtual Machine Filesystem (CVMFS) and containerized with Docker, Singularity, or Shifter. Similarly, the key science data are pre-staged on dedicated computing resources ahead of analysis, and distributed to shared computing resources via CVMFS or GridFTP as needed by computing tasks. Metadata that describe LIGO observations and candidate signals from data analysis are stored in databases with custom tools for ingestion and querying.

- ***A brief description (including a figure) of the facility CI (e.g., its architecture, key services/components, underlying infrastructure), how it is deployed/distributed, and its operation. What is the median age since deployment of the key CI components.***
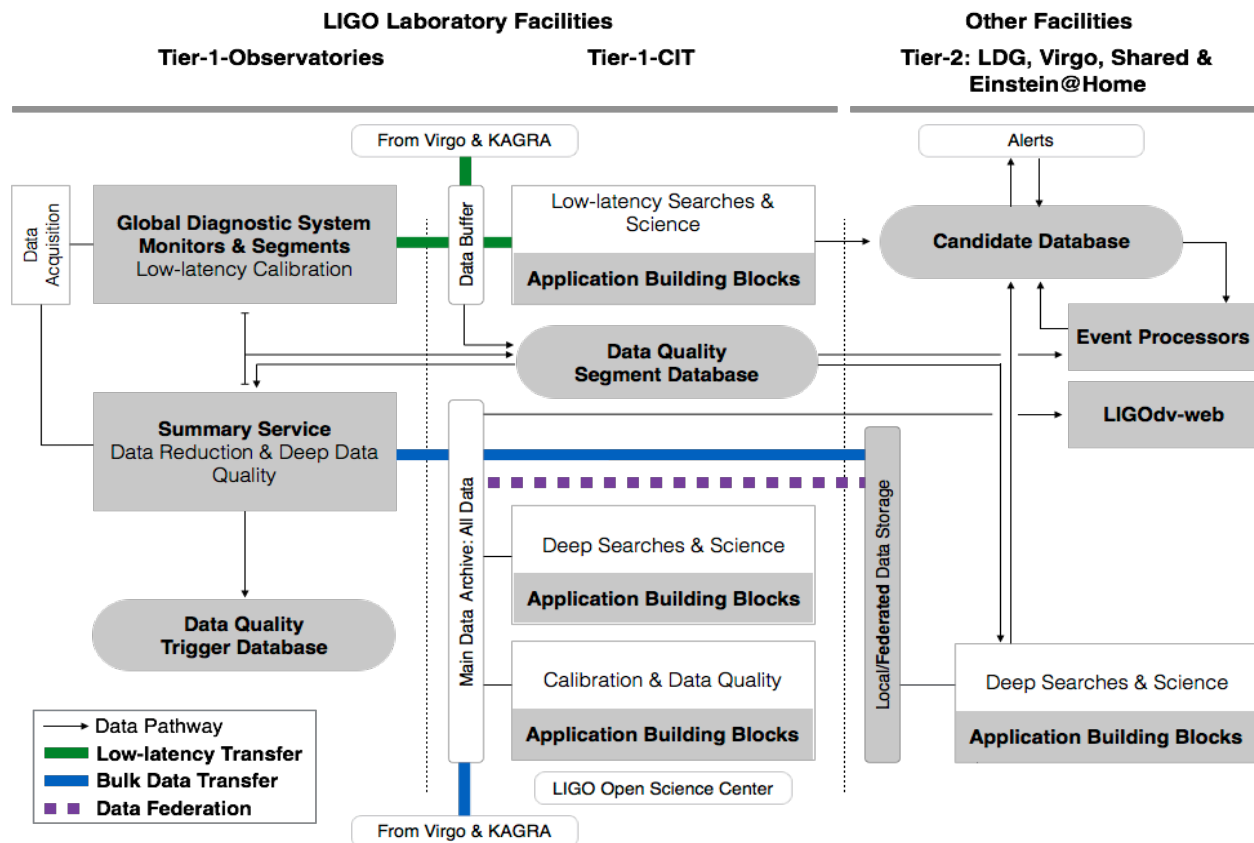
LIGO data analysis computing overwhelmingly consists of embarrassingly parallel workflows executed on high-throughput (HTC) resources. The majority of LIGO computing is provided by internal LIGO Scientific Collaboration (LSC)-managed clusters, but a growing fraction is provided by external shared resources. These resources are integrated into LIGO's computing environment via the Open Science Grid, and consist of a variety of dedicated and opportunistic campus, regional, and national clusters, Virgo scientific collaboration resources, and XSEDE allocations.

LIGO relies on HTCondor for its internal job scheduling, and uses both DAGMan and the Pegasus WMS for large-scale workflow management on top of HTCondor. In addition, LIGO uses the BOINC infrastructure to manage its single largest data analysis task (the search for continuous wave signals) via Einstein@Home running on volunteer computers as a screen saver. For Single Sign-On and other Identity

and Access Management functions, LIGO relies on Shibboleth, Grouper, InCommon, and CILogon. The underlying authentication infrastructure is built on Kerberos and authorization information if reflected in LDAP.

For distributed data management, LIGO relies on CVMFS, StashCache/Xrootd, Globus GridFTP, and a variety of in-house CI tools and services to complement and integrate these tools.

Unidata (http://www.unidata.ucar.edu) is a community data facility for the atmospheric and related sciences, established in 1984 by U.S. universities with sponsorship from the National Science Foundation (NSF). The Unidata Program Center (UPC), the program office for Unidata and the nexus of activities related to Unidata's mission, is managed by the University Corporation for Atmospheric Research (UCAR), a consortium of over 109 member universities and academic affiliates providing science in service to society.

Unidata exists to engage and serve researchers and educators dedicated to advancing the frontiers of Earth System science. The program's aim is to help transform the conduct of research and education in atmospheric and related sciences by providing well-integrated, end-to-end data services and tools that address many aspects of the scientific data lifecycle, from locating and retrieving useful data, through the process of analyzing and visualizing data either locally or remotely, to curating and sharing the results.

Specifically, the UPC:
- Acquires, distributes, and provides remote access to real-time meteorological data.
- Develops software for accessing, managing, analyzing, visualizing, and effectively using geoscience data.
- Provides comprehensive training and support to users of its products and services.
- In partnership with others, facilitates the advancement of tools, standards and conventions.
- Provides leadership in cyberinfrastructure and fosters adoption of new tools and techniques.
- Assesses and responds to community needs, fostering community interaction and engagement to promote sharing of data, tools, and ideas.
- Advocates on behalf of the community on data matters, negotiating data and software agreements.
- Grants equipment awards to universities to enable and enhance participation in Unidata.

Unidata is governed by its community. Representatives from universities populate standing and *ad hoc* committees that set policies for the program, provide first-hand feedback from users of program software and services, and offer guidance on individual projects

While Unidata's primary mission of serving universities engaged in atmospheric science education and research has remained unchanged through the years, the evolution and broad usefulness of its products and services have greatly enlarged its initial user base. Today, the Unidata community includes users from all sectors in over 200 countries, including nearly 2500 academic institutions and more than 80 research labs. Simultaneously, Unidata's activities and responsibilities have also grown as community needs have evolved. Despite the growth in users and enhanced scope of its activities, according to a 2010 survey conducted by the Unidata Users Committee, 97% of the respondents indicated that they were either satisfied or highly satisfied with Unidata's overall service to the community.

In the following sections we highlight some key quantitative and qualitative metrics that are used to gauge Unidata's success. These indicators offer a peek at Unidata's impact and how its cyberinfrastructure plays an irreplaceable role in advancing research, education, and outreach goals of its community. It should be noted that the UPC provides many of these metrics to its governing committees as part of its regular status reports.

Data services

Delivery of geoscience data to universities in near real time via the IDD system is at the core of Unidata's mission and is extremely

Table 1: Growth of IDD data volume	2008	2013	2016
Volume of data pushed to IDD sites	2.7 TB/day	13 TB/day	18.8 TB/day

important to our university community. Table 1 gives an idea of the explosive growth in the volume of data delivered via the IDD over the past decade.

While the IDD uses a "push" mechanism to deliver data automatically as it becomes available, Unidata's remote data access mechanisms (including THREDDS Data Servers, ADDE servers, RAMADDA servers, and EDEX servers) also provide roughly **670 GB/day** to community members.

Software and support

Unidata community members rely on the UPC to provide access to a variety of software packages for data transport, management, analysis, and visualization. Table 2 shows how many community members have downloaded the software packages that the UPC develops and supports over the past five years.

In addition to providing the software for download, UPC developers also provide the community with direct technical support via electronic mail. The support system is heavily used, with **more than 21000 support queries handled by UPC staff in the past five years**.

Table 2: Software Package Downloads	2012-2016
AWIPS	7700
GEMPAK	8400
IDV	43600
LDM	10100
McIDAS	300
netCDF-C Libraries*	566800
netCDF-Java Libraries (Common Data Model)	41900
TDS	9000
UDUNITS	22700

Appendix: A description of the key products/services

Data Distribution

The UPC coordinates the Internet Data Distribution system (IDD), in which hundreds of universities cooperate to disseminate near real-time earth observations via the Internet. While the "push" data services provided by the IDD system are the backbone of Unidata's data distribution services, the UPC also provides on-demand "pull" data services via THREDDS, ADDE, and RAMADDA data servers.

The UPC's data servers are not classified as "operational" resources, but they nonetheless have a 99.96% uptime record and are used heavily by educational sites that lack the resources to store IDD-provided data locally, or to operate their own data servers (see **Error! Reference source not found.**). UPC's servers are housed in a UCAR co-location computer facility for reliability, and share UCAR's Internet2/National Lambda Rail connectivity, which provides access to ample bandwidth for Unidata's needs.

Software

A variety of software packages are developed, maintained, and supported by the UPC:

NetCDF

Unidata's netCDF (network Common Data Form) is a freely distributed collection of data access libraries that provide a machine-independent data format that is self-describing, portable, scalable, appendable, sharable, and archivable – all important qualities for those who wish to create, access, and share array-oriented scientific data. NetCDF permits easy access to array-based, multi-dimensional datasets, a task that can be difficult when using other common storage schemes. NetCDF has been adopted widely by the atmospheric sciences community, and is especially popular among climate and ocean modelers. For example, model output datasets for the Sixth Assessment Report of the Intergovernmental Panel on Climate Change must be submitted in netCDF format, using the associated Climate and Forecast (CF) metadata conventions. The resulting large base of netCDF users and data has led to support for the format in more than 80 open source packages and many commercial applications including MATLAB and IDL.

Common Data Model & THREDDS Data Server

Unidata's Common Data Model (CDM) provides an interface for reading and writing files in netCDF and a variety of other scientific data formats. The CDM uses metadata to provide a high-level interface to geoscience-specific features of datasets, including geolocation and data subsetting in coordinate space. Unidata's THREDDS Data Server (TDS) builds on the CDM to allow for browsing and accessing collections of scientific data via electronic networks. Data published on a TDS are accessible through a variety of remote data access protocols including OPeNDAP, OGC Web Map Service (WMS) and Web Coverage Service (WCS), NetCDF Subset Service (NCSS), and HTTP.

Integrated Data Viewer

Unidata's Integrated Data Viewer (IDV) is a 3D geoscience visualization and analysis tool that gives users the ability to view and analyze a rich set of geoscience data in an integrated fashion. The IDV brings together the ability to display and analyze satellite imagery, gridded data (such as numerical weather prediction model output), surface observations (METARs), upper air soundings, NWS NEXRAD Level II and Level III RADAR data, NOAA National Profiler Network data, and GIS data, all within a unified interface. The IDV integrates tightly with common scientific data servers (including Unidata's TDS) to provide easy access to many real-time and archive datasets. It also provides collaborative features that enable users to easily share their own data holdings and analysis products with others.

AWIPS II & GEMPAK

AWIPS II is a weather forecasting, display, and analysis package currently being developed by the NWS and NCEP. Because many university meteorology programs are eager to use the same tools used by NWS

forecasters, Unidata community interest in AWIPS II is high. UPC staff have worked closely with NCEP staff during AWIPS II development in order to devise a way to make it available to the university community.

NCEP has stated that GEMPAK applications will be migrated from GEMPAK/NAWIPS into AWIPS II for the National Centers. The UPC will likewise facilitate a migration from GEMPAK/NAWIPS to AWIPS II for the university community.

Rosetta

The Rosetta project at the UPC is an effort to improve the quality and accessibility of observational data sets collected via datalogging equipment. The initial goal of Rosetta is to transform unstructured ASCII data files of the type commonly generated by datalogging equipment into the netCDF format, while minimizing disruption to existing scientific workflows.

Local Data Manager

The Unidata Local Data Manager (LDM) system includes network client and server programs designed for event-driven data distribution. It is the fundamental component of the IDD system. The LDM is used by hundreds of sites worldwide, and is integrated into the National Weather Service's AWIPS II package.

McIDAS

The Man-computer Interactive Data Access System (McIDAS) is a large, research-quality suite of applications used for decoding, analyzing, and displaying meteorological data. The older McIDAS-X system, developed by the University of Wisconsin's Space Science Engineering Center and supported by Unidata, is gradually being replaced by the IDV and by McIDAS-V (which is based on the IDV).

UDUNITS

Unidata's UDUNITS supports conversion of unit specifications between formatted and binary forms, arithmetic manipulation of units, and conversion of values between compatible scales of measurement.

RAMADDA

The Repository for Archiving, Managing and Accessing Diverse Data (RAMADDA) is a vibrant and growing technology initially developed by Unidata and now managed and developed as an open source project. Unidata integrates RAMADDA functionality into the IDV, provides training and support, and contributes code to the project. In addition, Unidata makes extensive use of RAMADDA to support community and collaborative projects, and actively facilitates its deployment in the university community.

2-Dimensional Crystal Consortium - Materials Innovation Platform (2DCC-MIP)

Facility Description:
2DCC Vision
Advance discovery-driven research into the growth, properties and applications of 2D chalcogenide crystals for next-generation electronics through the development of state-of-the-art synthesis and characterization tools within a multidisciplinary user environment to enable expansive national leadership in this important area.

2DCC Mission
1. Accelerate discovery in 2D chalcogenide materials by operating a world-class user facility that includes:
   a) a closed loop iterative collaboration of thin film and bulk growth synthesis techniques, *in situ* characterization, and predictive modeling of growth mechanisms and processes
   b) a community of practitioners that combines the expertise of an in-house research program and external users
   c) open sharing of knowledge, best practices, and publication-quality data
2. Provide access to synthesis, in-situ characterization and theory/simulation user facilities including instrumentation and expertise to users through a competitive proposal process
3. Maintain a vibrant in-house research program in synthesis, characterization and theory/simulation of 2D chalcogenides to drive advances in the field
4. Engage a diverse user base from academia, government and industry in the U.S. and internationally and increase participation of women and minorities underrepresented in science and technology through diverse representation in staffing and research activities.

Key products/services:
The 2DCC platform is defined by three major components: In-house research, user facility, and education/outreach in support of the research mission

Science Drivers (In-house research) -- The 2DCC research priorities are organized by four science drivers that are motivated by the unique properties of layered materials that often emerge in ultrathin or few-layer films, necessitating atomic-level control of film growth mode, stoichiometry, point defects and structural imperfections. The science drivers are: Physics of 2D Systems, Epitaxy of 2D Chalcogenides, Next-generation 2D Electronics, and Advanced Characterization and Modeling.

User Facility – The user program focuses on three main facility components:
(1) *Synthesis and In situ Characterization of Thin Films*
(2) *Bulk Crystal Growth*
(3) *Theory/Simulation*

The user program is focused on the synthesis of 2D chalcogenides for next generation electronics and includes priorities that are accomplished by a community of practitioners that collaborate among the in-house research and external user programs. Over time,

priorities will be adjusted by meritorious peer-reviewed proposals, user committee recommendations, and input from the 2DCC external advisory committee.

