

Report on

WORKSHOP ON CYBERINFRASTRUCTURE FOR POLAR SCIENCES

Minneapolis, MN
September 10–12, 2013



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ISSUES



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A Organizing Committee Members

B Workshop Participant Photo

C Acknowledgements

EXECUTIVE SUMMARY

Workshop Background

The Polar Cyberinfrastructure Program at the National Science Foundation has the potential to transform polar research by facilitating the transmission and integration of data and knowledge across the polar science and polar cyberinfrastructure (CI) communities. Community input is essential to ensuring that the infrastructure investments meet the on-the-ground requirements of scientists. For the program to meet the needs of the polar science community, stakeholders from the broadest range of science domains must be engaged in defining and communicating their CI needs and desires. NSF sponsored this Workshop on Cyberinfrastructure for Polar Sciences to engage polar and computer scientists and engineers to inform its Polar Cyberinfrastructure Program, to complement the EarthCube experience, and to ensure that the CI needs for this community are understood, articulated, integrated, and aligned with the overall plans and design of a Polar Cyberinfrastructure Strategic Plan.

Workshop Goal

The workshop goal was to identify, characterize, and provide recommendations to design, develop, and optimize a comprehensive CI for polar sciences.

The workshop and this report address engagement and connections between computer and polar sciences concerning what can be accomplished in the short term (2–5 years). The outcomes of this workshop will inform NSF's Polar Cyberinfrastructure Program concerning past and current polar CI activities and will provide support for a community-driven design and architecture development of a polar science CI that is aligned with the following end users' needs:

- 1 long-term sustainable curatorship, standardization, management, and discovery of data and metadata; visualization, manipulation, and analysis
- 2 high-performance computing (HPC) capability
- 3 infrastructure to handle big data and data access
- 4 interoperability with data from other domains
- 5 e-learning and educational tools based on CI components
- 6 virtual organizations

Workshop Recommendations

Workshop participants were asked to list top polar CI component needs. When responses were categorized and integrated, four stood out as priorities for the coming 2–5 years:

1 DATA AS A SERVICE (DAAS). DaaS is clearly a common denominator and should be emphasized in program opportunities within the next two years. The goals are to provide on-demand data sharing through discovery, access, transportation, and delivery to the end user. The DaaS recommendation includes both data production and consumption, since the interface between the two requires interoperability on each side; this should be viewed, managed, and implemented according to system engineering best practices to ensure openness and platform independence.

2 EDUCATION AND TRAINING. A variety of training forms, ranging from informal workshops to formal education, is essential to maintain a sustainable and cutting-edge polar CI to enable polar sciences.

3 COMMUNICATION AND NETWORKING. Networking continues to be a major bottleneck in polar sciences. This includes syncing data with data centers when conducting fieldwork and freely moving data for polar research across data centers.

4 COMMUNITY BUILDING. Polar CI is an emerging community crossing many disciplines, and the community needs proper mechanisms to improve awareness, advance building and utilization, and sustain the evolution of polar CI.

Other scientific workflow components, notably modeling and data analysis (including visualization and algorithms and software) should be addressed by subsequent workshops and their planning horizons blended with these recommendations. In addition, elements of analysis and visualization and algorithms and software that enter into the data production process should be more completely considered by future efforts.

The overall workshop goal was to identify, characterize, and provide recommendations to design, develop and optimize a comprehensive cyberinfrastructure for polar sciences. Plenary talks and breakout sessions were structured to work toward reaching community consensus on the definition of polar CI, the state of the art of CI for polar sciences, and the focused target areas for development and improvement in the next 2-5 years. Outcomes of this workshop, and the report recommendations, will serve as a reference for the polar CI program.

Workshop Description

The Polar Geospatial Center hosted the National Science Foundation–sponsored Workshop on Cyberinfrastructure for Polar Sciences on September 10–12, 2013, at the University of Minnesota McNamara Alumni Center. More than 60 scientists from the polar science and CI communities attended; others participated virtually.

