**NIST Big Data**

**General Requirements**

**Version 0.1**

**Requirements & Use Cases Subgroup**

**NIST Big Data Working Group (NBD-WG)**

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# Executive Summary

# Introduction

## Background

There is a broad agreement among commercial, academic, and government leaders about the remarkable potential of “Big Data” to spark innovation, fuel commerce, and drive progress. Big Data is the term used to describe the deluge of data in our networked, digitized, sensor-laden, information driven world. The availability of vast data resources carries the potential to answer questions previously out of reach. Questions like: How do we reliably detect a potential pandemic early enough to intervene? Can we predict new materials with advanced properties before these materials have ever been synthesized? How can we reverse the current advantage of the attacker over the defender in guarding against cybersecurity threats?

However there is also broad agreement on the ability of Big Data to overwhelm traditional approaches. The rate at which data volumes, speeds, and complexity are growing is outpacing scientific and technological advances in data analytics, management, transport, and more.

Despite the widespread agreement on the opportunities and current limitations of Big Data, a lack of consensus on some important, fundamental questions is confusing potential users and holding back progress. What are the attributes that define Big Data solutions? How is Big Data different from the traditional data environments and related applications that we have encountered thus far? What are the essential characteristics of Big Data environments? How do these environments integrate with currently deployed architectures? What are the central scientific, technological, and standardization challenges that need to be addressed to accelerate the deployment of robust Big Data solutions?

At the NIST Cloud and Big Data Forum held in January 15-17, 2013, the community strongly recommends NIST to create a public working group for the development of a Big Data Technology Roadmap. This roadmap will help to define and prioritize requirements for *interoperability*, *portability*, *reusability*, and *extensibility* for big data usage, analytic techniques and technology infrastructure in order to support secure and effective adoption of Big Data.

On June 19, 2013, the NIST Big Data Public Working Group (NBD-PWG) was launched with overwhelmingly participation from industry, academia, and government across the nation. The scope of the NBD-PWG is to form a community of interests from all sectors including industry, academia, and government, with the goal of developing a consensus in definitions, taxonomies, secure reference architectures, and a technology roadmap. Such a consensus would therefore create a vendor-neutral, technology and infrastructure agnostic framework which would enable Big Data stakeholders to pick-and-choose best analytics tools for their processing and visualization requirements on the most suitable computing platform and cluster while allowing value-added from Big Data service providers.

Currently NBD-PWG has created five subgroups namely the Definitions and Taxonomies, Use Case and Requirements, Security and Privacy, Reference Architecture, and Technology Roadmap. These subgroups will help to develop the following set of preliminary consensus working drafts by September 27, 2013:

1. Big Data Definitions
2. Big Data Taxonomies
3. Big Data Requirements
4. Big Data Security and Privacy Requirements
5. Big Data Reference Architectures White Paper Survey
6. Big Data Reference Architectures
7. Big Data Security and Privacy Reference Architectures
8. Big Data Technology Roadmap

Due to time constraints and dependencies between subgroups, the NBD-PWG hosted two hours weekly telecon meeting from Mondays to Fridays for the respective subgroups. Every three weeks, NBD-PWG called a joint meeting for progress reports and document updates from these five subgroups. In between, subgroups co-chairs met for two hours to synchronize their respective activities and identify issues and solutions

## Objectives

**Scope**

The focus of the NBD-PWG Use Case and Requirements Subgroup is to form a community of interest from industry, academia, and government, with the goal of developing a consensus list of Big Data requirements across all stakeholders. This includes gathering and understanding various use cases from diversified application domains.