Education/Outreach – The 2DCC offers programs that address *engagement of a diverse user base* from academia, government and industry in the U.S. and internationally and *broadening participation* of women and minorities underrepresented in STEM. Education/Outreach programs include: 1) an education series that includes executive course, tutorials and hands-on training; 2) a monthly webinar series that is broadcasted live; 3) major sponsorship and participation in the annual Graphene and Beyond workshop; 4) a travel extension program for 2DCC faculty to visit PUIs and MSIs and present the work of the 2DCC and highlight opportunities for involvement; and 5) Opportunities for summer extended stays for users wishing to spend intensive time training at the facility.

Facility CI:
Theory efforts in the 2DCC-MIP aims at accurately modeling the growth of two-dimensional chalcogenides with multiscale methods and simulating a broad range of characterization techniques from first-principles, both in deep collaboration with 2DCC experimentalists. As a user facility focused on synthesis, the 2DCC does not have a dedicated CI; computational work is divided between two facilities, with the majority of the current workload managed by the Penn State Institute for CyberScience Advanced CyberInfrastructure (ICS-ACI), and future works supported by XSEDE research allocation on the Louisiana State University superMIC (420k CPU hours).

The physical infrastructure of ICS-ACI located in the Penn State University Park campus, where about 50% of the facility's power and equipment resources are dedicated to supporting the infrastructure. The ICS-ACI cluster consists of over 1200 nodes on Linux 6, with high-performance Ethernet or Infiniband interconnects. The queueing system supports interactive and batch jobs. In addition, a Guaranteed-Response Time (GReaT) model is offered, guaranteeing queue times of at most one hour to participating subscribers (2DCC users included). In the current phase the 2DCC theory team accesses 60 256-GB nodes and 10 TB shared storage under an allocation of 1000k CPU hours released on a quarterly basis, with expansion planned for the next phase. Software required by the 2DCC team are provided in the ICS-ACI cluster software stack, including highly parallel quantum chemistry and molecular dynamics codes, along with software libraries that allow for custom compilation. The median age of key CI components is less than 1 year.

DesignSafe – Cyberinfrastructure for NSF Natural Hazards Engineering Research Infrastructure
https://www.designsafe-ci.org/

Natural hazards engineering plays an important role in minimizing the effects of natural hazards on society through the design of resilient and sustainable infrastructure. The DesignSafe cyberinfrastructure has been developed to enable and facilitate transformative research in natural hazards engineering, which necessarily spans across multiple disciplines and can take advantage of advancements in computation, experimentation, and data analysis. DesignSafe allows researchers to more effectively share and find data using cloud services, perform numerical simulations using high performance computing, and integrate diverse datasets such that researchers can make discoveries that were previously unattainable. This white paper describes the design principles used in the cyberinfrastructure development process, introduces the main components of the DesignSafe cyberinfrastructure, and illustrates the architecture of the DesignSafe cyberinfrastructure.

A cyberinfrastructure is a comprehensive environment for experimental, theoretical, and computational engineering and science, providing a place not only to steward data from its creation through archive, but also a workspace in which to understand, analyze, collaborate and publish that data. Our vision is for DesignSafe to be an integral part of research and discovery, providing researchers access to cloud-based tools that support their work to analyze, visualize, and integrate diverse data types. DesignSafe builds on the core strengths of the previously developed NEEShub cyberinfrastructure for the earthquake engineering community, which includes a central data repository containing years of experimental data. DesignSafe preserves and provides access to the existing content from NEEShub and adds additional capabilities to build a comprehensive CI for engineering discovery and innovation across natural hazards. DesignSafe has been developed along the following principles:

Create a flexible CI that can grow and change. DesignSafe is extensible, with the ability to adapt to new analysis methods, new data types, and new workflows over time. The CI is built using a modular approach that allows integration of new community or user supplied tools and allows the CI to grow and change as the disciplines grow and change.
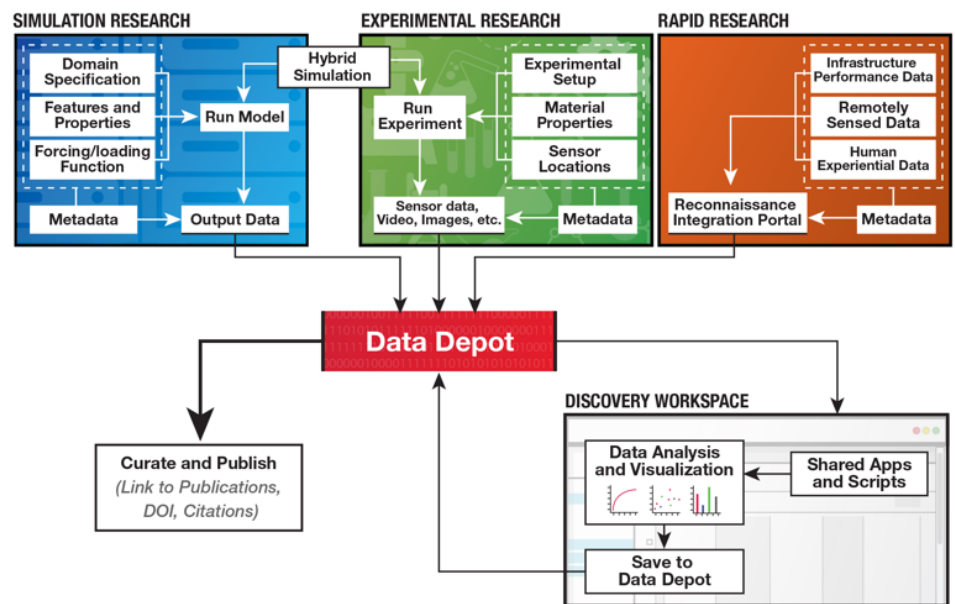
Provide support for the full data/research lifecycle. DesignSafe is not solely a repository for sharing experimental data, but is a comprehensive environment for experimental, simulation, and field data, from data creation to archive, with full support for cloud-based data analysis, collaboration, and curation in between. Additionally, it is the role of a cyberinfrastructure to continue to link curated data, data products, and workflows during the post-publication phase to allow for research reproducibility and future comparison and revision.

Provide an enhanced user interface. DesignSafe supplies a comprehensive range of user interfaces that provide a workspace for engineering discovery. Different interface views that serve audiences from beginning students to computational experts allow DesignSafe to move beyond being a "data portal" to become a true research environment.

Embrace simulation. Experimental data management is a critical need and vital function of the CI, but simulation also plays an essential role in modern engineering and must be supported. Through DesignSafe, existing simulation codes, as well as new codes developed by the community and SimCenter, are available to be invoked directly within the CI interface, with the resulting data products entered into the repository along with experimental and field data and accessible by the same analytics, visualization, and collaboration tools.

Provide a venue for internet-scale collaborative science. As both digital data captured from experiments and the resolution of simulations grow, the amount of data that must be stored, analyzed and manipulated by the modern engineer
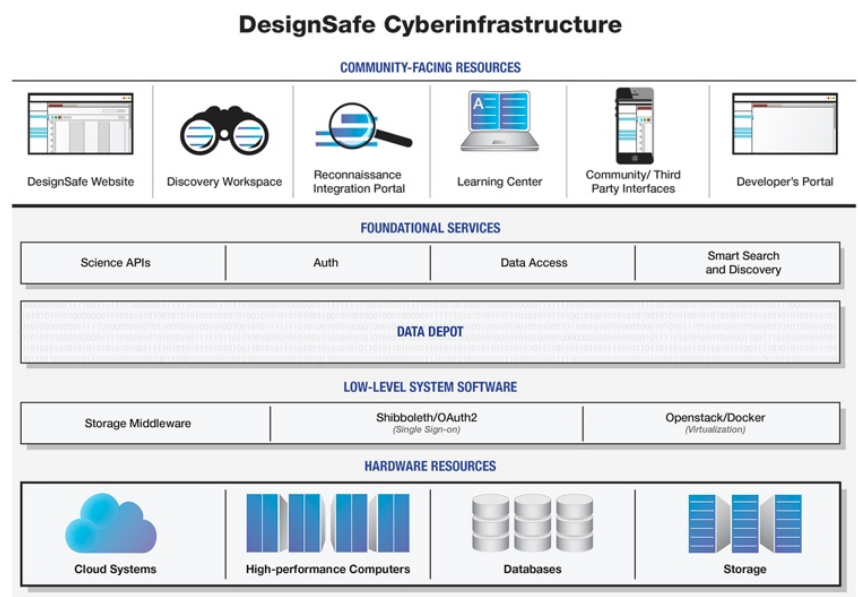
is rapidly scaling beyond the capabilities of desktop computers. DesignSafe embraces a cloud strategy for the big data generated in natural hazards engineering, with all data, simulation, and analysis taking place on the server-side resources of the CI, accessible and viewable from the desktop but without the limits of the desktop and costly, slow data transfers. **Develop skills for the cyber-enabled workforce in natural hazards engineering**. Computational skills are increasingly critical to the modern engineer, yet a degree in computer science should not be a prerequisite for using the CI. Different interfaces lower the barriers to HPC by exposing the CI's functionality to users of all skill levels, and best of breed technologies are used to deliver online learning throughout the CI to build computational skills in users as they encounter needs for deeper learning.

The DesignSafe infrastructure provides a comprehensive environment for experimental, theoretical, and computational engineering and science, providing a place not only to steward data from its creation through archive, but also the workspace in which to understand, analyze, collaborate and publish that data. The CI can be described in terms of the services it provides or in terms of the technical components that enable those services.

DesignSafe is architected to comprise the following services and components as shown in the figure:

- **DesignSafe** front end web portal

- The **Data Depot**, a multi-purpose data repository for experimental, simulation, and field data that uses a flexible data model applicable to diverse and large data sets and is accessible from other DesignSafe components. The Data Depot includes an intelligent search capability that allows dynamic creation of catalogs of the held data in an easily understandable way, and that can search ill-structured data with poor or incomplete metadata.

- A **Reconnaissance Integration Portal** that facilitates sharing of reconnaissance data within a geospatial framework.

- A web-based **Discovery Workspace** that represents a flexible, extensible environment for data access, analysis, and visualization.

- A **Learning Center** that provides training and online access to tutorials.

- A **Developer's Portal** that provides a venue for power users to extend the Discovery Workspace or Reconnaissance Integration Portal, and to develop their own applications to take advantage of the DesignSafe infrastructure's capabilities.

- A foundation of **storage and compute** systems at the Texas Advanced Computing Center (TACC), to provide both on-demand computing and access to scalable computing resources.

- A **middleware layer** to expose the capabilities of the CI to developers, and to enable construction of diverse web and mobile interfaces to data products and analysis capabilities

- A marketplace of **Community Defined Interfaces;** the extension capability of the CI allows other projects to leverage DesignSafe to build an interface of their own choosing.

The CI development was initiated in July 2015 upon receiving the NSF award, and was first deployed May 2016. As of June 2017 we have more than 1,100 registered users spanning dozens of institutions around the world.

Cyberinfrastructure at the National Nanotechnology Coordinated Infrastructure (NNCI) Site at Georgia Institute of Technology

The National Nanotechnology Coordinated Infrastructure (NNCI) is an NSF-funded program comprised of 16 sites, located in 17 states and involving 29 universities and other partners. This national network provides researchers from academia, government, and industry with access to university user facilities with leading edge fabrication and characterization tools, instrumentation and expertise within all disciplines of nanoscale science, engineering, and technology. Research undertaken within NNCI facilities is incredibly broad, with applications in electronics, materials, biomedicine, energy, geosciences, environmental sciences, consumer products, and many more. The toolsets of sites are designed to accommodate explorations that span the continuum from materials and processes through devices and systems. There are micro/nanofabrication tools, used in cleanroom environments, as well as extensive characterization capabilities to provide resources for both top-down and bottom-up approaches to nanoscale science and engineering. For more information about NNCI, please visit www.nnci.net. Georgia Tech serves as the coordinating office for the NNCI.

Modeling and simulation play a key role in enhancing nanoscale fabrication and characterization as they guide experimental research, reduce the required number of trial and error iterations, and enable more in-depth interpretations of the characterization results. Various NNCI sites provide a diverse set of software and hardware resources and capabilities. Some of these resources are only available to internal users and some to academic users and some to all interested parties. The rest of this white paper describes the rational behind a major cyberinfrastructure at Georgia Tech and its features and capabilities. This computing resource currently serves only students and faculty at Georgia Tech and is not available for external users.

Science and engineering research is the key to understanding everything in our universe and the best way we can improve the human condition. We are on the cusp of answering fundamental questions in the physical sciences, life sciences, social sciences, and mathematical and computational sciences. As our understanding deepens, we can leverage our basic fundamental knowledge to develop innovative and creative technologies that help drive solutions to the most pressing global problems all enabled by advances in cyberinfrastructure.

Investment in heterogeneous, sustainable, scalable, secure, and compliant cyberinfrastructure is critical to enable future discoveries. Significant resources are needed to address the storage, network bandwidth, and massive computational power required for simulation and modeling across multiple scales. Data-centric computing is also vital, necessitating high-throughput analysis and mining of massive datasets, as well as the ongoing demand for low cost, long-term, reliable storage. Sustained investment in cybersecurity will support sharing of datasets along with greater multi-institution and multi-disciplinary research collaboration. A significant investment in software engineering will enable researchers to leverage the promise offered by public-private, multi-cloud based cyberinfrastructure and emerging new architectures. Some of the greatest risks are an inability to meet workforce demand and the lack of a sustainable funding model. Addressing these issues includes maximizing the steady pipeline of students entering science and engineering careers; creating professional retooling programs; building specialized local and regional teams; and leveraging a range of investment sources including federal, state, municipal and local entities, as well as public-private partnerships (e.g. academic and industry, government and corporate).

Future breakthroughs are reliant on continued investment of national level resources in the path to exascale systems. That said, there are real limitations in an approach that primarily relies on "big iron" systems. More broadly, the perception is a general lack of resources to accommodate large simulations due to smaller jobs that require high-throughput computing. This problem is not likely to be addressed by reaching exascale capacity as there is essentially unbounded demand yet natural boundaries to scalability at many levels. Few researchers have access to funding to port code to new architecture introduced by these "big iron" systems. The national scale resources are also not well suited for small to medium-sized jobs and local institutional support is uneven and inconsistent.

Our existing cyberinfrastructure is also limiting for researchers who need more data-centric systems. Many modern computational tasks are "embarrassingly parallel" and have strong scalability, but available computer clusters and HPC systems are not designed or optimized for such HTC workloads. Examples include data analytics and deep learning workloads. We must develop new systems that can more efficiently support data intensive applications. There are promising technologies for this including modern memory hierarchies, GPUs, and other heterogeneous environments.