The workshop featured invited talks, plenary discussions, and breakout sessions. The third day was reserved for the organizing committee and select participants to begin framing and drafting the workshop report. Web-based access to the plenary presentations and discussion for remote participants was provided via UMConnect (Adobe Acrobat Connect) streaming. Plenary talks (downloadable as PDF documents) and videorecorded presentations are available at www.pgc.umn.edu/meetings/cyber2013.

Workshop Objectives

The goal of the workshop was to identify major research, data management and access, and modeling challenges and opportunities, and to provide feedback on potential directions for NSF's Polar Cyberinfrastructure Program.

The workshop sought to identify similarities and differences in how CI programs serve polar sciences and other disciplines. It also addressed engagement and connections between computer and polar sciences concerning what can be accomplished in the short term (2–5 years) and long term (5–10+ years). The outcomes of this workshop will inform the NSF's Polar Cyberinfrastructure Program concerning the past and current polar CI activities and will provide support for a community-driven design and architecture development of a polar science CI that is aligned with the

following end-user needs: (1) long-term sustainable curatorship, standardization, management, and discovery of data and metadata; visualization, manipulation, and analysis; (2) use of high-performance computing (HPC) for direct and sustainable advances in polar research; (3) infrastructure to handle big data and data access; (4) interoperability with data from other domains; (5) e-learning and educational tools based on CI components; and (6) virtual organizations.

The workshop was structured to provide responses to the following requests:

- Identify what CI support is currently available to the polar science community and whether it needs to be upgraded.
- Create a ranked list of science drivers and challenges made tractable by transformative CI that the community aims to tackle on a 1- to 5-year and 5- to 10-year time frame within the polar sciences, Arctic, and Antarctic communities.
- Develop a list of data and CI barriers/limits to further advancing polar science and suggest ways to overcome these barriers.
- Produce a list of community CI resources that should be developed, created, or made easier to allow polar scientists to do the important science they want to do now and in the future.
- Create use cases that illustrate the transformational science that could take place if provided sufficient CI and data tools.

SCIENCE DRIVERS

Two major research thrusts drive the need for improved polar CI.

First, because change at the poles influences and has become emblematic of the rapid change occurring across the globe, scientists are increasingly seeking to measure changes in the polar regions, understand the processes driving them, and put them into the framework of changes that have occurred through geologic time. These efforts are inherently multidisciplinary because the drivers of change occur across both physical and disciplinary boundaries. For example, understanding the processes that drive the rapid increase in flow in the Pine Island Glacier in West Antarctica demands interdisciplinary collaboration spanning atmospheric scientists, oceanographers, glaciologists and marine geologists, with a breadth spanning observational and modeling expertise. Quantifying the impact of change at the poles and developing strategies requires a more refined understanding of the rates of change and improved projections of future change than currently exists. Efforts to achieve this understanding are computationally intensive and will involve large quantities of data by today's standards, and increasingly will require improved linking of polar measurements and computer models. Beyond the global impacts, polar processes such as changing sea ice may influence large-scale features such as the location of the jet stream. Active research is ongoing to evaluate the role changing sea ice has on droughts in the Midwest, extreme precipitation, and the track of Hurricane Sandy. Polar processes are critical to global systems.

Antarctica and the Arctic are also important platforms for astronomical and upper atmosphere observatories. In addition to ongoing upper atmospheric research in both Antarctica and the high north, astronomical observatories on the high Antarctic plateau and the Antarctic coast regularly contribute to frontline astrophysical research. One current and large Antarctic-based experiment, IceCube, focuses on high-energy neutrinos, which can help us understand the origin of cosmic rays and seeks to learn more about gamma ray bursts, supernovae, and identify dark matter. Projects such as this, that use the poles as convenient platforms for science,



are equally challenged by many of the unique CI demands that befall Earth Science focused on the coldest, most remote parts of our planet. Therefore, the scope of polar CI extends to Space Science with the same logistical challenges as Antarctic and Arctic Geology, Geophysics, Oceanography, Meteorology, Glaciology, Hydrology, Biogeochemistry and Ecology and interdisciplinary research therein.