**Tasks**

* Gather input from all stakeholders regarding Big Data requirements.
* Analyze/prioritize a list of challenging general requirements that may delay or prevent adoption of Big Data deployment
* Develop a comprehensive list of Big Data requirements

**Deliverables**

1. Produce a working draft for Big Data General Requirements Document

## How This Report Was Produced

## Structure of This Report

# Use Case Summaries

## Government Operation

### Census 2010 and 2000 – Title 13 Big Data

*Vivek Navale & Quyen Nguyen, NARA*

**Application:** Preserve Census 2010 and 2000 – Title 13 data for a long term in order to provide access and perform analytics after 75 years. One must maintain data “as-is” with no access and no data analytics for 75 years; one must preserve the data at the bit-level; one must perform curation, which includes format transformation if necessary; one must provide access and analytics after nearly 75 years. Title 13 of U.S. code authorizes the Census Bureau and guarantees that individual and industry specific data is protected.

**Current Approach:** 380 terabytes of scanned documents

### National Archives and Records Administration Accession NARA, Search, Retrieve, Preservation

*Vivek Navale & Quyen Nguyen, NARA*

**Application:** Accession, Search, Retrieval, and Long term Preservation of Government Data.

**Current Approach:** 1) Get physical and legal custody of the data; 2) Pre-process data for virus scan, identifying file format identification, removing empty files; 3) Index; 4) Categorize records (sensitive, unsensitive, privacy data, etc.); 5) Transform old file formats to modern formats (e.g. WordPerfect to PDF); 6) E-discovery; 7) Search and retrieve to respond to special request; 8) Search and retrieve of public records by public users. Currently 100’s of terabytes stored centrally in commercial databases supported by custom software and commercial search products.

**Futures:** There are distributed data sources from federal agencies where current solution requires transfer of those data to a centralized storage. In the future, those data sources may reside in multiple Cloud environments. In this case, physical custody should avoid transferring big data from Cloud to Cloud or from Cloud to Data Center.

### Statistical Survey Response Improvement (Adaptive Design)

*Cavan Capps, U.S. Census Bureau*

**Application:** Survey costs are increasing as survey response declines. The goal of this work is to use advanced “recommendation system techniques” that are open and scientifically objective, using data mashed up from several sources and historical survey para-data (administrative data about the survey) to drive operational processes in an effort to increase quality and reduce the cost of field surveys.

**Current Approach:** About a petabyte of data coming from surveys and other government administrative sources. Data can be streamed with approximately 150 million records transmitted as field data streamed continuously, during the decennial census. All data must be both confidential and secure. All processes must be auditable for security and confidentiality as required by various legal statutes. Data quality should be high and statistically checked for accuracy and reliability throughout the collection process. Use Hadoop, Spark, Hive, R, SAS, Mahout, Allegrograph, MySQL, Oracle, Storm, BigMemory, Cassandra, Pig software.

**Futures:** Need to improve recommendation systems similar to those used in e-commerce (see Netflix use case) that reduce costs and improve quality while providing confidentiality safeguards that are reliable and publically auditable. Data visualization is useful for data review, operational activity and general analysis. It continues to evolve; mobile access important.

### Non-Traditional Data in Statistical Survey Response Improvement (Adaptive Design)

*Cavan Capps, U.S. Census Bureau*

**Application:** Survey costs are increasing as survey response declines. This use case has similar goals to that above but involves non-traditional commercial and public data sources from the web, wireless communication, electronic transactions mashed up analytically with traditional surveys to improve statistics for small area geographies, new measures and to improve the timeliness of released statistics.

**Current Approach:** Integrate survey data, other government administrative data, web scrapped data, wireless data, e-transaction data, potentially social media data and positioning data from various sources. Software, Visualization and data characteristics similar to previous use case.

**Futures:** Analytics needs to be developed which give statistical estimations that provide more detail, on a more near real time basis for less cost. The reliability of estimated statistics from such “mashed up” sources still must be evaluated.

## Commercial

### Cloud Eco-System, for Financial Industries (Banking, Securities & Investments, Insurance) transacting business within the United States

*Pw Carey, Compliance Partners, LLC*

**Application:** Use of Cloud (Bigdata) technologies needs to be extended in Financial Industries (Banking, Securities & Investments, Insurance).