In 2009, Georgia Tech created a technology model for central hosting of computing resources that would be capable of supporting multiple science disciplines with shared resources, private resources, and a group of expert support personnel, in support of campus research community. This project is called "Partnership for an Advanced Computing Environment (PACE)." Since its inception, PACE has acquired more than 50,000 cores of high performance computing capability and more than 8 Petabytes of total storage used by approximately 3000 (1500 active) faculty and graduate students. This project provides power, cooling, and high-density racks, as well as a three tiered storage system including home directory, project space, and high transfer rate scratch space across the whole system. On top of storage, compute capabilities are provided both as private resources for a researcher or research group, or as a public resource with access open to researchers on campus through a proposal process for requesting compute cycles. PACE is funded through a mix of central and faculty funding that has proven sustainable is expected to continue with increased growth into the future (Figure 1). Due to this rapid growth, more hosting capability is being planned.
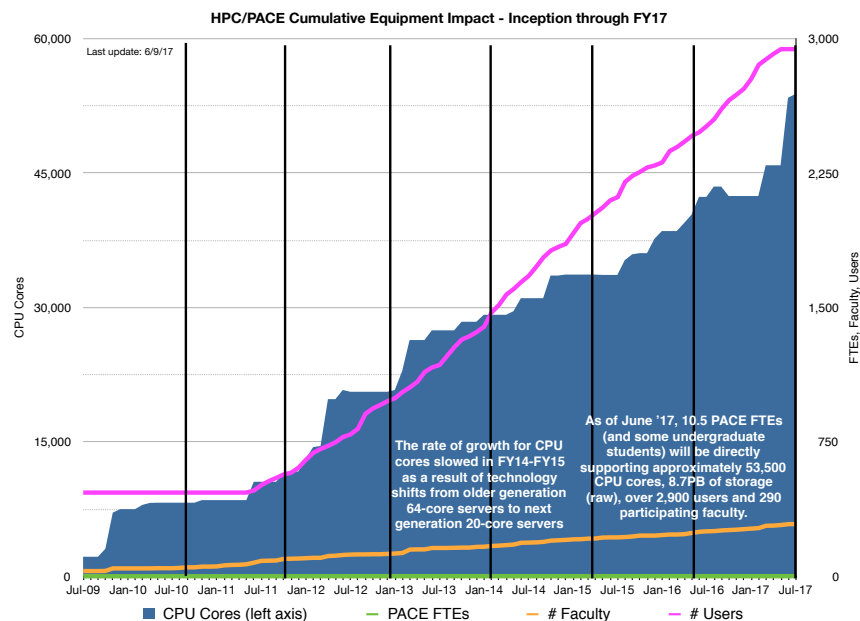

HPC/PACE Cumulative Equipment Impact - Inception through FY17

Last update: 6/9/17

The rate of growth for CPU cores slowed in FY14-FY15 as a result of technology shifts from older generation 64-core servers to next generation 20-core servers

As of June '17, 10.5 PACE FTEs (and some undergraduate students) will be directly supporting approximately 53,500 CPU cores, 8.7PB of storage (raw), over 2,900 users and 290 participating faculty.

CPU Cores (left axis) — PACE FTEs — # Faculty — # Users

Figure 1. Growth at PACE, represented in cumulative terms of CPU Cores in blue, users in pink, faculty in orange, and PACE full-time employees (FTEs) in green.

A significant investment in software engineering will enable researchers to leverage the promise offered by public-private, multi-cloud based cyberinfrastructure and emerging new architectures. Some of the greatest risks are an inability to meet workforce demand and the lack of a sustainable funding model. Addressing these issues includes maximizing the steady pipeline of students entering science and engineering careers; creating professional retooling programs; building specialized local and regional teams; and leveraging a range of investment sources including federal, state, municipal and local entities, as well as public-private partnerships (e.g. academic and industry, government and corporate).

NRAO Whitepaper Submission to the NSF Large Facilities Cyberinfrastructure Workshop

B.E. Glendenning, Assistant Director, NRAO Data Management and Software Department

1   NRAO TELESCOPES

The National Radio Astronomy Observatory (NRAO, https://public.nrao.edu/) operates the Karl G. Jansky Very Large Array (VLA) near Socorro New Mexico, and is the operating partner (Executive) for the North American part of the Atacama Large Millimeter/Submillimeter Array (ALMA), which operates at a high site near San Pedro, Chile.

Both telescopes are very general purpose. Telescope time is allocated based on a peer-review process from many sub-fields of astronomy. Hundreds of PI groups per year get data, and in addition once the proprietary period has expired (usually one year), the data may be used by other groups for Archival research.

Both telescopes are radio interferometers, which operate by coherently combining the signals of the relocatable antennas (27 for the VLA, 66 for ALMA) in complex central electronics (notably the correlators, which are approximately 0.1 Exa-Op very parallel special purpose supercomputers) which produces raw data, essentially a noisy (electronics, radio-frequency-interference, atmospheric and other environmental effects) irregularly sampled spatial Fourier transform of sky "stacked" over separate frequency channels for up to 4 polarizations.

The electronics are capable of sustaining 1 (VLA) and 16 (ALMA) Gigabytes per second of raw data output, although the data rates are usually averaged down (in time, and frequency) to a small fraction of that (typically 25 Megabytes/second for the VLA, and 6 MB/s for ALMA). This averaging is done both to reduce the computing that is needed, and because many times the science application do not need high data rates. However there are some classes of science observations that are not made because computing capacity is not available.

The raw data is turned into regularly gridded 2-4 dimensional images (axes: position on the sky, frequency or Doppler velocity, polarization) using multi-million line of code software systems produced by the NRAO and our partners. These images (currently: Giga-pixel, coming Tera-pixel, Possible: Peta-pixel) are then typically processed through analysis codes (both produced by NRAO and the wider community) to enable the science to be extracted from the data.

2   CURRENT NRAO COMPUTING PARADIGM

The raw science data from each telescope is buffered at the telescope site (to allow for network outages and periods of high data rate observing), from which it is transferred and ingested into the master archive (in Santiago in the case of ALMA, Socorro NM in the case of the VLA). In the case of ALMA the data is then replicated from the master archive to the "regional" archives, which for North America resides at Charlottesville Virginia. Through an archive search web interface the raw data may be

downloaded by operations staff and the PI group that proposed the observations (after QA in the case of ALMA). The raw data may be freely downloaded by anyone after the (typically) 1-year proprietary period has expired.

After the raw-data for the entire project has arrived in the archive (this could take several different observing sessions), "pipelines" are executed which automatically make derived data products, currently flagged and calibrated raw data for both telescopes, and reference images for the case of ALMA. After some QA is performed, these data products may be downloaded by the PI groups, or by anyone after the proprietary period has expired. NRAO has initiated a "Science Ready Data Products" (SRDP) project to improve the quality of the automatically generated data products, with a goals that: the images should be directly usable for science, to improve the user interfaces, and to allow a human to be in the loop to optimize via high-level guidance the derived data products to be well suited for use in answering particular science questions.

At the moment, almost all VLA derived data products, and many ALMA ones, which are used for the actual science analysis are produced through the manual (including ad-hoc Python scripting) execution of programs from suites of data processing, analysis, and visualization tasks produced by the NRAO. These programs are developed by the NRAO with significant contributions from our ALMA partners, and total about 3M SLOC. This software is available under an open source license, although the NRAO generates executables for common Linux variants and recent versions of MacOS.

The software is executed at a combination of NRAO and user facilities. Our software is downloaded several thousand times per year for use by users (laptops through small clusters). In addition the NRAO allows our users to use our in-house computing facilities through a reservation system. Although our resources are relatively modest (150 16-core compute nodes, 2 PB of fast Lustre filesystem with Inifiniband interconnects), they are well tuned to our software stack, have fast access to the raw data archives, and we allow them to be used interactively (we also have batch queues). That is, they are convenient to use and very suitable for modest problem sizes. Our computing resources are used by a few hundred PI groups per year.

We have experimented with commercial cloud providers (AWS) and national supercomputing centers (XSEDE), but have not made extensive use of either yet, nor have our users.

Key CI improvements areas we would identify are:

- In-the-cloud Elastic, Interoperable, Data Center accessibility
- Machine learning applications (vs. ad-hoc expert knowledge capture in scripts)
- Software sustainability infrastructure
- Visualization and information extraction from multi-peta-pixel multi-dimensional image data

We look forward for the opportunity to discuss these topics at the workshop.

CHESS Facility and Cyberinfrastructure Overview

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June 19, 2017

Abstract

We present an overview of the Cornell High Energy Synchrotron Source (CHESS), focusing on the facility and key cyberinfrastructure components.

1   CHESS Facility

The Cornell High Energy Synchrotron Source (CHESS) is a NSF-funded National User Facility located on the Cornell University campus in Ithaca, New York. The mission of CHESS is to provide a national hard x-ray synchrotron radiation facility for individual investigators, on a competitive, peer reviewed, proposal basis. With 11 experimental stations, the facility is used by approximately 1,100 investigators per year from over 150 academic, industrial, government, non-profit, and international institutions. CHESS impacts a wide range of disciplines, serving researchers from the physical, biological, engineering, and life sciences, as well as cultural specialists such as anthropologists and art historians. CHESS users conduct studies encompassing, but not limited to, the atomic and nanoscale structure, properties, operando, and time-resolved behavior of electronic, structural, polymeric and biological materials, protein and virus crystallography, environmental science, radiography of solids and fluids, and micro-elemental analysis, and other technologies for x-ray science.

The CHESS facility is hosted by the Cornell Laboratory for Accelerator-based Sciences and Education (CLASSE), which also operates the Cornell Electron Storage Ring (CESR) as the x-ray source for CHESS. Computing services for CHESS are provided centrally by the CLASSE-IT department. The primary computing services used by CHESS are:

- high-speed data acquisition for x-ray detectors at the CHESS experimental stations

- access to and long-term storage of x-ray data collected by CHESS users

- software libraries and parallel computation resources for CHESS staff and users.

More information about the CHESS facility may be found at http://www.chess.cornell.edu.

2   CHESS Cyberinfrastructure

The CLASSE cyberinfrastructure (CI) consists of an interconnected series of high-availability server clusters (HACs), data acquisition systems, control systems, compute farms, and workstations. Most of these systems run either Scientific Linux or Windows on commodity 64-bit Intel-based hardware and are centrally managed using Puppet. The median age of key CI components is approximately 5 years, with an average refresh rate of once every 10 years. The CLASSE CI components most relevant to CHESS are described below and are shown in Figure 1.

2.1   Central Infrastructure

The central Linux infrastructure cluster runs the core CLASSE infrastructure services, including name services, file systems, databases, and web services. Recently, a dedicated oVIrt cluster has been commissioned to run centrally-provisioned virtual machines. These clusters utilize shared 10Gb iSCSI storage domains, and they provide file systems and other basic services to the rest of the lab.
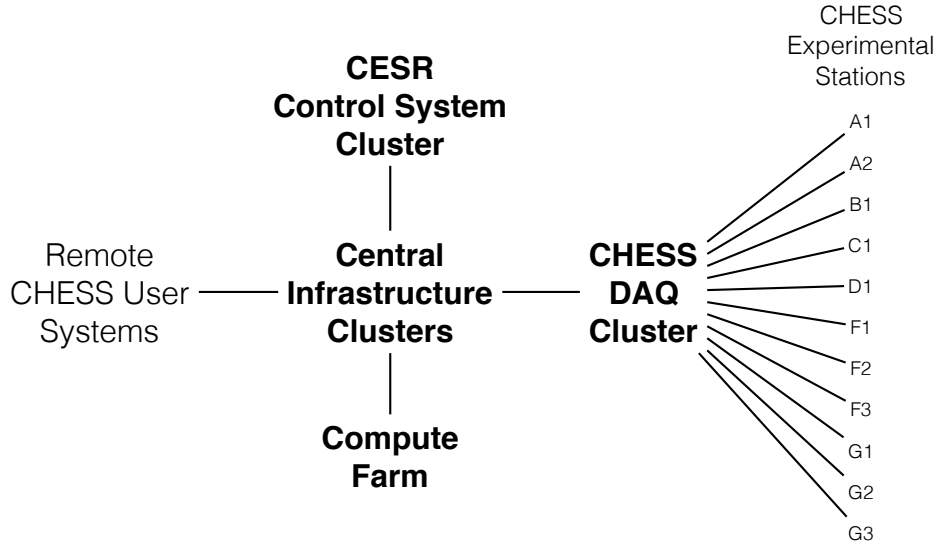
Figure 1: Main components of the CHESS cyberinfrastructure.

2.2 CHESS Data Acquisition (DAQ)

The CHESS data acquisition system runs on a dedicated HAC and provides 10Gb network connections to each experimental station. Data collected at the stations are written directly to the data acquisition system over either NFS or Samba, where it can then be processed on the CLASSE Compute Farm or end-user workstations. CHESS users can also download their data remotely using a Globus server endpoint or via SFTP.

2.3 Compute Farm

The CLASSE Compute Farm is a central resource consisting of approximately 60 enterprise-class Linux nodes (with around 400 cores) with a front-end queueing system that distributes jobs across the Compute Farm nodes. This queueing system supports interactive, batch, parallel, and GPU jobs, and it ensures equal access to the Compute Farm for all users.

2.4 CESR Control System

The CESR control system, responsible for running the particle accelerator that produces x-rays for CHESS, consists of a dedicated Linux HAC. Although the CESR, CLASSE, and CHESS DAQ clusters are essentially identical, the CESR cluster runs many more control system services and is able to operate independently from the CLASSE central infrastructure. This isolation ensures continuity of CESR operations in the event of a power failure or general network outage.

2.5 User Connectivity

Based on their requirements, CHESS users are either granted restricted "external" CLASSE accounts (providing access to station computers and remote access to data) or full CLASSE accounts (providing access to the CLASSE Compute Farm and full interactive desktops, both local and remote).

While collecting data at the experimental stations, CHESS users generally connect their instruments and experimental equipment to a private subnet that is selectively firewalled from the rest of the CLASSE infrastructure. If users require direct write access to the CHESS DAQ filesystems, they may use dedicated station and kiosk computers located at the experimental stations and in other restricted-access locations. Outside the experimental stations, CHESS user data is made available for read-only access through the CLASSE public network.

Research Vessels: Seagoing Datacenters

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Introduction

Scripps Institution of Oceanography (SIO) is a graduate school of UC San Diego and is a world leader in oceanographic field research. SIO supports the operation and/or scientific research of 3 research vessels, a research platform, and is in the primary role in a multi-institution partnership that works with the US Coast Guard to conduct arctic oceanographic research. SIO also manages a cost-saving satellite-based Internet project for research vessels at sea, serving the network-based needs of the majority of University-National Oceanographic Laboratory System (UNOLS) participants.

Key Products/Services

The Ship Operations & Marine Technical Support (SOMTS) department within SIO offers basic and specialized services.

Our most basic (and obvious) service is that of functional and fully equipped seagoing platforms for oceangoing research. These platforms range from a regional research vessel (R/V Robert Gordon Sproul), and Ocean Class research vessel (R/V Sally Ride -- America's newest research vessel) and a Global Class vessel (R/V Roger Revelle -- our flagship). We also support a specialized platform, R/P Flip, which is a platform designed to stably study ocean currents by inverting itself 90 degrees in the water. All platforms come equipped with instrumentation and information systems to acquire commonly useful information about the environment: from seawater temperature and salinity, ocean floor, ocean currents, wind and weather, etc. These systems often operate with other devices as a system of systems, providing cohesive information about a vessel's movement in order to better understand the environment around that vessel.

We also support a number of specialized projects: repeat hydrography, arctic research aboard the USCGC Healy (in partnership with other academic institutions and the US Coast Guard), and support a multi-dish satellite earth station through the HiSeasNet project which has provided affordable Internet to the UNOLS community for the better part of a decade.

Finally, we are in the process of exploring the data delivery mechanism(s) upon completion of scientific missions. At present, data is delivered via "sneakernet" to a data archive/curation project, but as Internet connectivity improves, standardized realtime delivery of data from oceanographic ships at sea should to. Further, modern instrumentation data needs are growing. Newer vessels are installing instruments that produce 100 times more data than other systems; a cohesive, modern data management plan is being sought for these standalone environments.

Deployment

We are in the process of upgrading SIO's mobile platforms to datacenter-grade computing to provide the redundancy, resiliency and the graceful degradation of equipment that only a no-single-point-of-failure system can provide. Despite redundancies, severe weather and rough seas can make off-ship communication difficult at times; as such a ship needs to be somewhat self-contained when communications go awry.

Working oceanographic equipment (along with the attached computing systems) tend to have a slow upgrade path. Many ships work the majority of the year; an idle ship is expensive. As such, equipment upgrades and maintenance have to be targeted to be as non-disruptive as possible. As such, we are constantly seeking opportunities to proactively deploy and maintain equipment. That said, some of the equipment on-hand does not have clear upgrade paths and it is not rare to find a 10+ year old computer system aboard a ship. Getting such systems to behave reliably can be a losing battle.

Internet connectivity at sea remains challenging to engineer consistently and keep ships online. After a decade of successes, HiSeasNet is looking to the future to re-equip all of UNOLS with modern, maintained satellite communications. Older installations in the fleet are showing signs of wear, and proactivity is needed to keep the fleet communicating well.