CI APPROACHES INFORMED BY SCIENCE DRIVERS

Polar science is a particularly challenging environment for CI because it often takes place in regions with poor Internet communications. The need for CI support occurs at every stage of the Data-Information-Knowledge-Wisdom (DIKW) pipeline (FIGURE 1).

An example of the DIKW process is the Center for Remote Sensing of Ice Sheets (CReSIS, University of Kansas) use case #43, recorded at bigdatawg.nist.gov/usecases.php. Raw data is taken from instruments and loaded onto disks that are used for spot field analysis or transported to CONUS (Continental US) where they are loaded onto disk/tape with metadata, including geolocation, added. Images of ice sheets, glaciers, and snow are run through radar analysis codes to produce a set of images recording radar signals. The result is processed, corrected, labeled data (Information). The radar

images are then analyzed by manual or (semi)-automatic machine learning codes to determine ice sheet or snow layers (Knowledge). This knowledge can be used in simulations or other analyses that give models for glacier melting and feed into IPCC assessments (Wisdom).

Data as a Service (DaaS) will serve as a key building block in the future development of polar CI. In the context of this report, we define DaaS as: On-demand data sharing through discovery, access, transportation, and delivery to polar scientists. Five research areas—data management, data services, data curation, metadata, and data portal—were identified. In terms of data management, concerns were raised for maintaining the long-term polar data. Several efforts, including Advanced Cooperative Arctic Data and Information Service (ACADIS), Integrated Earth Data Applications (IEDA), and National Snow and Ice Data Center (NSICD) are in place to maintain polar