**Current Approach:** Currently within Financial Industry, Bigdata and Hadoop are used for fraud detection, risk analysis and assessments as well as improving the organizations knowledge and understanding of the customers. At the same time, the traditional client/server/data warehouse/RDBM (Relational Database Management) systems are used for the handling, processing, storage and archival of the entities financial data. Real time data and analysis important in these applications.

**Futures:** One must address Security and privacy and regulation such as SEC mandated use of XBRL (extensible Business Related Markup Language) and examine other cloud functions in the Financial industry.

### Mendeley – An International Network of Research

*William Gunn, Mendeley*

**Application:** Mendeley has built a database of research documents and facilitates the creation of shared bibliographies. Mendeley uses the information collected about research reading patterns and other activities conducted via the software to build more efficient literature discovery and analysis tools. Text mining and classification systems enables automatic recommendation of relevant research, improving the cost and performance of research teams, particularly those engaged in curation of literature on a particular subject

**Current Approach:** Data size is 15TB presently, growing about 1 TB/month. Processing on Amazon Web Services with Hadoop, Scribe, Hive, Mahout, Python. Standard libraries for machine learning and analytics, Latent Dirichlet Allocation, custom built reporting tools for aggregating readership and social activities per document.

**Futures:** Currently Hadoop batch jobs are scheduled daily, but work has begun on real-time recommendation. The database contains ~400M documents, roughly 80M unique documents, and receives 5-700k new uploads on a weekday. Thus a major challenge is clustering matching documents together in a computationally efficient way (scalable and parallelized) when they’re uploaded from different sources and have been slightly modified via third-part annotation tools or publisher watermarks and cover pages.

### Netflix Movie Service

*Geoffrey Fox, Indiana University*

**Application:** Allow streaming of user selected movies to satisfy multiple objectives (for different stakeholders) -- especially retaining subscribers. Find best possible ordering of a set of videos for a user (household) within a given context in real-time; maximize movie consumption. Digital movies stored in cloud with metadata; user profiles and rankings for small fraction of movies for each user. Use multiple criteria – content based recommender system; user-based recommender system; diversity. Refine algorithms continuously with A/B testing.

**Current Approach:** Recommender systems and streaming video delivery are core Netflix technologies. Recommender systems are always personalized and use logistic/linear regression, elastic nets, matrix factorization, clustering, latent Dirichlet allocation, association rules, gradient boosted decision trees and others. Winner of Netflix competition (to improve ratings by 10%) combined over 100 different algorithms. Uses SQL, NoSQL, MapReduce on Amazon Web Services. Netflix recommender systems have features in common to e-commerce like Amazon. Streaming video has features in common with other content providing services like iTunes, Google Play, Pandora and Last.fm.

**Futures:** Very competitive business. Need to aware of other companies and trends in both content (which Movies are hot) and technology. Need to investigate new business initiatives such as Netflix sponsored content

### Web Search

*Geoffrey Fox, Indiana University*

**Application:** Return in ~0.1 seconds, the results of a search based on average of 3 words; important to maximize quantities like “precision@10” or number of great responses in top 10 ranked results.

**Current Approach:** Steps include 1) Crawl the web; 2) Pre-process data to get searchable things (words, positions); 3) Form Inverted Index mapping words to documents; 4) Rank relevance of documents: PageRank; 5) Lots of technology for advertising, “reverse engineering ranking” “preventing reverse engineering”; 6) Clustering of documents into topics (as in Google News) 7) Update results efficiently. Modern clouds and technologies like MapReduce have been heavily influenced by this application. ~45B web pages total.

**Futures:** A very competitive field where continuous innovation needed. Two important areas are addressing mobile clients which are a growing fraction of users and increasing sophistication of responses and layout to maximize total benefit of clients, advertisers and Search Company. The “deep web” (that behind user interfaces to databases etc.) and multimedia search of increasing importance. 500M photos uploaded each day and 100 hours of video uploaded to YouTube each minute.