Summary

Oceanographic field research is fraught with challenges of being both self-sufficient where it matters, available via network in locations with little infrastructure. SIO is looking to meet these challenges with 21st century solutions, and help lead the charge to produce excellent data from its seagoing research that will be useful and have impact for many years.

National Science Foundation Ocean Observatories Initiative (OOI) Cyberinfrastructure White Paper

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INTRODUCTION

The NSF Ocean Observatories Initiative (OOI) is a networked ocean research observatory with arrays of instrumented water column moorings and buoys, profilers, gliders and autonomous underwater vehicles within different open ocean and coastal regions. OOI infrastructure also includes a cabled array of instrumented seafloor platforms and water column moorings on the Juan de Fuca tectonic plate. This networked system of instruments, moored and mobile platforms, and arrays will provide ocean scientists, educators and the public the means to collect sustained, time-series data sets that will enable examination of complex, interlinked physical, chemical, biological, and geological processes operating throughout the coastal regions and open ocean.

The seven arrays built and deployed during construction support the core set of OOI multidisciplinary scientific instruments that are integrated into a networked software system that will process, distribute, and store all acquired data. The OOI has been built with an expectation of operation for 25 years. This unprecedented and diverse data flow is coming from 89 platforms carrying over 830 instruments which provide over 100,000 scientific and engineering data products.

The OOI is funded by the National Science Foundation and is managed and coordinated by the OOI Program Office at the Consortium for Ocean Leadership (COL). Implementing organizations, subcontractors to COL, are responsible for construction and development of the different components of the program. Woods Hole Oceanographic Institution (WHOI) is responsible for the Coastal Pioneer Array and the four Global Arrays, including all associated vehicles. Oregon State University (OSU) is responsible for the Coastal Endurance Array. The University of Washington (UW) is responsible for cabled seafloor systems and moorings. Rutgers, The State University of New Jersey, is implementing the Cyberinfrastructure (CI) component. The OOI data evaluation and education and public engagement team is co-located with the Cyberinfrastructure group at Rutgers University.

OOI CYBER-INFRASTRUCTURE SERVICES

The primary functions of the OOI CI are data acquisition/collection, storage, processing and delivery. The overall architecture of the OOI CI network is shown in Figure 1.

(a) Data Collection and Transmission to the OOI CI: Data is gathered by both cabled and un-cabled (wireless) instruments located across multiple research stations in the Pacific and Atlantic oceans. Once acquired, the raw data (consisting mostly of tables of raw instrument values – counts, volts, etc.) are transmitted to one of three operations centers: Pacific City, directly connected via fiber optic cable to all cabled instruments in the Cabled Array; OSU, an Operational Management Center (OMC) responsible for all un-cabled instrument data on the Pacific coast; and WHOI, the OMC for Atlantic coast-based un-cabled instrument data. The data from the operations centers is transferred to the OOI CI for processing, storage and dissemination.

(b) Data Management, Storage, and Processing: Two primary CI centers operated by the Rutgers Discovery Informatics Institute (RDI²) are dedicated to OOI data management: the West Coast CI in Portland, OR, and the East Coast CI, at Rutgers University. While data from the Cabled Array components are initially received at the Shore Station in Washington, it is the East Coast CI that houses the primary computing servers, data storage and backup, and front-facing CI portal access point, all of which are then mirrored to the West Coast CI over a high-bandwidth Internet2 network link provisioned by MAGPI (Mid-Atlantic GigaPOP in Philadelphia) on the east coast and PNWGP (Pacific-Northwest GigaPOP) on the west coast. The data stores at the OMCs at OSU and WHOI are continuously synchronized with the data repositories located at the East and West Coast CI sites.

(c) Data Safety & Integrity: Data safety and protection is ensured in two ways: data security and data integrity. Data security is addressed through the use of a robust and resilient network architecture that employs redundant, highly available next-generation firewalls along with secure virtual private networks. Data integrity is managed through a robust and resilient information life-cycle management architecture.
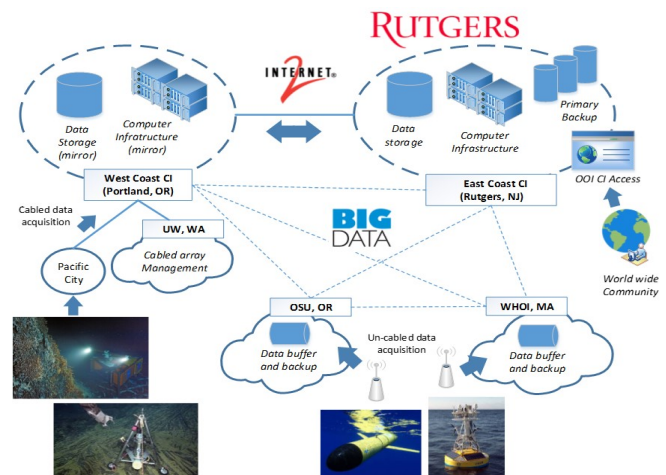

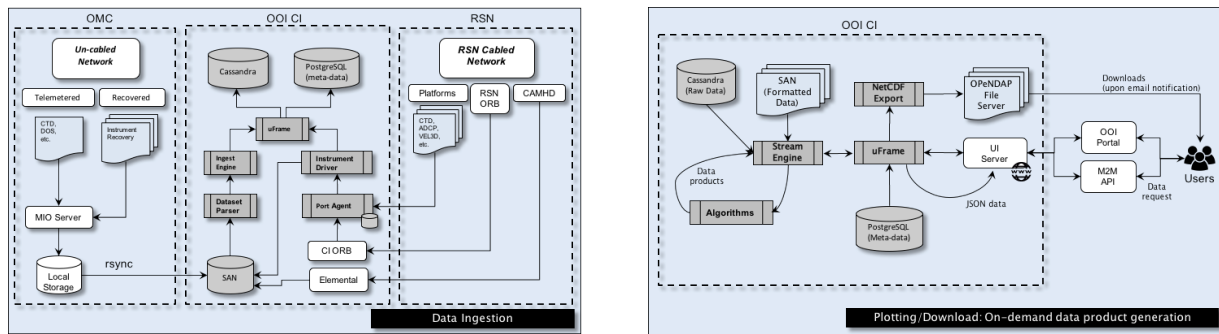*Fig. 1. OOI CI Network Architecture*

Fig. 2. UFrame-based OOINet software data workflow (left: data ingestion, right: data plotting/download)

(d) Public Data Access: The OOI CI software ecosystem (OOINet) employs the uFrame software framework that processes the raw data and presents it in visually meaningful and comprehensible ways in response to user queries, which is accessible over the Internet through the CI web-based portal access point. A machine-to-machine (M2M) API provides programmatic access to OOINet through a RESTful API. In addition to the portal and API, OOI CI provides the following data delivery methods: (1) *THREDDS Data Server*: delivers data products requested through the CI portal (i.e., generated asynchronously); (2) *Raw Data Archive*: delivers data as they are received directly from the instrument, in instrument-specific format, and (3) *Alfresco Server*: provide cruise data, including shipboard observations. OOI CI software ecosystem permits 24/7 connectivity to bring sustained ocean observing data to a user any time, any place. Anyone with an Internet connection can create an account or use CILogon and access OOI data.

DESING AND IMPLEMENTATION ISSUES

The OOI CI design and implementation principles are based on industry best practises for the different aspects of the CI. The approach is based on a decentralized but coordinated architecture, which is driven by requirements, e.g., data storage capabilities, system load, security, etc.

(a) Redundancy and resiliency: The OOI CI is a mirrored infrastructure for high availability, disaster recovery and business continuity. It implements a resilient information life-cycle management architecture that integrates redundant enterprise storage area network (disk-based) and a robotic library (tape-based). Redundancy is implemented at different layers, for example, an enterprise-level storage network of multiple hard drives managed by an intelligent device manager, reduces the data footprint by reducing data duplication while maintaining data integrity and access performance through storage redundancy, and tape storage, a "last tier" storage that is not dependent on power or cooling, supports longer-term backup and archiving, disaster recovery, and data transport.

(c) Service-oriented Architecture: The core of the OOI CI software ecosystem (Uframe-based OOINet, see Figure 2) is based on a service oriented architecture, a set of data dataset, instrument, platform drivers and data product algorithms, which plug in to the uFrame framework. Uframe-based OOINet uses latest generation technologies for big management data such as Apache Cassandra,

which is a state-of-the-art, scalable and highly available distributed database management system designed to handle large amounts of data. Uframe-based OOINet services are exposed through a RESTful API and are available as the M2M interface for external access through a secure endpoint. The use of a well-defined API based on standard protocols enables other systems to interface and interact with OOI CI programmatically.

(c) Cyber-security: The system is based on a multi-tier security approach with dedicated and redundant (highly available) appliances at the CI perimeter. The OOI CI implementation supports encryption of traffic, network traffic segregation, multi-layer traffic filtering, multi-layer access control and comprehensive monitoring. Further, data delivery to external users is implemented through dedicated and distinct storage appliances (i.e., physical and logical isolation from core storage infrastructure) In addition to implementing industry best practices, the OOI CI cyber-security effort includes a comprehensive cyber-security program based on engagement with the NSF Center for Trustworthy Scientific Cyber-Infrastructure. This program encompasses a set of policies and procedures. Regular vulnerability scans/audits (internally and externally) are also performed to the OOI CI.

CONCLUSION

OOI CI has initiated its operational phase and data (including science, engineering and data products) flowing from those instruments is freely available to users. The OOI CI portal provides all data, metadata and data processed via conventional algorithms or direct retrieval from OOI storage or data archives. Data quality and data management will utilize generally accepted protocols, factory calibrations and at sea calibration procedures.

During its early operation (1.5 years), OOI community has been growing every day and is made up of a diverse set of users from 180 different organizations from around the world. At least 500 people has already registered on the OOI Data Portal, which has over 3,000 unique visitors each month[1].

The NSF Cybersecurity Center of Excellence: Large Facilities Services

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June 19, 2017

Overview of the NSF CCoE

The genesis of the NSF Cybersecurity Center of Excellence (trustedci.org) is with a series of two workshops, the Scientific Software Security Innovation Institute (S3I2) workshops. The S3I2 workshops, held in 2010 [1] and 2011 [2], included representatives of 35 major NSF-funded projects. The original goal of the workshops was to explore a software institute focused on IT security for the NSF community. What the workshops found is that the NSF community faces strong challenges in obtaining access to IT security expertise. Projects are forced to divert their resources to develop that expertise, address risks haphazardly, unknowingly reinvent basic cybersecurity solutions, and struggle with interoperability. The workshops further determined the need for access to expertise was more critical than any new software product.

In 2012, based on these workshop findings, the NSF funded the Center for Trustworthy Scientific Cyberinfrastructure (CTSC) to provide security expertise to the NSF community. Building on the success of CTSC, the NSF Cybersecurity Center of Excellence (CCoE) was funded in 2016 as an expansion of the CTSC. The CCoE draws is a collaboration of four internationally recognized institutions: Indiana University, the University of Illinois, the University of Wisconsin-Madison, and the Pittsburgh Supercomputing Center.

CCoE Services in support of Large Facilities

Science projects manage a number of risks to their scientific missions including risks typically managed by cybersecurity, i.e. malicious entities who attack IT infrastructure to further their own ends at the expense of legitimate users or to explicitly harm those users. To be effective cybersecurity must be tailored for the science community, taking the community's risks, tolerances, and technologies into account. The CCoE's mission is to provide the NSF Large Facility community expertise in cybersecurity for science This mission is accomplished through one-on-one engagements with projects to address their specific challenges; education, outreach, and training to raise the state of security practice across the scientific enterprise; and leadership in advancing the overall state of knowledge on cybersecurity for science through applied research and community building. Examples of these mechanisms follow. Details can be found on trustedci.org.

One-on-one engagements:

- DKIST: DKIST and the CCoE collaborated to develop a cybersecurity planning guide for DKIST that addresses these terms and conditions, aligns with existing institutional

policies, and can be implemented within DKIST's budgetary limitations. This guide was made generally available for other NSF large facilities and projects [3].

- LIGO: The CCoE, LIGO and the Open Science Grid collaborated to establish an international identity federation in support of LIGO's scientific mission.
- Icecube, LSST, NEON: The CCoE helped with the development, assessment, and improvement of operational cybersecurity programs.
- Globus, Pegasus, OSG: The CCoE provided software security consulting and assurance evaluation to helping the NSF community develop more secure software and assess software they are using (or considering using).

Education, outreach and training:

- Situational awareness: The CCoE provides situational awareness of the current cyber threats to the research and education environment, including those that impact scientific instruments, by providing timely email notifications about relevant software vulnerabilities.
- Webinars: The CCoE offers a monthly webinar series to allow NSF projects to share findings and experiences with each other.
- Training: The CCoE regularly provides training, tailored to the science community, on a number on a number of topics, including log analysis, incident response, federated identity management, and developing a cybersecurity program.

Advancing the state of knowledge through applied research and community building:

- Large Facility Security Working Group: to develop a working relationship between those responsible for cybersecurity across the LFs and to advance the development and implementation of best practices, standards and requirements within the community.
- NSF Cybersecurity Summit for Large Facilities and Cyberinfrastructure:The CCoE organizes this annual event to bring together leaders in NSF cyberinfrastructure and cybersecurity to build a trusting, collaborative community, and to address that community's core cybersecurity challenges.

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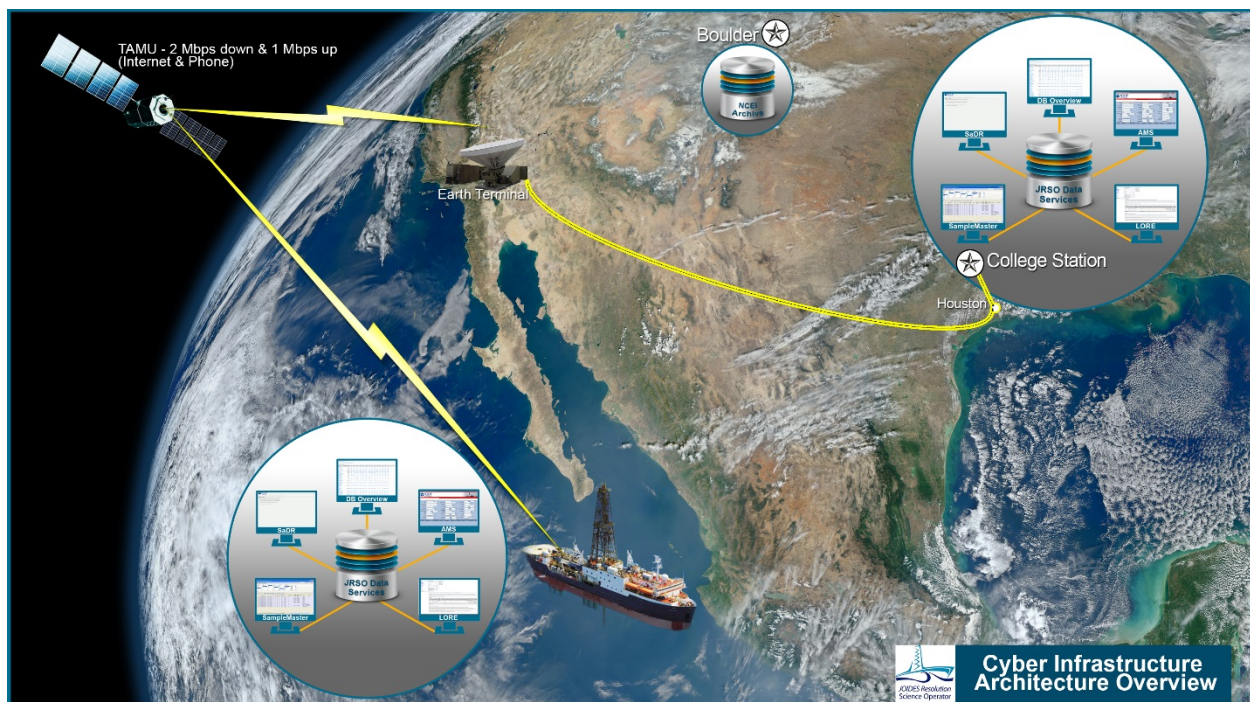
JOIDES Resolution Science Operator
Cyberinfrastructure Overview