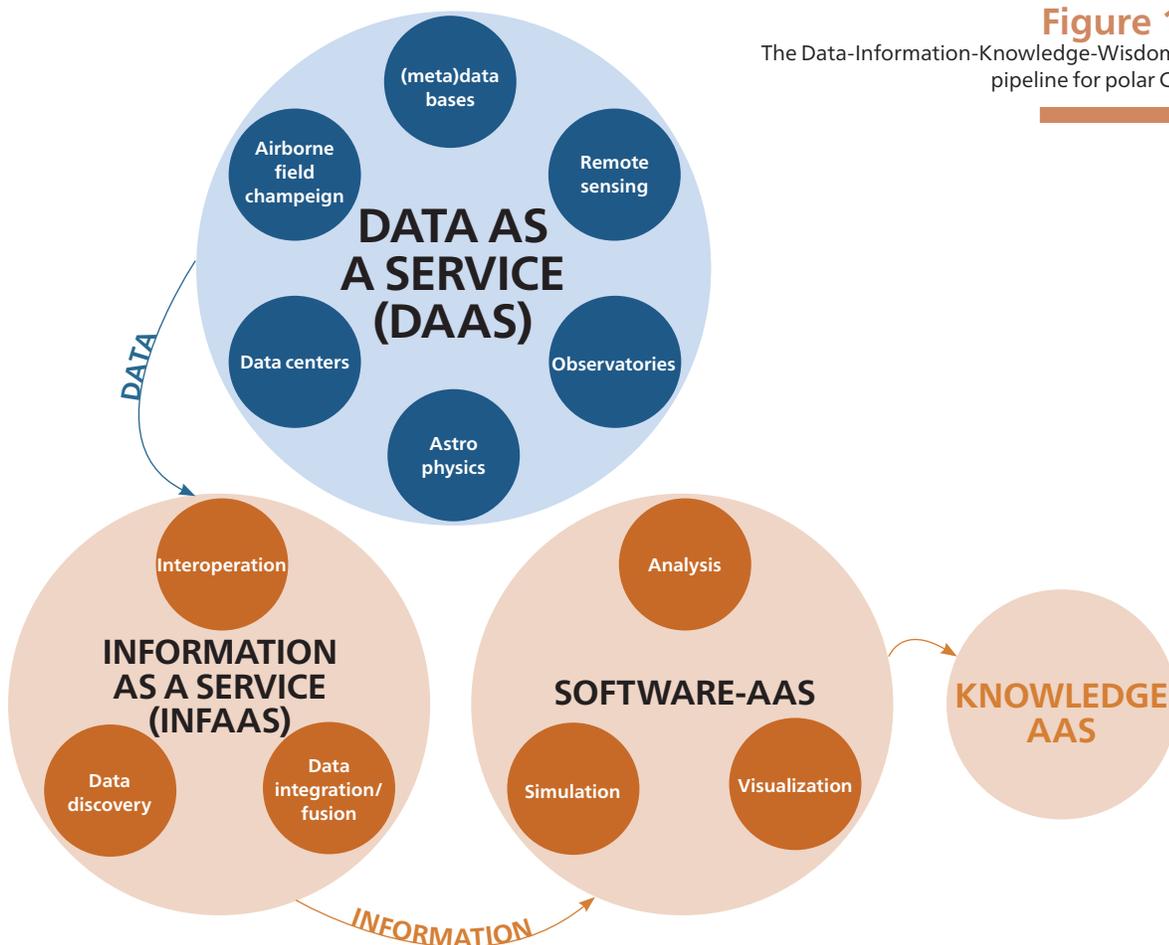


Figure 1
The Data-Information-Knowledge-Wisdom pipeline for polar CI

CI Approaches Informed by Science Drivers

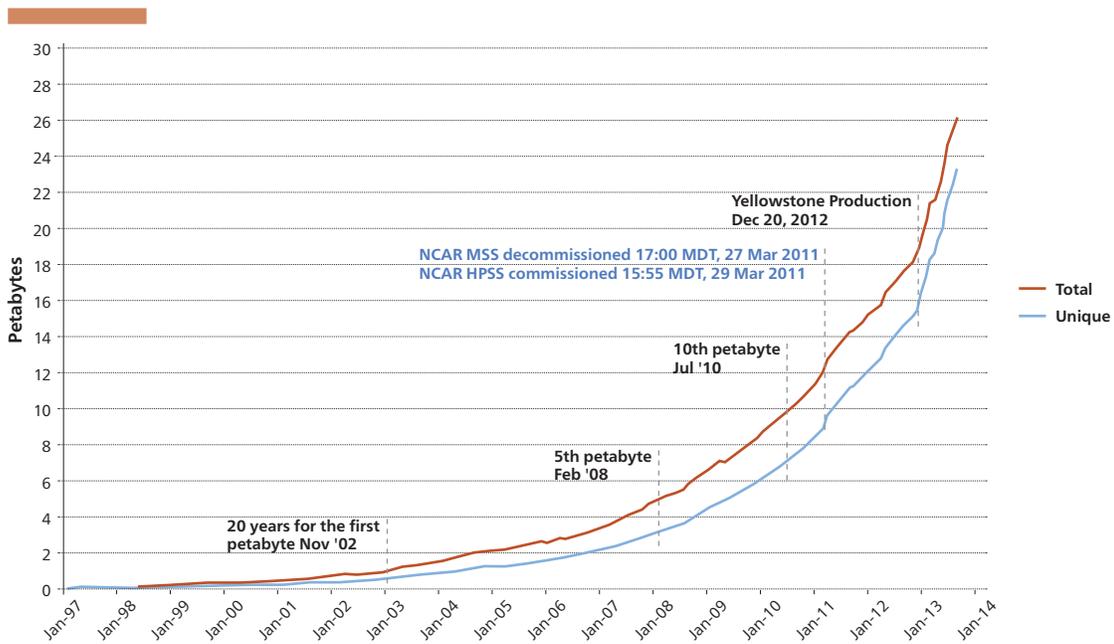


datasets acquired via Earth-observing satellites, airborne field campaigns, observatories, etc. Each data center/repository provides an interface/portal to help users find relevant datasets. Datasets are highly heterogeneous, structured in formats ranging from ASCII text, to Excel files, to self-describing binaries using established metadata protocols, such as NetCDF files using the Climate and Forecast (CF) convention. Interoperability among datasets across polar

data centers/repositories is a huge challenge. This is a result of many factors, including security, management difficulty, policy, social behavior, field convention and the legacy of past disciplinary conventions.