### IaaS (Infrastructure as a Service) Big Data Business Continuity & Disaster Recovery (BC/DR) Within a Cloud Eco-System

*Pw Carey, Compliance Partners, LLC*

**Application:** BC/DR (Business Continuity/Disaster Recovery) needs to consider the role that the following four overlaying and inter-dependent forces will play in ensuring a workable solution to an entity's business continuity plan and requisite disaster recovery strategy. The four areas are; people (resources), processes (time/cost/ROI), technology (various operating systems, platforms and footprints) and governance (subject to various and multiple regulatory agencies).

**Current Approach:** Cloud Eco-systems, incorporating IaaS (Infrastructure as a Service), supported by Tier 3 Data Centers provide data replication services. Replication is different from Backup and only moves the changes since the last time a replication occurs, including block level changes. The replication can be done quickly, with a five second window, while the data is replicated every four hours. This data snap shot is retained for seven business days, or longer if necessary. Replicated data can be moved to a Fail-over Center to satisfy an organizations RPO (Recovery Point Objectives) and RTO (Recovery Time Objectives). Technologies from VMware, NetApps, Oracle, IBM, Brocade are some of those relevant. Data sizes are terabytes up to petabytes

**Futures:** The complexities associated with migrating from a Primary Site to either a Replication Site or a Backup Site is not fully automated at this point in time. The goal is to enable the user to automatically initiate the Fail Over sequence. Both organizations must know which servers have to be restored and what are the dependencies and inter-dependencies between the Primary Site servers and Replication and/or Backup Site servers. This requires a continuous monitoring of both.

### Cargo Shipping

*William Miller, MaCT USA*

**Application:** Monitoring and tracking of cargo as in Fedex, UPS and DHL.

**Current Approach:** Today the information is updated only when the items that were checked with a bar code scanner are sent to the central server. The location is not currently displayed in real-time. An architectural diagram is in full description.

**Futures:** This Internet of Things application needs to track items in real time. A new aspect will be status condition of the items which will include sensor information, GPS coordinates, and a unique identification schema based upon a new ISO 29161 standards under development within ISO JTC1 SC31 WG2.

### Materials Data for Manufacturing

*John Rumble, R&R Data Services*

**Application:** Every physical product is made from a material that has been selected for its properties, cost, and availability. This translates into hundreds of billion dollars of material decisions made every year. However the adoption of new materials normally takes decades (two to three) rather than a small number of years, in part because data on new materials is not easily available. One needs to broaden accessibility, quality, and usability and overcome proprietary barriers to sharing materials data. One must create sufficiently large repositories of materials data to support discovery.

**Current Approach:** Currently decisions about materials usage are unnecessarily conservative, often based on older rather than newer materials R&D data, and not taking advantage of advances in modeling and simulations.

**Futures:** Materials informatics is an area in which the new tools of data science can have major impact by predicting the performance of real materials (gram to ton quantities) starting at the atomistic, nanometer, and/or micrometer level of description. One must establish materials data repositories beyond the existing ones that focus on fundamental data; one must develop internationally-accepted data recording standards that can be used by a very diverse materials community, including developers materials test standards (such as ASTM and ISO), testing companies, materials producers, and R&D labs; one needs tools and procedures to help organizations wishing to deposit proprietary materials in data repositories to mask proprietary information, yet to maintain the usability of data; one needs multi-variable materials data visualization tools, in which the number of variables can be quite high.

### Simulation driven Materials Genomics

*David Skinner, LBNL*

**Application:** Innovation of battery technologies through massive simulations spanning wide spaces of possible design. Systematic computational studies of innovation possibilities in photovoltaics. Rational design of materials based on search and simulation. These require management of simulation results contributing to the materials genome.

**Current Approach:** PyMatGen, FireWorks, VASP, ABINIT, NWChem, BerkeleyGW, and varied materials community codes running on large supercomputers such as 150K core Hopper machine at NERSC produce results that are not synthesized.

**Futures:** Need large scale computing at scale for simulation science. Flexible data methods at scale for messy data. Machine learning and knowledge systems that integrate data from publications, experiments, and simulations to advance goal-driven thinking in materials design. The current 100TB of data will become 500TB in 5 years.