The *JOIDES Resolution* Science Operator (JRSO) manages and operates the riserless drillship, *JOIDES Resolution*, for the International Ocean Discovery Program (IODP). The JRSO (http://iodp.tamu.edu) is based in the College of Geosciences at Texas A&M University.
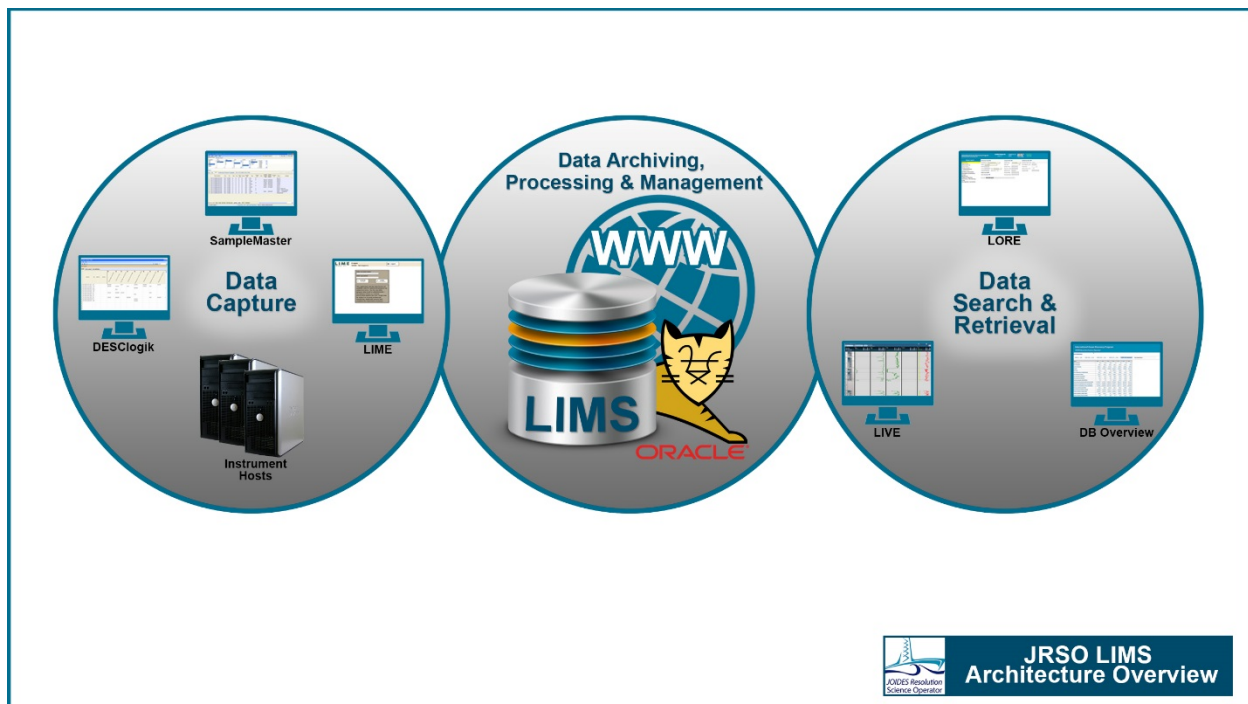
The JRSO is responsible for overseeing the science operations of the riserless drilling vessel *JOIDES Resolution* (JR), archiving the scientific data, samples and logs that are collected, and disseminated via web applications and online publications. The drillship travels throughout the oceans sampling the sediments and rocks beneath the seafloor. The scientific samples and data are used to study Earth's past history, including plate tectonics, ocean currents, climate changes, evolutionary characteristics and extinctions of marine life, and mineral deposits.

The JR is an NSF large facility that serves the global geosciences community. In addition to NSF funding through a cooperative agreement, JRSO operations are partly funded by 22 IODP member nations, including Australia, Austria, Brazil, Canada, China, Denmark, Finland, France, Germany, India, Ireland, Italy, Japan, Korea, Netherlands, New Zealand, Norway, Portugal, Spain, Sweden, Switzerland, and the United Kingdom.

The cyberinfrastructure team supports a split based operations construct, providing cyberinfrastructure, cybersecurity and data management services at sea on board the JR and on shore in College Station, TX. VSAT (very small aperture terminal) satellite services are used to provide connectivity services between ship and shore. Currently, this is a dedicated asynchronous wide area network circuit offering 2 Mbps down to the ship and 1 Mbps up.

The JRSO's Laboratory Information Management System (LIMS) architecture (see picture below) is designed to capture, archive, process, manage, and disseminate data using several JRSO-developed instrument uploaders, client applications and web application tools. LIMS comprises the database that stores the data, the web services that pull and push the data, and the applications and hardware that capture and disseminate the data. One JRSO goal is to make this data, along with the data stored a legacy system (JANUS), more human and machine discoverable. JRSO is hopeful that the NSF-funded Open Core Data project will soon provide the data discovery capability it is seeking.

The cyberinfrastructure team serves approximately 115 internal JRSO staff, 150 international scientists who sail on the JR each year, and the broader global geosciences community.

Under its capital equipment replacement program, the JRSO routinely updates infrastructure services on ship and shore (i.e., servers, storage, backup services, battery backup, and high-speed network). The median age for JRSO infrastructure equipment is approximately six years.

JRSO leverages Texas A&M University policies and tools to maintain its cybersecurity program. JRSO conducts a security self-assessment once per year using RSA Archer GRC in order to remain in compliance with university and state regulations.

JRSO science data is permanently achieved at the NCEI facility in Boulder, CO.

NATIONAL SUPERCONDUCTING CYCLOTRON LABORATORY

The overall mission of the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University is to provide forefront research opportunities with stable and rare isotope beams. A broad research program is made possible by the large range of accelerated primary and secondary (rare isotope) beams provided by the facility. The major research thrust is to determine the nature and properties of atomic nuclei, especially those near the limits of nuclear stability. Other major activities are related to nuclear properties that influence stellar evolution, explosive phenomena in the cosmos (e.g. supernovae and x-ray bursts), and the synthesis of the heavy elements; and research and development in accelerator and instrumentation physics, including the development of superconducting radiofrequency cavities and design concepts for future accelerators for basic research and societal applications. In all activities an important part of the NSCL program is the training of the next generation of scientists. Upon completion of the DOE-funded Facility for Rare Isotope Beams (FRIB), the laboratory will transition to programs with beams from this facility.

NSCL operates two coupled cyclotrons, which accelerate stable ion beams to energies of up 170 MeV/u. Rare isotope beams are produced by projectile fragmentation and separated in-flight in the A1900 fragment separator. For experiments with high-quality rare isotope beams at an energy of a few MeV/u, the high-energy rare isotope beams are transported to a He gas cell for thermalization, and then sent to the ReA linear post-accelerator for reacceleration. Rare isotope beams in this energy range allow nuclear physics experiments such as low-energy Coulomb excitation and transfer reaction studies as well as for the precise study of astrophysical reactions. The facility has produced over 904 rare isotope beams for experiments, and 65 new isotopes have been discovered at NSCL.

NSCL is a national user facility and has a large user community with over 800 actual, active users in a given year. Most experiments conducted at NSCL involve international collaborations with about 75% of the experiments lead by a US spokesperson.

NSCL provides beams to approximately 30 experiments per year. Experiments are short (~3-7 days) with many changes during and in between experiments. Data acquisition and analysis and simulation framework need to support fast online decision making. Experiments have increased significantly in complexity with an increase of the number of channels read out, often together with high-resolution digitized waveform data. Each experiment can generate up to 10 TB of experimental data set. Storage and backup systems must match such data sizes. Data sets are analyzed on-line during the data acquisition and later off-line either at NSCL or at the spokesperson's institution. Experiments with in-house spokespersons require long-term storage (usually a few years) of the full data set and adequate computing resources for analysis. A computing cluster in the order of 1000 cores dedicated for online analysis is foreseen. Network bandwidths of 100 Gbit/s will be required. External data transfer capabilities must continue to accommodate the needs of a large and distributed user community with increased data set sizes. Data sets are provided to experimenters via magnetic tape, though other methods are available.

NSCL CI supports and enables the Laboratory overall mission. CI includes a broad range of functional areas: business support information technology, networking, accelerator controls, experimental controls and DAQ, and offline simulation and analysis. Internally developed and commercial solutions are used. Systems are primarily managed and maintained by Laboratory

personnel. CI challenges include increasing security requirements, Laboratory growth with FRIB planning and construction, and increasing and foreseen experimental needs.

The Business IT department provides a range of enterprise IT services directly supporting business processes including an internally hosted ERP suite and other customized COTS solutions. Windows based services including Active Directory, Exchange, SharePoint are deployed. More than 500 Windows desktop PCs are maintained.

Business IT department also maintains the Lab-wide network, servers and storage used by DAQ and NSCL Controls and is responsible for overall IT security.

Internet is provided via MSU with MSU assisting with Internet security. Laboratory wired networks are managed internally with MSU supporting wireless access.

The Controls department is responsible for hardware and software controls for accelerators, beamlines, and other experimental equipment. The controls system uses EPICS protocols with graphical monitoring using CS-Studio. NSCL personnel are active in development of both projects. A number of associated systems provide alarms, access controls, archiving etc. for EPICS.

With construction of the FRIB accelerator progressing, new accelerator and cryogenic controls networks are being deployed. These are also EPICS based. The designs emphasis security with FRIB Controls network isolated from other Laboratory systems.

In house developed software forms the core of the DAQ systems. NSCLDAQ is a modular system supporting a range of experiment arrangements. SpecTcl is a compatible analysis software. DDAS is an internally developed digital-DAQ, supporting XIA Pixie-16 Digitizer and compatible with NSCLDAQ. As a user facility, NSCL provides DAQ assistance to visiting experimenters. Typical experiments produce approximately 100 GB of data per day with experiments storing digitized waveforms producing ~1 TB per day. Currently, most experiments' needs are met with 1GE networking and several DAQ computers. Data is recorded to ZFS/Linux servers. Reliability is critical as experiments' beam times are generally limited for less than one week. Visiting experimenters may make use of DAQ systems while present at NSCL.

Increasingly, flexible CPU and software systems are used for DAQ. One purpose is distinguishing overlapping waveform signals from higher rate experiments. The GRETINA experiment is active at NSCL currently utilizing a dedicated farm of approximately 100 PC nodes (1000 cores) for selecting events based on digitized waveforms.

Offline simulations and analysis systems are provided for Laboratory students, faculty and staff. Clustered interactive Linux hosts and a small (~50 node) Linux SLURM batch system are available. Approximately 1 PB of networked research storage is available using ZFS/Linux systems with NFS. Increasing detector complexity, data volumes and analysis complexity require increasing simulation and analysis capacity. Free and widely used applications such as ROOT and GEANT are the norm.

IceCube Computing Infrastructure Overview

Contact: Gonzalo Merino, gonzalo.merino@icecube.wisc.edu
Computing Facilities Manager

IceCube is a neutrino detector built at the South Pole by instrumenting about a cubic kilometer of ice with 5160 light sensors. It uses Cherenkov light, emitted by charged particles moving through the ice to realize the enormous detection volume required for detecting neutrinos. One of the primary goals for IceCube is to elucidate the mechanisms for production of high-energy cosmic rays by detecting high-energy neutrinos from astrophysical sources. The Detector construction started in 2005 and finished in December 2010. Data taking started in 2006 and it is expected to be operated for at least 20 years. The United States National Science Foundation (NSF) supplied funds for the design, construction, and operations of the detector. As the host institution, the University of Wisconsin-Madison, with support from the NSF, has responsibility on the maintenance and operations of the detector. The scientific exploitation is carried out by an international Collaboration of about 300 researchers from 48 institutions in 12 countries (see http://icecube.wisc.edu).

The IceCube data processing is divided in two regimes: online at the South Pole and offline at the UW-Madison main data processing center. Computing equipment is lifecycle replaced on average every ~4 years at the South Pole and ~5 years at UW-Madison. Several collaborating institutions also contribute to the offline computing infrastructure at different levels. Two Tier1 sites provide tape storage services for the long term preservation of the IceCube data products: NERSC in the US and DESY-Zeuthen in Germany. About 20 additional IceCube sites in the US, Canada, Europe and Asia provide computing resources for simulation and analysis.
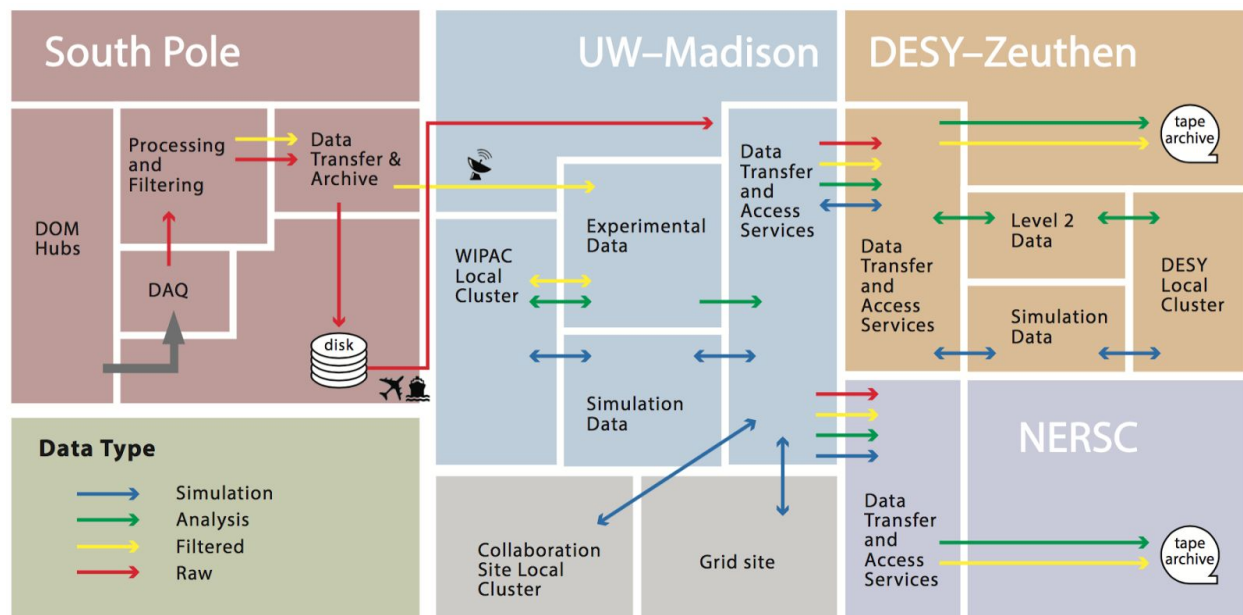

Figure 1 - The IceCube data flow and computing infrastructure.

Online Computing Infrastructure

Aggregation of data from the light sensors begins in the IceCube Laboratory (ICL), a central computing facility located on top of the detector hosting about 100 custom readout DOMHubs and 50 commodity servers. Data is collected from the array at a rate of 150 MB/s. After triggering and event building, the data is split into two independent paths. First, RAW data products are written to disks at a rate of about 1 TB/day, awaiting physical transfer north once per year. In addition, an online compute farm of 22 servers does near-real-time processing, event reconstruction, and filtering. Neutrino candidates and other event signatures of interest are identified within minutes, and notifications are dispatched to other astrophysical observatories worldwide via the Iridium satellite system. Approximately 100 GB/day of filtered events are queued for daily transmission to the main data processing facility at UW–Madison via high-bandwidth satellite links. Once in Madison, filtered data is further processed to a level suitable for scientific analysis.

Offline Computing Infrastructure

The main data processing facility at UW-Madison currently consists of ~7600 CPU cores, ~400 GPUs and ~6 PB of disk. This facility is used mainly for user analysis, but also for data processing and simulation production. Data products that need to be preserved for long time are replicated to two different locations: NERSC and DESY-Zeuthen.