Model output for polar regions is usually curated separately from observational data, often organized around requirements for intercomparison or reanalysis, and typically housed by organizations responsible for model development. As a result the

Figure 2
NCAR Archive Data Growth



NCAR unique and total (includes duplicate copies) archive storage has grown exponentially since 1997 with the milestones of the Mass Storage System (MSS), High Performance Storage System (HPSS) and upgrade to the Yellowstone high performance computer (figure courtesy of the National Center for Atmospheric Research Computational and Information Systems Laboratory).



National Research Council (2012) has advocated CI targeted to better support distributed model development and analysis. Needed functions include effortless creation and sharing of code repositories without hosting a server, cloud-based model inputs and output, and sophisticated analysis tools to meld observations with output from model hierarchies and ensembles.

Also needed are sufficient capacity to accommodate model horizontal resolutions less than 10 km for land, atmosphere, ocean-sea ice, ice sheet, and glacial codes, with compatible high vertical and temporal resolution, and the ability to partition these services into restricted and public access cloud spaces. A critical issue facing the polar modeling community is that efforts to improve parallel computing resources to meet polar science's demand for increased resolution are outpacing capacity to transmit, analyze, and store the output (FIGURE 2).

Another major issue is the need for well-established documentation for all kinds of metadata. Though multiple metadata standards exist, interoperability is not a pressing issue, since this has been well studied in the GIScience field. What captured workshop attendees' attention is whether the metadata is informative enough. Polar scientists need provenance, content, format, and quality information to identify the right dataset, evaluate uncertainty, and ensure the replicability of scientific workflows.

In addition, polar datasets need to be accessible. Each data center/repository serves as an access point to its own data holdings, and few efforts have been made to provide an integrated picture of what datasets are available for polar studies. Scientists tend to use datasets

they have ready access to, so limited awareness of resources may be a limiting factor in our ability to understand the polar ecosystem. Tools that can automatically discover and provide central access to distributed polar data resources are urgently needed.

The workshop also touched on other building blocks, such as computing infrastructure, for moving polar CI forward. These tend to be at the “Information to Knowledge” stage of the DIKW pipeline. One example is the GPS data for the GNET and ANET polar networks (about 110 polar stations), which measure loading due to ice changes around the ice sheets in order to find the Glacial Isostatic Adjustment correction that forms (by far) the largest uncertainty in the GRACE satellite cryosphere mass budget. Currently it takes 12 weeks on a 128-core cluster to process the data.

Another major area of need discussed at the workshop relates to large-scale simulation of glacier flow and other snow and ice phenomena. Here CI has developed sophisticated algorithms and software, and environments like XSEDE provide major supercomputer resources. Software includes libraries to support simulations, data storage and transport, and portals and workflow that can support, for example, multidisciplinary ocean, atmosphere, and polar models. These simulations produce large output datasets, causing storage challenges.

Finally, workshop discussions relating to open access to data recognized the emergence of evolving community standards and conventions for data citation and release—notably the use of digital object identifiers for data citation in the context of open-access to data CODATA-ICST 2013.

RECOMMENDATIONS

Workshop participants were asked to list top polar CI component needs. When responses were categorized and integrated, four stood out as priorities for the coming two years:

- 1 DATA AS A SERVICE (DAAS)**
- 2 EDUCATION AND TRAINING**
- 3 COMMUNICATION AND NETWORKING**
- 4 COMMUNITY BUILDING**

Other scientific workflow components, notably modeling and data analysis (including visualization, algorithms, and software) need to be addressed by subsequent workshops and their planning horizons blended with these recommendations. In addition, elements of analytics, visualization, tools, and scientific modeling that enter into the data life cycle should be more completely considered by future efforts.