## Defense

### Cloud Large Scale Geospatial Analysis and Visualization

*David Boyd, Data Tactics*

**Application:** Need to support large scale geospatial data analysis and visualization. As the number of geospatially aware sensors increase and the number of geospatially tagged data sources increases the volume geospatial data requiring complex analysis and visualization is growing exponentially.

**Current Approach:** Traditional GIS systems are generally capable of analyzing a millions of objects and easily visualizing thousands. Data types include Imagery (various formats such as NITF, GeoTiff, CADRG), and vector with various formats like shape files, KML, text streams. Object types include points, lines, areas, polylines, circles, ellipses. Data accuracy very important with image registration and sensor accuracy relevant. Analytics include closest point of approach, deviation from route, and point density over time, PCA and ICA. Software includes Server with Geospatially enabled RDBMS, Geospatial server/analysis software – ESRI ArcServer, Geoserver; Visualization by ArcMap or browser based visualization.

**Futures:** Today’s intelligence systems often contain trillions of geospatial objects and need to be able to visualize and interact with millions of objects. Critical issues are Indexing, retrieval and distributed analysis; Visualization generation and transmission; Visualization of data at the end of low bandwidth wireless connections; Data is sensitive and must be completely secure in transit and at rest (particularly on handhelds); Geospatial data requires unique approaches to indexing and distributed analysis.

### Object identification and tracking from Wide Area Large Format Imagery (WALF) Imagery or Full Motion Video (FMV) – Persistent Surveillance

*David Boyd, Data Tactics*

**Application:** Persistent surveillance sensors can easily collect petabytes of imagery data in the space of a few hours. The data should be reduced to a set of geospatial object (points, tracks, etc.) which can easily be integrated with other data to form a common operational picture. Typical processing involves extracting and tracking entities (vehicles, people, packages) over time from the raw image data.

**Current Approach:** It is unfeasible for this data to be processed by humans for either alerting or tracking purposes. The data needs to be processed close to the sensor which is likely forward deployed since it is too large to be easily transmitted. Typical object extraction systems are currently small (1-20 node) GPU enhanced clusters. There are a wide range of custom software and tools including traditional RDBMS’s and display tools. Real time data obtained at FMV (Full Motion Video) – 30-60 frames per/sec at full color 1080P resolution or WALF (Wide Area Large Format) with 1-10 frames per/sec at 10Kx10K full color resolution. Visualization of extracted outputs will typically be as overlays on a geospatial (GIS) display. Analytics are basic object detection analytics and integration with sophisticated situation awareness tools with data fusion. Significant security issues so that sources and methods cannot be compromised so the enemy should not be able to know what we see

**Futures:** Typical problem is integration of this processing into a large (GPU) cluster capable of processing data from several sensors in parallel and in near real time. Transmission of data from sensor to system is also a major challenge.

### Intelligence Data Processing and Analysis

*David Boyd, Data Tactics*

**Application:** Allow Intelligence Analysts to a) Identify relationships between entities (people, organizations, places, equipment) b) Spot trends in sentiment or intent for either general population or leadership group (state, non-state actors) c) Find location of and possibly timing of hostile actions (including implantation of IEDs) d) Track the location and actions of (potentially) hostile actors e) Ability to reason against and derive knowledge from diverse, disconnected, and frequently unstructured (e.g. text) data sources f) Ability to process data close to the point of collection and allow data to be shared easily to/from individual soldiers, forward deployed units, and senior leadership in garrison.

**Current Approach:** Software includes Hadoop, Accumulo (Big Table), Solr, Natural Language Processing, Puppet (for deployment and security) and Storm running on medium size clusters. Data size in 10s of Terabytes to 100s of Petabytes with Imagery intelligence device gathering petabyte in a few hours. Dismounted warfighters would have at most 1-100s of Gigabytes (typically handheld data storage).