Conversion of event rates into physical fluxes ultimately relies on knowledge of detector characteristics numerically evaluated by running Monte Carlo simulations that model fundamental particle physics, the interaction of particles with matter, transport of optical photons through the ice, and detector response and electronics. Large amounts of simulations of background and signal events must be produced for use by the data analysts. The computationally expensive numerical models necessitate a distributed computing model that can make efficient use of a large number of clusters at many different locations.

Up to 50% of the computing resources used by IceCube simulation and analysis are distributed (i.e. not at UW-Madison). The HTCondor software is used to federate these heterogeneous resources and present users a single consistent interface to all of them:

- Local clusters at IceCube collaborating institutions

- UW campus shared clusters

- Open Science Grid

- XSEDE supercomputers

Overview of UNAVCO

UNAVCO, a non-profit university-governed consortium, facilitates geoscience research and education using geodesy. The website is at http://www.unavco.org.

The UNAVCO consortium membership consists of more than 100 US Full Members and over 80 Associate Members (domestic and international). Through our Geodetic Infrastructure and Geodetic Data Services Programs, UNAVCO operates and supports geodetic networks, geophysical and meteorological instruments, a free and open data archive, software tools for data access and processing, cyberinfrastructure management, technological developments, technical support, and geophysical training. The UNAVCO Education and Community Engagement Program provides educational materials, tools and resources for students, teachers, university faculty and the general public.

Under a 2013 award from the National Science Foundation (NSF), UNAVCO operates the Geodesy Advancing Geosciences and EarthScope (GAGE) Facility. In this role, UNAVCO deploys and operates instrumentation that collects a variety of data to support geodetic with instrumentation systems are deployed globally. UNAVCO provides data management, curation, archiving and distribution services for geodetic data collected or acquired by UNAVCO and by US investigators performing geodesy research with NSF funding. Under certain circumstances non-NSF or NASA funded contributed research data and products are also handled. UNAVCO has been a Regular Member of the ICSU World Data System since 2015.

The Geodetic Data Services (GDS) program manages a complex set of metadata and data flow operations providing a wide range of geodetic/geophysical observations to scientific and educational communities. Sensors currently include Global Navigation Satellite System (GNSS) (downloaded files and high rate data streaming in real time (RTGNSS), borehole geophysics instrumentation (strainmeters, tiltmeters, seismometers, accelerometers, pore pressure and meteorological sensors), long baseline laser strainmeters, and terrestrial laser scanners. Field data are acquired either from continuously operating sites or episodic "campaign" surveys conducted by the community. UNAVCO also acquires and distributes satellite synthetic aperture radar (SAR) data from foreign space agencies. GDS services include data operations (managing metadata; data downloading, ingesting and preprocessing); data products and services (generating processed results and QA/QC and state-ofhealth monitoring); data management and archiving (distribution and curation); cyberinfrastructure; and information technology (systems and web administration). In order to perform this work, GDS maintains a highly specialized technical staff, onsite and offsite computer facilities with networking, servers and storage, and manages a number of sub awards to university groups who provide additional products, software and training.

Key Data and Products
Key data products include GNSS unprocessed and processed data from over 3,000 continuous stations; Terrestrial and Airborne Laser Scanning swaths, point clouds and rasters; raw and processed space borne SAR (Synthetic Aperture Radar) and InSAR (Interferometric Synthetic Aperture Radar) images; borehole strain and seismic data (raw and processed); and raw and processed meteorological observations collocated at selected geodetic stations. Key software developed and supported by UNAVCO for community use include GNSS preprocessing codes, and GNSS data and metadata management software

systems. Through sub awards UNAVCO provides community support for GNSS processing codes.

Facility CI
UNAVCO's CI is intended to provide robust, reliable, secure hardware and software systems that ensure data and metadata integrity from the field sensor to the user. Data are managed through multiple software and systems processes covering acquisition, data communications, ingestion, quality checking, preprocessing and processing, and archiving. Increasingly, web services are used to deliver capability for internal handling as well as discovery tools, visualization, and data delivery processes. UNAVCO maintains internet connectivity with two routes to the outside: a primary link on Internet2 through the Front Range Gigapop, and a failover Comcast commercial Internet link. In-house virtualization with VMWare on newer (less than 5-year old) Dell servers hosts the majority of services; this is supplemented by older Sun server and storage hardware (ten years old); SAN storage technology (Oracle, Infotrend) is supplemented with cloud-based IaaS. A colocation service is used for critical backups and failover capability. The wide range of data types and tools for processing and preprocessing is supported by a variety of software stacks developed starting in the 1990's and evolving through the present with 10 years as the median age. In addition, UNAVCO is investigating deploying several services in the cloud (commercial and NSF XSEDE) through the Earthcube GeoSciCloud project.
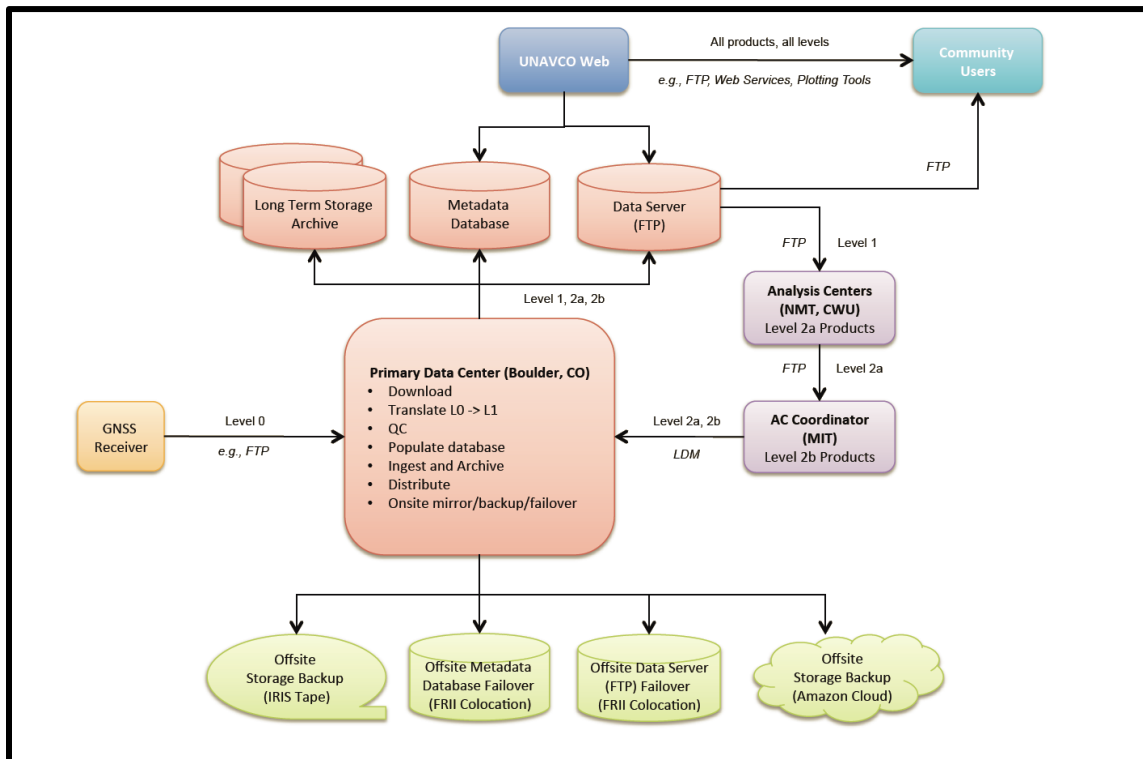

Figure 1. Schematic for UNAVCO's CI for GNSS data and products showing data coming from the field through data and products delivered to users. This schematic, though limited to the GNSS data type, is generally representative of the CI used for other data types (TLS, SAR, borehole strain and seismic, meteorological) handled by UNAVCO.

IRIS Data Services
Tim Ahern
Director of Data Services

The central component of IRIS Data Services (DS) is the IRIS Data Management Center in Seattle, Washington. The DMC relies on other DS components in Albuquerque, La Jolla, University of Washington, LLNL, and Almaty, Kazakhstan to realize its full functionally but the heart of the DS is the DMC. The major CI components are in place at the DMC. We run a fully functional Auxiliary Data Center that is unmanned at LLNL.

1. ***A brief description of the facility, its science mission, and the community (including size, make up – number of individual, number of institutions, etc.). Please include a URL for more information.***

The IRIS DMC is a domain specific facility that meets the needs of the seismological community both within and outside the US. The DMC facilitates science within our domain but does not DO any science. Our science mission can be found in our strategic plan:
http://www.iris.edu/hq/files/programs/data_services/policies/Strategic_Plan_v7.pdf
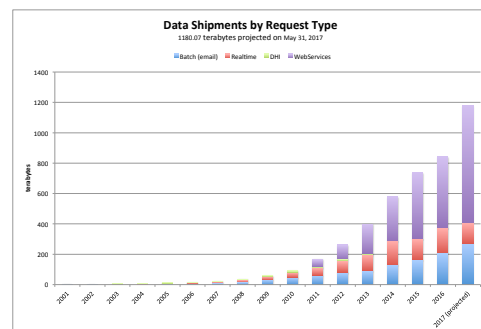Our science community numbers in the thousands worldwide.

Mission: *To provide reliable and efficient access to high quality seismological and related geophysical data, generated by IRIS and its domestic and international partners, and to enable all parties interested in using these data to do so in a straightforward and efficient manner.*

IRIS is university consortium with approximately 125 members (US academic institutions with graduate degrees in seismology) and roughly the same number of foreign affiliates scattered all over the globe. We are a 501c3 Delaware corporation. We distribute primary data to roughly 25,000 (3rd level IP address) distinct users or IP addresses per quarter from roughly 12,000 distinct organizations (2nd level IP address). IRIS ingests roughly 75 terabytes of new observable data per year and we project we will more than one petabyte in 2017.

2. ***A description of the key products/services of the facility (data, software, services, etc.)?***

IRIS' primary products are (Level 0, raw and Level 1 quality controlled) time series data. The time series come from roughly 30 types of sensors deployed on/in the ground, in the water column or water bottom, and in the atmosphere. IRIS also produces Level 2 derived products, and manages community developed Level 2 and higher products. (See http://ds.iris.edu/spud/). Level 0 and 1 products are fully documented (metadata) time series data from geophysical sensors distributed globally generated form NSF and other national and international sources. We distribute roughly one petabyte of level 0 and 1 data per year.

Figure 1 shows volume of time series data shipped from the IRIS DMC to end users and or monitoring agencies since 2001. Major types of shipments include legacy requests in the blue, real time data distribution in the red, and web service distribution in the purple.

IRIS also produces a great deal of community software and offers both IRIS developed and community developed software and tools in Redmine and GitHub repositories. IRIS develops and maintains specific client applications for accessing and working with IRIS data.

All IRIS data assets (Level 0-3) are available through service APIs. Some of the APIs have been adopted internationally (FDSN web services) and other APIs are IRIS developed and maintained and not yet adopted internationally. (see http://service.iris.edu). IRIS also maintains comprehensive documentation and is also the source of documentation for the SEED format, which is the international seismological domain format. (www.fdsn.org)

 3. A brief description (including a figure) of the facility CI (e.g., its architecture, key services/components, underlying infrastructure), how it is deployed/distributed, and its operation. What is the median age since deployment of the key CI components.

The figure could be provided at a later date, it is very complex obviously and difficult to provide something at a high enough level as to be useful.

The IRIS DMC operates a primary data center in Seattle as well as an unmanned, fully functional Auxiliary Data Center (ADC) in Livermore California. Major components of CI at the DMC and ADC consist of the following

- **Storage** – IRIS operates large volume Hitachi RAID systems that emphasis storage over performance. We improve performance by indexing the RAID contents in a PostgreSql DBMS. We have roughly 700 terabytes of storage RAID at both the DMC and the ADC. We also operate high performance RAID systems made by NetApp both for reception of real time data and PostgreSql database transactions.
- **Servers**- IRIS runs virtual servers on physica Dell Servers. Virtualization software is VMWare.
  IRS operates Forcepoint Firewalls and A10 Load Balancers. Load Balancers are configured so that a failure at the DMC or the ADC does not remove outsides user's access to services,
- **LANs-** We run 10 gigabit/second LANs sometimes in parallel to form a data backbone internal to the DMC and ADC. We connect to the Internet through the University of Washington.

Storage access to observational data has been abstracted through web services for both internal and external use. Access to data is transitioning from direct SQL access to abstractions thorugh web services. We are very close to running a SOA for both internal and external access.

Our goal is to refresh all major computational and storage hardware infrastructure every four years. Budget pressues sometimes pushes this to 5 years.

We are currently testing operating our software in XSEDE and AWS to see if this is viable.

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NSF Cyberinfrastructure Facilities Whitepaper
S. Berukoff, E. Cross
Daniel K. Inouye Solar Telescope
National Solar Observatory

Introduction

The Daniel K. Inouye Solar Telescope (DKIST) (http://dkist.nso.edu) is a four-meter, off-axis Gregorian solar telescope currently under construction by the National Solar Observatory and AURA on Haleakala, Maui, Hawai'i. When complete in 2019, it will be the largest solar telescope in the world, providing facility-class, high-resolution solar observations to a small but growing community of students, researchers, and the general public. In full operations, planned to last fifty years, the DKIST will house five complex instruments and a state-of-the-art adaptive optics system, generating over three petabytes of raw data annually. Key to its success, then, is a cyberinfrastructure providing facility and instrument control, scientific and operational data acquisition, and data management, processing, and distribution services. In this whitepaper, we provide a high-level description of primary components of the cyberinfrastructure.

Cyberinfrastructure

The DKIST cyberinfrastructure is comprised of three primary components: the systems and infrastructure providing services to operate the telescope and its supporting subsystems ("Summit"), the core services and infrastructure needed to support science and engineering activities related to observatory operations and network services ("DKIST IT"), and the services and infrastructure performing long-term data management, processing, discovery, and distribution ("Data Center"). These components are highlighted in Figure 1, and discussed in more detail below.