Data as a Service

Data was the most highly emphasized CI component during this workshop and the most mentioned term in the workshop priorities survey. DaaS is clearly a common denominator and should be emphasized in program opportunities within the next two years. The goal is to provide on-demand data sharing through discovery, access, transportation, and delivery to polar scientists. The motivation is to accelerate scientific progress and interdisciplinary research within and beyond the polar science communities. DaaS recommendations include both data production and data consumption, since the interface between the two requires interoperability on each side and this should be viewed, managed, and implemented according to system engineering best practices to ensure openness and platform independence. The goal is to achieve a balance between standardization and innovation on both sides of the interface.

Data Curation

To implement DaaS, data curation should consider sustainability, storage, and open access to data through community data, metadata, and Application Program Interface (API) standards as follows:

- Understand and automate, where possible, the components supporting the polar science workflow.
- Allocate funding in NSF awards to support data management.
- Recommend investigators include in grant applications a plan for working with data curation specialists (e.g.,

- federal data centers) at the beginning of their project to establish data management strategies and mechanics.
- Establish a matrix of CI components for inclusion in the data management plan to assess data management gaps and share the data management responsibility among sponsor institutes and individual PIs.
- Require investigators to harmonize their proposed data with the system science perspective and provide incentives to follow through.
- Encourage interoperability (e.g., standards-based interface protocols) across all steps of the scientific workflow.
- Provision storage in a way that improves capacity and reduces latency in support of the DaaS goals.
- Develop methods for data quality assurance, uncertainty characterization and propagation of errors, and provenance articulation.
- Provide for the sustainability of long-term data for polar regions.
- Provide curators and mediators to mediate between information stakeholders and science experts.
- Leverage implementers who can help scientists better collect and document data.
- Ensure data curators are aware of limitations due to data quality, and that these limitations are accurately reflected in metadata.

Data producers and consumers should jointly support community-specified best practices in line with these further recommendations:

- Understand and support the role of curators who can mediate between data producers and consumers.
- Ensure data curators understand the scientific basis underlying data and metadata content in support of the need for complete and consistent searching and sharing of metadata.
- Encourage investigators to work with data curators in their disciplines (e.g., federal data centers) at beginning of their project in support of their data management plans.

Data Management

Data management should take a system engineering approach that considers data sustainability and storage capacity and encourages data sharing through community consensus standards when designing and implementing projects. The workshop yielded these detailed recommendations:

- Understand and automate, if possible, the components supporting the workflow from data to information to knowledge.
- Add a percentage for data management to all

- NSF awards.
- Encourage interoperability (e.g., standard-based) protocols for data collection, metadata generation, data sharing, data services, data analytics, modeling, and cross-domain integration.
- Build large-scale (10–50 PB) server farms at geographically optimized locations, such as Alaska, Minnesota, Antarctica, and California.
- Maintain data quality, uncertainty, and provenance.
- Develop a strategy for maintaining a long-term data record for polar regions.
- Establish a CI matrix as part of a data management plan to assess data management gaps and share the data management responsibility among sponsor institutes and individual investigators.

Data Services

Serving data online by leveraging the latest CI advancements is critical to help polar scientists better conduct research. Workshop participants made the following recommendations:

- Post all data center holdings, especially the polar gridded/raster data, via web services, such as OGC web services.
- Leverage technologies, such as cloud computing, that foster near real-time data availability to the community, and ensure that key technologies currently relied upon for near-real-time data are adequately funded and maintained.
- Build a set of services for data processing.
- Promote as examples projects demonstrating strength of open data access and zero latency in providing data service by encouraging awardees to use both their own data and other available data via an online data service.
- Ensure data services are sharable within and across communities.
- Build interfaces to incorporate Long Term Ecological Research Network (LTER) into observational data to create hybrid datasets of timeline Earth Observing System (EOS).