**Futures:** Data currently exists in disparate silos which must be accessible through a semantically integrated data space. Wide variety of data types, sources, structures, and quality which will span domains and requires integrated search and reasoning. Most critical data is either unstructured or imagery/video which requires significant processing to extract entities and information. Network quality, Provenance and security essential.

## Healthcare and Life Sciences

### Electronic Medical Record (EMR) Data

*Shaun Grannis, Indiana University*

**Application:** Large national initiatives around health data are emerging, and include developing a digital learning health care system to support increasingly evidence-based clinical decisions with timely accurate and up-to-date patient-centered clinical information; using electronic observational clinical data to efficiently and rapidly translate scientific discoveries into effective clinical treatments; and electronically sharing integrated health data to improve healthcare process efficiency and outcomes. These key initiatives all rely on high-quality, large-scale, standardized and aggregate health data. One needs advanced methods for normalizing patient, provider, facility and clinical concept identification within and among separate health care organizations to enhance models for defining and extracting clinical phenotypes from non-standard discrete and free-text clinical data using feature selection, information retrieval and machine learning decision-models. One must leverage clinical phenotype data to support cohort selection, clinical outcomes research, and clinical decision support.

**Current Approach:** Clinical data from more than 1,100 discrete logical, operational healthcare sources in the Indiana Network for Patient Care (INPC) the nation's largest and longest-running health information exchange. This describes more than 12 million patients, more than 4 billion discrete clinical observations. > 20 TB raw data. Between 500,000 and 1.5 million new real-time clinical transactions added per day.

**Futures:** Teradata, PostgreSQL, MongoDB running on Indiana University supercomputer supporting information retrieval methods to identify relevant clinical features (tf-idf, latent semantic analysis, mutual information). Natural Language Processing techniques to extract relevant clinical features. Validated features will be used to parameterize clinical phenotype decision models based on maximum likelihood estimators and Bayesian networks. Decision models will be used to identify a variety of clinical phenotypes such as diabetes, congestive heart failure, and pancreatic cancer.

### Pathology Imaging/digital pathology

*Fusheng Wang, Emory University*

**Application:** Digital pathology imaging is an emerging field where examination of high resolution images of tissue specimens enables novel and more effective ways for disease diagnosis. Pathology image analysis segments massive (millions per image) spatial objects such as nuclei and blood vessels, represented with their boundaries, along with many extracted image features from these objects. The derived information is used for many complex queries and analytics to support biomedical research and clinical diagnosis. The full description has examples of 2-D and 3-D pathology images.

**Current Approach:** 1GB raw image data + 1.5GB analytical results per 2D image. MPI for image analysis; MapReduce + Hive with spatial extension on supercomputers and clouds. GPU’s used effectively. The full description shows the architecture of Hadoop-GIS, a spatial data warehousing system over MapReduce to support spatial analytics for analytical pathology imaging.

**Futures:** Recently, 3D pathology imaging is made possible through 3D laser technologies or serially sectioning hundreds of tissue sections onto slides and scanning them into digital images. Segmenting 3D microanatomic objects from registered serial images could produce tens of millions of 3D objects from a single image. This provides a deep “map” of human tissues for next generation diagnosis. 1TB raw image data + 1TB analytical results per 3D image and 1PB data per moderated hospital per year.

### Computational Bioimaging

*David Skinner, Joaquin Correa, Daniela Ushizima, Joerg Meyer, LBNL*

**Application:** Data delivered from bioimaging is increasingly automated, higher resolution, and multi-modal. This has created a data analysis bottleneck that, if resolved, can advance the biosciences discovery through Big Data techniques.

**Current Approach:** The current piecemeal analysis approach does not scale to situation where a single scan on emerging machines is 32TB and medical diagnostic imaging is annually around 70 PB excluding cardiology. One needs a web-based one-stop-shop for high performance, high throughput image processing for producers and consumers of models built on bio-imaging data.