Summit

The DKIST Summit cyberinfrastructure comprises integrated facility, instrument control and safety systems, enabling telescope and dome control, optical alignment and routing, mechanical controls, observation execution and monitoring, instrument data acquisition, management, and distribution, and environmental monitoring and control. These systems are comprised of a High Level Software suite written primarily in Java and Python, utilizing CORBA. They are deployed through configuration-controlled provisioning stacks, including SaltStack, and sit atop an HPC architecture comprising many dedicated nodes interconnected through 10 Gb Ethernet and FDR InfiniBand. The Summit cyberinfrastructure is currently being readied for integration testing as a prelude to observatory integration efforts coming in the next 12-18 months.
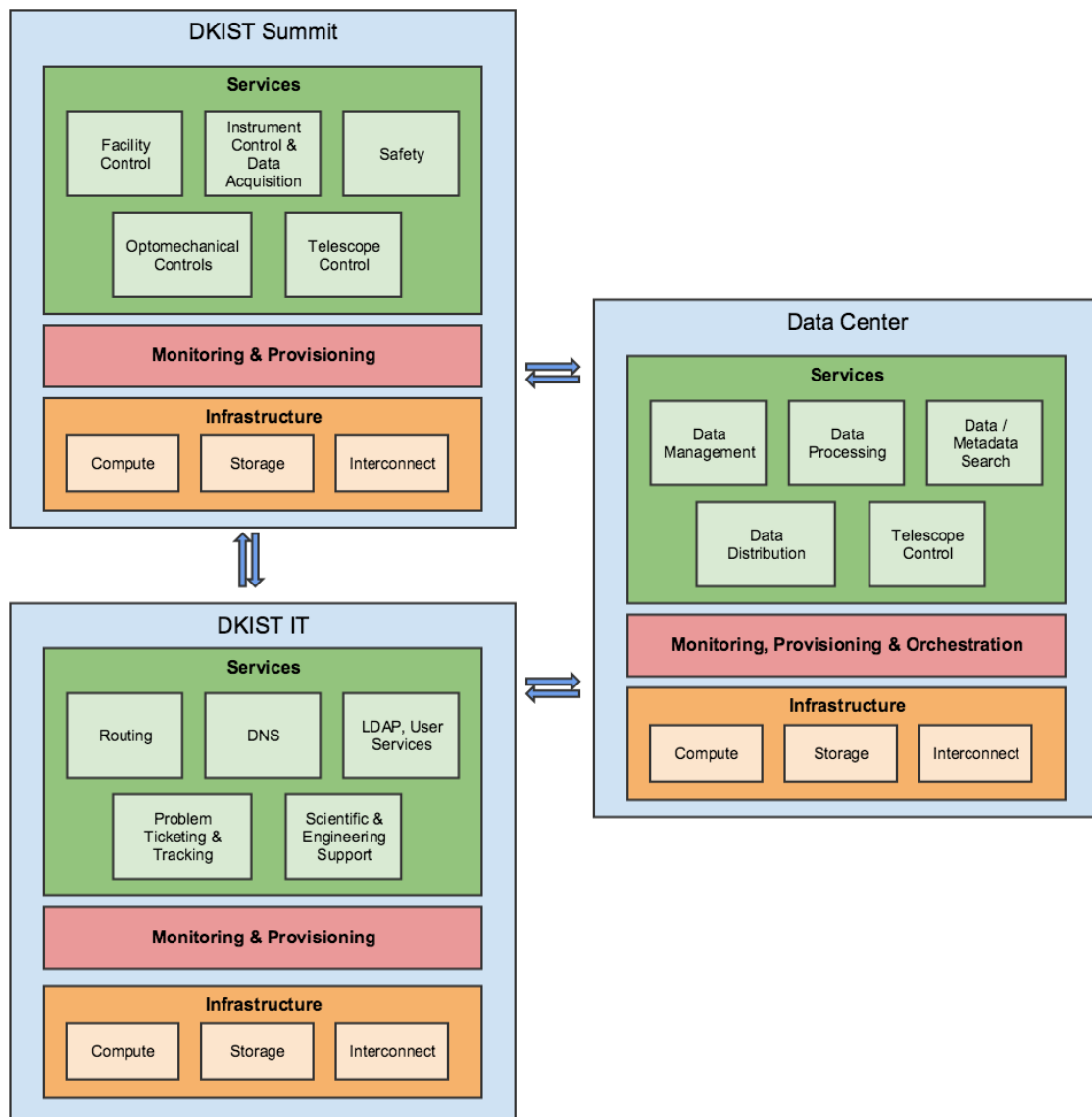
Figure 1: DKIST Cyberinfrastructure

DKIST IT

The DKIST IT supports the observatory through deployment of core services such as routing, DNS, LDAP, and network maintenance and monitoring for the summit and a remote support building, as well ensuring SLAs and/or contracts with partner organizations (U. Hawai'I in Maui and U. Colorado in Boulder at the NSO Headquarters) are met and maintained. In addition, the DKIST IT provides operational support for physical infrastructure (optical fiber, Ethernet and InfiniBand networking, and routing hardware) on the Summit and the remote support building. Services are deployed through configuration-controlled provisioning stacks, sitting atop commodity equipment including Cisco switching. The DKIST IT is ramping its efforts, particularly with regard to network buildout on the Summit and the remote support facility.

Data Center

The DKIST Data Center will provide long-term data management, scientific processing, search, and distribution services for the observatory. It will manage 3.2 PB of data per year, comprised of hundreds of millions of observations and tens of billions of metadata, exported by the Summit and, after calibration, intended for end-user consumption. Thus, data management and processing services must scale effectively with little rework, while data search depends on appropriate data modeling and well-developed use cases to allow end-users to effectively target data of interest. Key aspects of the architecture include a combined microservices and virtual machine deployment, provisioned through SaltStack and managed with Elastic and related tooling. While it is planned for the Data Center to reside at the NSO Headquarters, economies of scale are shifting, indicating a need to ensure "deploy-anywhere" (e.g., commercial cloud providers) can be supported effectively. The Data Center is currently completing its design phase, with development expected to occur in 2018-2020, with phased delivery of critical services occurring as DKIST comes online.

When combined with a rigorous systems-engineering approach, including detailed requirements and interface controls, these three primary components will support DKIST use and scientific data exploitation. Despite the bespoke nature of the Summit CI, there is a significant focus on leveraging open source technologies in the DKIST, rather than relying on integration of commercial products. This is partly due to the long-term nature of the program and tight budgetary constraints. However, there are no free lunches – significant open source adoption without proactive forward replacement planning can leave obsolesced components underpinning critical systems. Given the long development timeline for the DKIST – the first CI work began in 2005 – these issues are already creeping into a yet-to-operate facility. Yet, the state of system development shows significant progress forward, and a bright future, for the DKIST CI.

Summary

This whitepaper briefly discusses the DKIST end-to-end cyberinfrastructure, focusing on the three primary entities and their roles. Each is in a different developmental state, emphasizing the importance of clear requirements and interfaces, effective team communication strategies, and stakeholder management.

Gemini Observatory

White Paper for NSF Cyberinfrastructure Workshop, Sept 2017

Facility Description

The Gemini Observatory consists of twin 8.1-meter diameter optical/infrared telescopes located on two of the best observing sites in the world: Maunakea in Hawaii and Cerro Pachon in Chile. From these two locations, Gemini's telescopes can collectively provide access to the entire sky. Gemini was built and is operated by an international partnership of five countries including the United States, Canada, Brazil, Argentina and Chile. These Participants and the University of Hawaii, which has regular access to Gemini, each maintain a "National Gemini Office" to support their local users. Any astronomer in these countries can apply for time on Gemini, which is allocated in proportion to each Partcipant's financial stake. For the US, Gemini provides the largest publicly-accessible optical/infrared telescopes.

Formally, the Mission Statement is "To advance our knowledge of the Universe by providing the international Gemini Community with forefront access to the entire sky." Gemini's achieves this by supporting peer-reviewed science proposed by the astronomical communities in the participating nations, and providing competitive instrumentation and observing modes in doing so. Over the five-year period between 2012 and 2016, more than 1000 individual Principal Investigators applied for Gemini observing time, from more than 300 academic institutions across the Gemini Partnership.

The Gemini web site: http://www.gemini.edu/

Key products/services

The direct product of Gemini observatory is observational data, taken in appropriate observing conditions, and placed in an archive for access by Principal Investigators (PIs). The service provided to PIs, jointly between the observatory and the NGOs, is to help prepare their observations, then to execute them on the telescopes or support the PI in executing them. Some PIs visit the telescope to make observations, others have their observations taken for them by staff operators. Gemini provides the preparation tool for PIs to create their observations. It also provides a data reduction package for all facility-class instruments. Currently this is based on the standard "IRAF" package distributed by NOAO.

Facility CI

The Gemini Observatory CI (computers, storage and networking; we do not include software in the definition) addresses the combined requirements of telescope operations, data handling and administrative support functions. Each of the four Gemini sites operates identical key services; a redundant core network service to support the distributed network environment, a redundant data storage system capable of replicating data offsite/cross-site in real time, a virtual machine cluster, a physical server farm, a virtual tape library backup environment, which also replicates data offsite, and

instrumentation support infrastructure - such as per-instrument server hardware, network connectivity, remote power management and system monitoring.

The two main Gemini sites (Gemini North and Gemini South) are connected via site-to-site VPN tunnels, that utilize the Internet 2 network infrastructure in the US, with interconnections to the REUNA research network in Chile.

Additionally the two base facility sites in La Serena, Chile and Hilo, Hawaii are equipped with high power computers. These units offer Gemini scientist the possibility of efficiently processing data locally to support their research. While for the most part the consumption of these key services and components is separated, non-operational functions, such as research, project and document management, telecommunications and internet access, enjoy the benefits of increased redundancy and high availability.

The median age of these key CI components is largely dictated by the manufacturers recommendations and enterprise support capabilities and experience in the field. These numbers are in turn transposed to the observatories longevity/obsolescence plan and are therefore understood in advance of the budget cycles. The networking equipment, for example, has a general operating age of around eight years, at which point the support contracts are no longer offered and spares are difficult to procure. The current core network hardware was replaced in 2014 and is set to be replaced in 2022. Similar examples can be made for each key CI component within Gemini, ensuring that the technology will also meet the observatory's long term requirements.

National Ecological Observatory Network (NEON)
Cyberinfrastructure Overview (July 2017)

Science Mission: Through a Cooperative Agreement with the National Science Foundation, Battelle is constructing the National Ecological Observatory Network (NEON) as a research platform designed to study the biosphere at regional and continental scales and to conduct real-time ecological studies at the scales required to address grand challenges in ecology. www.NEONScience.org

Facility Description: NEON is a new nationwide, "shared-use" research platform of field-deployed instrumented towers and sensor arrays, sentinel measurements, specimen collection protocols, remote sensing capabilities, natural history archives, and facilities for data analysis, modeling, visualization, and forecasting. NEON assets are managed with a cyberinfrastructure of networked processing routines, repositories, and interfaces. The Observatory also supports multi-sensor aircraft payloads (AOPs) operated from leased Twin Otter aircraft, and five mobile deployment platforms (MDPs) that contain both terrestrial and aquatic instrumentation. NEON construction will be completed within the next year.

Key Products & Services: The continental-scale cyberinfrastructure serves 181 data products from 20 regional eco-climatic domains which consist of terrestrial, aquatic, and aerial sampling from over 350 staff. To enable researchers to answer major ecological questions, NEON collects data on a suite of biotic and abiotic variables. As a national research platform, infrastructure, sampling methods, and measurements are being standardized and provided via extensive metadata associated with each downloadable data product. Consistency in collection across locations, through the use of standardized sensors, protocols, and processes, is required to ensure the validity and usability of NEON data by the scientific community and other stakeholders. NEON staff, in concert with automated procedures, evaluate data quality.

The NEON cyberinfrastructure includes models and related computational resources for delivering a range of value-added "data products" based on the in-situ, experimental, and remote sensing components. These models and algorithms perform quality control processing, classification, scaling and interpolation functions, as well as provide a platform for external researchers accessing the data to detect patterns, test hypotheses, and project ecological forecasts against seamless, continental scale data layers.

The cyberinfrastructure, which is headquartered in Colorado, publishes both real-time provisional data, and annual releases of observatory-wide versions of results. The cyberinfrastructure architecture is built across facilities which range from the central, commercial data center, to headquarters development environments, to cloud-based data acquisition/staging applications, to distributed sites with dedicated local unmanned facilities, communications, routing controls, and local data logging. Repository content is managed via a central object store, a portfolio of relational databases, and shared code libraries. The cyberinfrastructure includes numerous operational subsystem including: ingest; archival; calibration; processing pipelines; metadata management; specimen custody management, and publishing functions. NEON's web presence consists of interactive portals to data assets, community services, and application programming interfaces (API).

The cyberinfrastructure development team uses best practices approaches to software development via an iterative approach to development (using industry-standard Agile methodology) that stresses the evolving nature of requirements gathering and development. The team emphasizes best practices engineering principles, including code re-use and definition of interfaces to facilitate object-oriented software integration and provide a basis for future growth. Formalized QA methods are applied to in unit, integrated, and regression testing. Segregated development, test, integration, and production environments control releases. The NEON cyberinfrastructure is designed to invite incremental improvements through incorporation and testing of open-source code from community members.
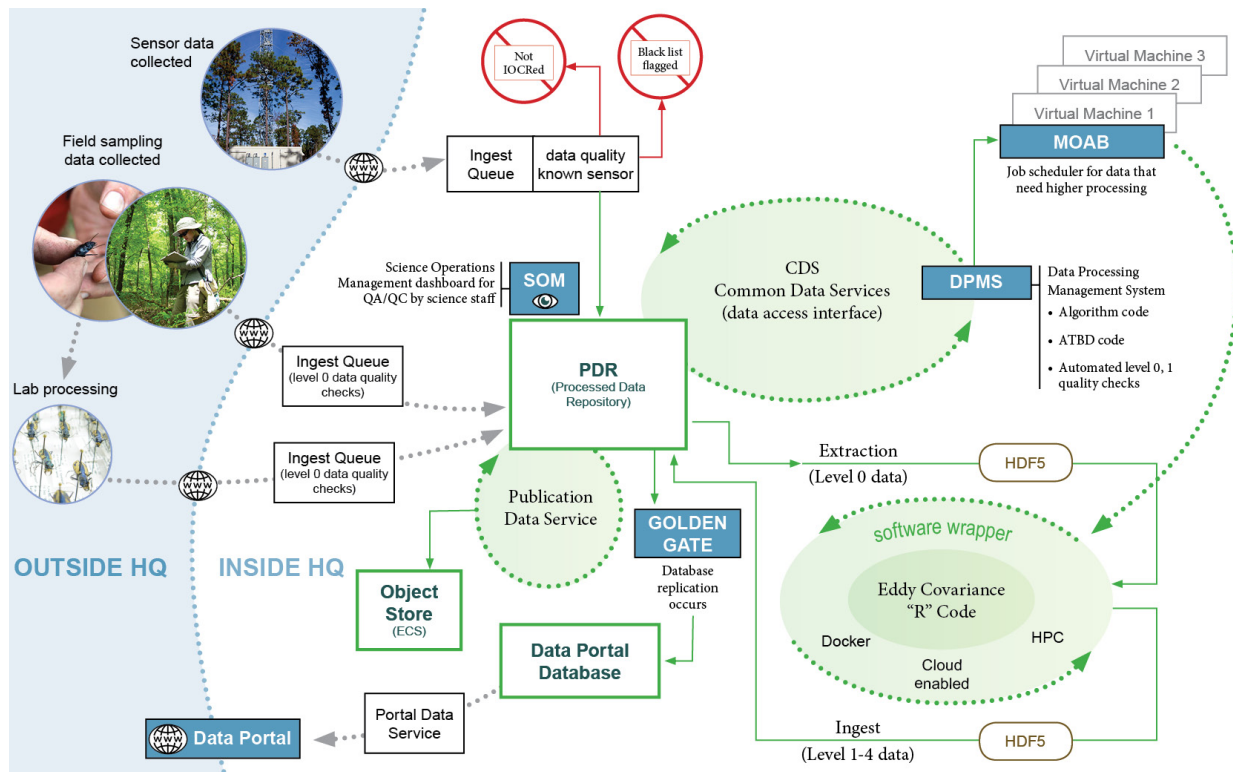
Figure 1. Generalized landscape of data flow through the NEON cyberinfrastructure.

Management & Community Engagement: Leadership is conducted from the NEON Project headquarters in Boulder, Colorado, where core science, management, and administrative functions for the Observatory is managed through the 30-year operational life. NEON's operation is periodically adapted through guidance from the Science, Technology, and Education Advisory Committee (STEAC). Community input is facilitated by 20+ Technical Working Groups. Some NEON products are hosted by community partner organizations: BOLD; SRA; MG-RAST; PhenoCam; AeroNet; AmeriFlux, and DataOne. NEON participants include dozens of laboratories, universities, and agencies. Initial user statistics reflect over 10,000 users from domestic and international organizations.

OCEAN NETWORKS CANADA'S OCEANS 2.0 DIGITAL INFRASTRUCTURE

BENOÎT PIRENNE, DIRECTOR, USER ENGAGEMENT, OCEAN NETWORKS CANADA, VICTORIA, BC

Ocean Networks Canada (ONC) is a world-leading organization supporting ocean discovery and technological innovation. ONC is a not-for-profit society that operates and manages innovative cabled observatories on behalf of the University of Victoria, in British Columbia. These observatories supply continuous power and Internet connectivity to various scientific instruments located in coastal, deep-ocean, and Arctic environments. ONC's arrays host hundreds of sensors distributed in, on and above the seabed along with mobile and land-based assets strategically located. The instruments address key scientific and policy issues (subsea earthquakes and tsunamis, ocean acidification, marine biodiversity, etc.) within a wide range of environments. (See Fig. 1).