Data Archiving, Discovery, and Access

Polar data are diversified, heterogeneous, and hard to find. Workshop participants recommended that polar CI efforts consider putting polar data online and making it possible to:

- Access existing data repositories and approaches.
- Access all polar data through interfaces with existing catalogs.
- More easily search using ontology and semantics.
- Post all data center holdings, especially the polar gridded/raster data, via web services such as OGC web services.
- Leverage technologies, such as cloud computing, that foster near real-time data availability to the community.

- Build popular and lightweight processing (e.g., reprojection, integration, subsetting).
- Improve consumer searching of existing data repositories.
- Unify interfaces or build a one-stop portal to provide discovery and access to all available polar data across existing metadata catalogs.
- Improve searching using community-based ontology and semantics.

Data Analysis and Modeling

Workshop participants recommended that polar CI efforts:

- Promote tools for sharing high-throughput computing (HTC) or high-performance computing (HPC) resources from different labs.
- Promote the creation of an “NFSCloud” infrastructure to facilitate broader access to big (efficient, cheap) data centers.
- Develop cloud-based analytical tools.
- Carry out data fusion demonstration projects.

Education and Training

Training, ranging from informal workshop to formal education, is essential to maintain a sustainable and cutting-edge polar CI. Workshop participants made the following detailed recommendations:

- Hold sessions at professional meetings to improve understanding of the importance of data management.
- Provide data, metadata, and CI best practice training as a part of field training.
- Encourage mutual workshops/training to help polar CI experts understand science drivers and help polar scientists understand CI capabilities.
- Provide best practices for how CI experts and investigators can collaboratively leverage CI to foster polar research.
- Promote opportunities for data users and providers to learn how to implement and use web services.
- Develop courses to prepare new scientists with skills needed to solve data-driven problems in geoscience research.
- Develop a training curriculum/certificate for polar CI.
- Encourage early-career polar CI investigators.

Communication and Networking

Networking to sync data with data centers when conducting field work and to freely move data for polar research across data centers is still a big bottleneck in polar sciences. The committee recommends polar CI:

- Establish smart phone sensor polar network communication.
- Increase satellite bandwidth for scientists conducting polar field trips to move the data from/to the

Recommendations

- pole regions.
- Supply fast and reliable Internet connection for polar research.
- Share and standardize tools for moving data to/from polar regions.