**Futures:** Our goal is to solve that bottleneck with extreme scale computing with community-focused science gateways to support the application of massive data analysis toward massive imaging data sets. Workflow components include data acquisition, storage, enhancement, minimizing noise, segmentation of regions of interest, crowd-based selection and extraction of features, and object classification, and organization, and search. Use ImageJ, OMERO, VolRover, advanced segmentation and feature detection software.

### Genomic Measurements

*Justin Zook, NIST*

**Application:** NIST/Genome in a Bottle Consortium integrates data from multiple sequencing technologies and methods to develop highly confident characterization of whole human genomes as reference materials, and develop methods to use these Reference Materials to assess performance of any genome sequencing run.

**Current Approach:** The storage of ~40TB NFS at NIST is full; there are also PBs of genomics data at NIH/NCBI. Use Open-source sequencing bioinformatics software from academic groups (UNIX-based) on a 72 core cluster at NIST supplemented by larger systems at collaborators.

**Futures:** DNA sequencers can generate ~300GB compressed data/day which volume has increased much faster than Moore’s Law. Future data could include other ‘omics’ measurements, which will be even larger than DNA sequencing. Clouds have been explored.

### Comparative analysis for metagenomes and genomes

*Ernest Szeto, LBNL (Joint Genome Institute)*

**Application:** Given a metagenomic sample, (1) determine the community composition in terms of other reference isolate genomes, (2) characterize the function of its genes, (3) begin to infer possible functional pathways, (4) characterize similarity or dissimilarity with other metagenomic samples, (5) begin to characterize changes in community composition and function due to changes in environmental pressures, (6) isolate sub-sections of data based on quality measures and community composition.

**Current Approach:** integrated comparative analysis system for metagenomes and genomes, front ended by an interactive Web UI with core data, backend precomputations, batch job computation submission from the UI. Provide interface to standard bioinformatics tools (BLAST, HMMER, multiple alignment and phylogenetic tools, gene callers, sequence feature predictors…).

**Futures:** Management of heterogeneity of biological data is currently performed by relational database management system (Oracle). Unfortunately, it does not scale for even the current volume 50TB of data. NoSQL solutions aim at providing an alternative but unfortunately they do not always lend themselves to real time interactive use, rapid and parallel bulk loading, and sometimes have issues regarding robustness.

### Individualized Diabetes Management

*Ying Ding, Indiana University*

**Application:** Diabetes is a growing illness in world population, affecting both developing and developed countries. Current management strategies do not adequately take into account of individual patient profiles, such as co-morbidities and medications, which are common in patients with chronic illnesses. Need to use advanced graph-based data mining techniques applied to EHR converted into a RDF graph, to search for Diabetes patients and extract their EHR data for outcome evaluation.

**Current Approach:** Typical patient data records composed of 100 controlled vocabulary values and 1000 continuous values. Most values have a timestamp. Need to change traditional paradigm of relational row-column lookup to semantic graph traversal.

**Futures:** Identify similar patients from a large Electronic Health Record (EHR) database, i.e. an individualized cohort, and evaluate their respective management outcomes to formulate most appropriate solution suited for a given patient with diabetes. Use efficient parallel retrieval algorithms, suitable for cloud or HPC, using open source Hbase with both indexed and custom search to identify patients of possible interest. Use Semantic Linking for Property Values method to convert an existing data warehouse at Mayo Clinic, called the Enterprise Data Trust (EDT), into RDF triples that enables one to find similar patients through linking of both vocabulary-based and continuous values. The time dependent properties need to be processed before query to allow matching based on derivatives and other derived properties.

### Statistical Relational Artificial Intelligence for Health Care

*Sriraam Natarajan, Indiana University*

**Application:** The goal of the project is to analyze large, multi-modal medical data including different data types such as imaging, EHR, genetic and natural language. This approach employs the relational probabilistic models that have the capability of handling rich relational data and modeling uncertainty using probability theory. The software learns models from multiple data types and can possibly integrate the information and reason about complex queries. Users can provide a set of descriptions – say for instance, MRI images and demographic data about a particular subject. They can then query for the onset of a particular disease (say Alzheimer’s) and the system will then provide a probability distribution over the possible occurrence of this disease.