ONC has built Oceans 2.0, the digital infrastructure that manages vast amounts of complex data streams. Oceans 2.0 is unique in that it supports the continuously increasing volume (currently at 500 terabytes), the variety of data types (dozens of instrument types and over 5000 individual sensors), the data structures that enable rapid access and delivery of analytically-derived alerts, the consistency of data through an instrument management system with robust and rich metadata, as well as automatic and manual QA/QC.

Ocean Networks Canada's Oceans 2.0 sensor network data management can also host and distribute data for 3rd parties, and has features for attribution and access restrictions. Some of its unique data access features include a distributed, live video annotation (SeaScribe) and a video search capability (SeaTube); tools for viewing and searching a hydrophone data archive; tools for the continuous browsing of complex time series data, etc. It also includes an integrated suite of observatory management tools to monitoring and control the infrastructure (electrical, communication and data flow control — see Fig. 2).

Oceans 2.0 is solidly founded on a Service Oriented Architecture based on a core Enterprise

Fig. 1: Ocean Networks Canada ocean and coastal observing facilities include the VENUS and NEPTUNE systems off British Columbia (see inset), together with a number of community observatories across Canada (including in the Arctic). With over 400 instruments reporting real-time data from the deep ocean to the coast, ONC's Oceans 2.0 data management system makes big data and products available to scientists, governments, municipalities and first nations.

Fig. 2: ONC's Oceans 2.0 system offers integrated monitoring and control tools for managing power, data flow and communication with the "Device Console" tool. The navigation follows the tree structure of the network topology. The same interface allows operators control over any part of the infrastructure regardless of where it is located.

Service Bus. This provides a high performance platform based on a modular, loosely-coupled component architecture, and allows for the simplified addition of the constituent modules on an as needed basis.

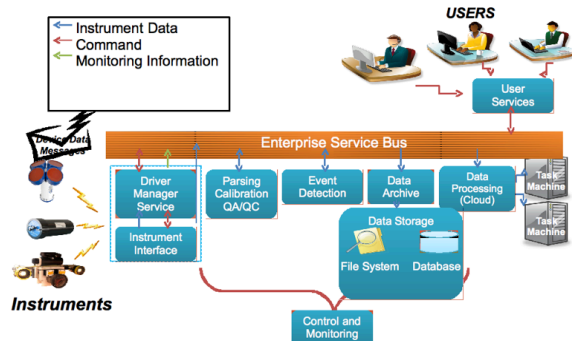With this architectural foundation, Oceans 2.0 provides a simplified, well-defined, event-driven and "pluggable" system which can be scaled as the organization's requirements change. (See Fig. 3). The Oceans 2.0 components include: The *Enterprise Service Bus,* which is the message passing system that allows all parts of Oceans 2.0 to interact and pass information and data. All functional components of Oceans 2.0 use it to asynchronously intercommunicate.

The *Driver Manager Service and Instrument Interface* represent the part of the software that interacts with instruments and their integrated sensors. The software standardizes access to instruments and generalizes their data structures so that they can be used downstream by other software

Figure 3. Elements of Oceans 2.0 and their relationship from sensor data generation to the archive and users.

components. Another critically important role of the drivers is their time stamping function that guarantees the same time reference across all the instruments connected to all of the supported networks. Once a raw data record is obtained from an instrument, the driver publishes it to the service bus that subsequently makes it available for other software elements in the system. Oceans 2.0 has drivers for more than 100 different types of instruments from a variety of manufacturers.

Parsing & Calibration, QA/QC is the software module that takes the raw readings from instruments and turns them into meaningful, corrected values, possibly after an optional calibration stage. Moreover, a level 0 automated calibration can be configured to flag sensor values that are out of range.

Event Detection is used to create custom reactions for real-time events. Users can create event definitions using algebraic formulas or other triggers, and associate appropriate reactions if the event occurs. Event Detection currently has several use cases within Oceans 2.0: it is used to perform Quality Assurance and Quality Control (QA/QC) evaluations, and to synchronize acoustic device sampling so as to prevent interference. Another, significantly more advanced event detection system is the ability to detect P-wave from accelerometers, helping with the detection and characterization of earthquakes.

Data Archive takes all data traffic between the instruments and the "surface" side and archives them.

Data Processing indicates the part of the system where data products are generated from the raw data. These include data format conversion, plots and images, etc.

User Services includes a combination of data access and visualization tools, using either a web interactive interface, an application programming interface consisting of standard-abiding web services and a "sandbox" where users upload data processing codes and run them.

Security and resilience. The security of the system against malevolent or accidental access by unexpected parties is provided by isolation of all the key component in secure, private and non-routable networks. The Oceans 2.0 architecture has also been designed around resilience, in particular for the data acquisition component including: fault tolerance in case of network path breakdown, multiple safeguards to minimize data loss in case of unexpected anomalies; and, support of multiple archive centres containing integral data copies.

Americas Lightpaths (AmLight) supporting NSF Large Facilities and CI in the Americas

White Paper for NSF Large Facilities Cyberinfrastructure Workshop

Florida International University (FIU) is the awardee of the NSF International Research Network Connections (IRNC) program, under cooperative agreements, to build and operate the network infrastructure that links the U.S. research networks with peer networks in South America and the Caribbean. This network infrastructure, referred to as AmLight, consists of multiple 10/100 Gbps links, presently totaling 240Gbps of aggregate bandwidth capacity between the U.S. and South America; an international exchange point facility in Miami, Florida, called AMPATH, which terminates the many network connections that depart from the U.S. to, and that arrive from, the research and education networks of the nations of South America, and the Caribbean. FIU has been performing this role on behalf of the NSF since 2005.

Science data flows between NSF Large Facilities or CI, operating in South America or the Caribbean, benefit from the use of the AmLight network links and the network infrastructure that connect these large facilities or CI back to the U.S. AmLight network links are built and operated by network operators whose purpose it is to support research and education communities.   The commitment to collaborate and coordinate among the network operators is underpinned by agreements (MOUs) FIU established with the network operators participating in AmLight. For example, in the U.S., network operators are primarily FIU, Florida LambdaRail (regional network in Florida), Internet2 (U.S. national research and education network), ESnet (U.S. national research and education network), and a few others. In South America, network operators are primarily RedCLARA (regional network of Latin America), RNP (national research and education network of Brazil), ANSP (Academic Network of Sao Paulo), REUNA (national research and education network of Chile), and others.

Remote users of NSF Large Facilities in South America or the Caribbean depend on reliable network services to access CI for their research. For example, this could be a low latency network service to remotely control a telescope in Chile, or a higher throughput network service to transfer a large LHC data set from a data center in Sao Paulo to Fermi Lab. Impacts to network services, caused by fiber cuts, power outages, retransmits, etc., will significantly impact applications using CI at NSF Large Facilities. The impact could render the science application inoperative when the NSF Large Facility and the CI are continents apart. For example, a fiber cut will impact a science data flow from an observatory in Chile to the NCSA data center in Champaign, Illinois. Fortunately, networks participating in AmLight have instrumented their networks with monitoring and measurement instruments to detect network impacting events. Data collected from these instruments enable network operators to represent the conditions on the networks that constitute the end-to-end path of the data flow. To inform users of CI at NSF Large Facilities, a web-based interface is available that shows network conditions for many of the interconnection points along the networks between the U.S., South America and the
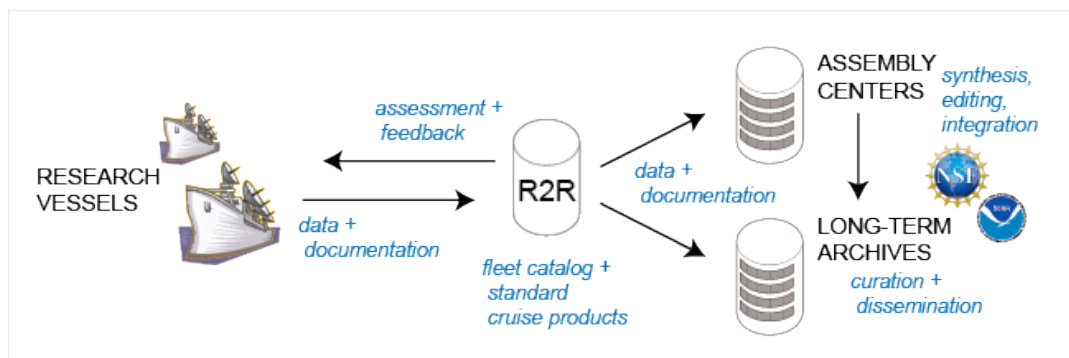
Caribbean. With the web-based interface and other deployed tools, AmLight is achieving its goal to improve detection of network impacting events and to minimize their impacts on science data flows.

Flows of science data between endpoints is a very important unit of measure for AmLight. Flows should experience little to no friction along the end-to-end path. The end-to-end path should be instrumented to monitor and measure network conditions that could impact science data flows. Mechanisms, such as a Science DMZ or Data Transfer Nodes (DTN), should be considered as best practices to reduce friction on science data flows. AmLight can facilitate the implementation and use of these mechanisms for NSF Large Facilities and CI.

The Rolling Deck to Repository Program Marine Data Services for the US Academic Research Fleet

Mission

The Rolling Deck to Repository (R2R; www.rvdata.us) program documents and preserves environmental sensor data acquired during scientific expeditions on U.S. academic research vessels. The program is a collaborative effort between Lamont-Doherty Earth Observatory, Florida State University, Scripps Institution of Oceanography, and Woods Hole Oceanographic Institution; and works closely with the University-National Oceanographic Laboratory System (UNOLS; www.unols.org), whose membership includes 58 U.S. academic institutions supporting oceanographic research worldwide. R2R is funded primarily by the National Science Foundation with support from the Office of Naval Research and the Schmidt Ocean Institute.

Products and Services

Each research vessel delivers a package of original/unprocessed navigational, geophysical, oceanographic, and meteorological data from its permanently installed sensor systems to R2R at the end of an expedition, along with a manifest that provides the vessel ID, cruise ID, title, start/end dates and ports, and science party members. R2R deposits a copy of each package to private offline storage segments at both the NOAA National Centers for Environmental Information (NCEI) and Amazon Glacier. Each package is then broken out into individual datasets according to sensor type, make, model, and file format; and a master catalog of expeditions and datasets is published online via the R2R Web site. A Digital Object Identifier (DOI) is published for each expedition as well as for each dataset. After permission is granted by the Chief Scientist, individual datasets are posted for public download via the R2R Web site. Selected datasets are submitted to NCEI for dissemination and inclusion in global syntheses.

R2R assesses the quality of selected data types, using a scripted workflow and criteria developed in collaboration with specialists in the science community. The assessment results are published online via the R2R Web site, and standard ratings are calculated as part of feedback to vessel technicians. R2R also produces a standard set of data products after each expedition including quality-controlled shiptrack navigation, underway geophysical profiles (gravity, magnetics, bathymetry), water column depth profiles from CTD hydrocasts, and real-time

meteorology/near-surface oceanography; all of which are posted for public download via the R2R Web site. R2R supports an Event Logger application, including a shipboard microserver, to assist science parties in documenting their scientific sampling while underway.

The R2R program interoperates with 14 other data repositories, primarily NSF-sponsored, that manage other kinds of marine data content related to cruises inventoried in the R2R Catalog. The data content hosted in these repositories includes data acquired with specialized science party instruments and national instrument facilities, scientific sampling logs and associated laboratory analyses, as well as processed data products derived from field data, global synthesis products, and links to articles in scientific journals. A suite of Web-based services support interoperability including a OGC Web Feature Service (WFS) that provides shiptrack geometries; a Catalog Service for Web (CSW) that provides ISO 19139 XML records for expeditions; a W3C "Linked Data" graph and associated RDF Query Language (SPARQL) endpoint for Semantic Web clients; and customized Atom+GeoRSS feeds for partner programs such as OOI and ECS. The complete inventory of expeditions and datasets in the R2R Catalog are discoverable in global research indexes such as DataCite (http://search.datacite.org).

Infrastructure

R2R's computer infrastructure is primarily located on the LDEO campus of Columbia University in Palisades, New York, with selective extensions to commercial providers. The LDEO campus cluster consists of six Dell Linux-based servers, six ACNC fiber storage arrays, and a supporting local network of switches/routers, firewalls, and environmental monitors, split between two buildings. Hardware is typically refreshed on a 5-year cycle. Monitoring and backups are implemented via the Nagios and Bacula open-source packages. The application infrastructure is open-source software consisting of Apache Httpd/Tomcat, PostgreSQL, and PostGIS backends. Programming is primarily PHP and Shell scripting, managed in GitHub private repositories, using open-source libraries such as GDAL and MB-System. Commercial provisioning is used for outward-facing Web services such as the R2R Search page (Linode.com), and an off-site backup copies of R2R data packages received from all research vessels are stored in a Amazon Web Services Glacier vault in the US-West-2 (Oregon) zone.

NSF Large Facilities Cyberinfrastructure Workshop

Oregon State University College of Earth, Ocean, and Atmospheric Sciences:

Regional Class Research Vessel Project, http://ceoas.oregonstate.edu/ships/rcrv/

<u>Science Mission:</u> The coastal ocean encompasses the most complex range of oceanic phenomena on the globe. Coastal regions are sensitive to human alteration from water and air pollution, resource extraction, transportation, and recreational activities. Wind- and freshwater-driven coastal ocean flows directly affect regional climate. As conveyors for heat and salt and regions of strong vertical mixing, boundary currents play an outsized role in the large-scale ocean circulation. Vigorous interactions between the coastal ocean and the atmosphere control many biogeochemical processes (e.g., the exchange of macronutrients and micronutrients between the land, ocean, and continental margin sediments).

The coastal oceans are extremely productive, accounting for a large percentage of the world's wild seafood and most of the aquaculture. They are the dominant sites for burial of organic matter, important in net marine uptake of atmospheric CO_2, and locations of major hydrocarbon resources, including oil, gas, and methane gas hydrate. The coastal oceans can be sites of wind and wave energy extraction, play host to the deposition of river sediments, including dredge spoils, and are sites of tectonic activity, including hazardous earthquakes and tsunamis. To better understand such coastal phenomena and their importance in the Earth system, ocean scientists and educators must accelerate exploration and sustained regional observations of marine physical, chemical, biological, and geological processes.

Even with the development of new platforms to study the ocean—such as cabled observatories and underwater robots— coverage is scant, and ships are more vital than ever for multi-disciplinary observations and sampling of the ocean. The RCRVs will feature advanced sensors and sampling systems, and through telepresence capabilities and satellite communications, will bring science at sea to classrooms, the public, and researchers ashore. Oregon State is proud to be leading the charge in developing next-generation vessels that promise state-of-the-art platforms for the nation's scientists and students to explore our ocean planet

<u>Facility size & composition during construction:</u> Core team - OSU = 15 (members), Engineering & Design Support - The Glosten Associates = 4, Science Oversight Committee = 11

<u>Facility size & composition when operational:</u> OSU Class Management Office = 4, OSU Ship Operations = 15, Institution Two = approx. 15, Institution Three = approx. 15.

<u>Key Products and Services:</u> Oceanographic research ships, and the Regional Class Research Vessels specifically, are the primary platform from which ocean science is conducted. A research vessel must function as observatory, lab, and accommodation.   Therefore the facility must provision cyberinfrastructure for the research enterprise, for vessel operations and for quality of life. In addition to these core services the RCRV facility shall also provide a system

for real-time bi-directional transfer of data and information between shipboard and shoreside parties.

To support these requirements we've developed a system for sensor data transmission, capture, archive, replication, and use. The system incorporates a variety of open-source and commercial products including, Enterprise DB Postgres Advanced Server, Apache, Django, Highcharts, Tableau, Mapserver, Leaflet, and ERDDAP.

Facility Cyberinfrastructure: The figure below describes the basic architecture, components, and services of the RCRV Datapresence System. The system is currently under development and testing and has been deployed successfully during prototype cruises.