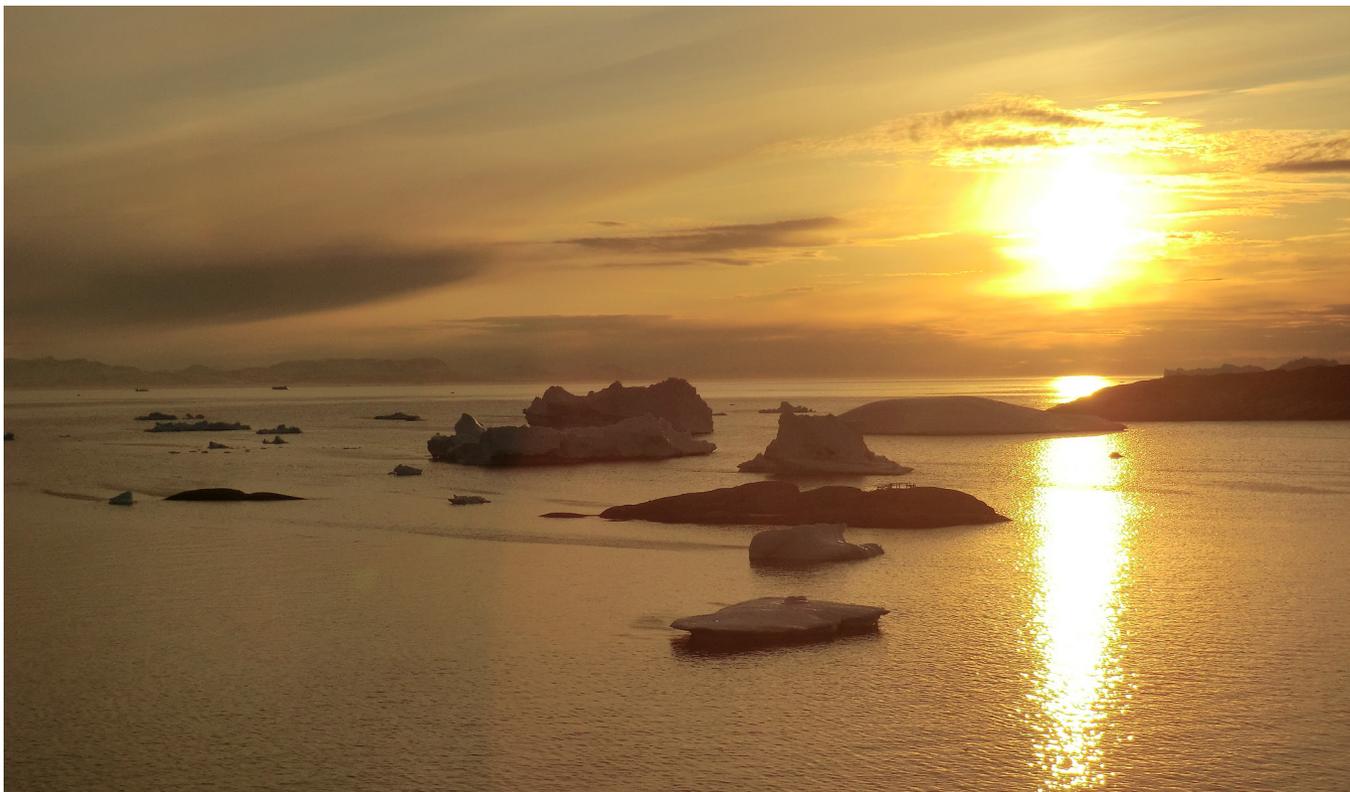
Community Building

The emerging interdisciplinary polar CI community needs mechanisms to improve the awareness, advance the building and utilization, and sustain the evolution of polar CI. Specific recommendations include:

- Provide an environment for CI experts and polar scientists to collaborate.
- Encourage CI experts and polar scientists to share experiences, problems, solutions, and lessons learned.
- Form an alliance of polar scientists, CI researchers, open source communities, government agencies, and data centers to identify additional strategies for working toward an integrated, effective polar CI.
- Continue community coordination through NSF Research Coordination Networks (RCN).
- Collaborate with other initiatives and integrated research programs, such as IARPC.
- Establish a technical working group to develop a comprehensive conceptual system architecture.
- Establish a technical working group to identify best practices for polar CI from other CI projects.

- Establish a community portal to:
 - Create a virtual, online collaboratory where polar scientists can meet, exchange ideas, and do science.
 - Host an inventory of software tools, contacts, experts, collaborators, and locations so community members can easily identify available resources.
 - Facilitate the development of a common language and definitions (ontology and semantics).
 - Provide a one-stop listing of polar CI resources (funded by NSF, NASA, NOAA, USGS and other agencies), such as those from GINA, PGC, NSIDC, NASA DAACs, NGDC and the Antarctic and Southern Ocean Data Portal at Lamont-Doherty Earth Observatory.

As outlined in this report, there are many fundamental issues that need to be addressed to meet the challenges of polar CI. Data was the most highly emphasized CI component during the workshop and the most mentioned term in the workshop priorities survey. The developments we envision have the potential to dramatically change the way polar scientists interact with data, whether through discovery of existing data, providing context for new data, characterizing and comparing disparate datasets, or archiving data, in ways that will enable new questions to be answered and existing challenges to be addressed.



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APPENDICES



NSF Workshop on Cyberinfrastructure for Polar Sciences group participants at the University of Minnesota McNamara Alumni Center. Photo courtesy of Mark Parsons, Rensselaer Polytechnic Institute.

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