**Current Approach:** A single server can handle a test cohort of a few hundred patients with associated data of 100’s of GB.

**Futures:** A cohort of millions of patient can involve petabyte datasets. Issues include availability of too much data (as images, genetic sequences etc) that can make the analysis complicated. A major challenge lies in aligning the data and merging from multiple sources in a form that can be made useful for a combined analysis. Another issue is that sometimes, large amount of data is available about a single subject but the number of subjects themselves is not very high (i.e., data imbalance). This can result in learning algorithms picking up random correlations between the multiple data types as important features in analysis.

### World Population Scale Epidemiological Study

*Madhav Marathe, Stephen Eubank or Chris Barrett, Virginia Tech*

**Application:** One needs reliable real-time prediction and control of pandemic similar to the 2009 H1N1 influenza. In general one is addressing contagion diffusion of various kinds: information, diseases, social unrest can be modeled and computed. All of them can be addressed by agent-based models that utilize the underlying interaction network to study the evolution of the desired phenomena.

**Current Approach:** (a) Build a synthetic global population. (b) Run simulations over the global population to reason about outbreaks and various intervention strategies. Current 100TB dataset generated centrally with MPI based simulation system written in Charm++. Parallelism is achieved by exploiting the disease residence time period.

**Futures:** Use large social contagion models to study complex global scale issues

### Social Contagion Modeling for Planning, Public Health and Disaster Management

*Madhav Marathe or Chris Kuhlman, Virginia Tech*

**Application:** Model Social behavior including national security, public health, viral marketing, city planning, disaster preparedness. In a social unrest application, people take to the streets to voice unhappiness with government leadership. There are citizens that both support and oppose government. Quantify the degrees to which normal business and activities are disrupted owing to fear and anger. Quantify the possibility of peaceful demonstrations, violent protests. Quantify the potential for government responses ranging from appeasement, to allowing protests, to issuing threats against protestors, to actions to thwart protests. To address these issues, must have fine-resolution models (at level of individual people, vehicles, and buildings) and datasets.

**Current Approach:** The social contagion model infrastructure includes different types of human-to-human interactions (e.g., face-to-face versus online media) to be simulated. It takes not only human-to-human interactions into account, but also interactions among people, services (e.g., transportation), and infrastructure (e.g., internet, electric power). These activity models are generated from averages like census data.

**Futures:** Data fusion a big issue; how should one combine data from different sources and how to deal with missing or incomplete data? Take into account heterogeneous features of 100s of millions or billions of individuals, models of cultural variations across countries that are assigned to individual agents? How to validate these large models?

### Biodiversity and LifeWatch

*Wouter Los, Yuri Demchenko, University of Amsterdam*

**Application:** Research and monitor different ecosystems, biological species, their dynamics and migration with a mix of custom sensors and data access/processing and a federation with relevant projects in area. Particular case studies: Monitoring alien species, monitoring migrating birds, wetlands. See ENVRI for integration of LifeWatch with other environmental e-infrastructures.

**Futures:** LifeWatch initiative will provide integrated access to a variety of data, analytical and modeling tools as served by a variety of collaborating initiatives. Another service is offered with data and tools in selected workflows for specific scientific communities. In addition, LifeWatch will provide opportunities to construct personalized ‘virtual labs', also allowing one to enter new data and analytical tools. New data will be shared with the data facilities cooperating with LifeWatch. LifeWatch operates the Global Biodiversity Information facility and Biodiversity Catalogue that is Biodiversity Science Web Services Catalogue. Data includes ‘omics, species information, ecological information (such as biomass, population density etc.), ecosystem data (such as CO2 fluxes. Algal blooming, water and soil characteristics)

### Large-scale Deep Learning

*Adam Coates, Stanford University*

**Application:** Increase the size of datasets and models that can be tackled with deep learning algorithms. Large models (e.g., neural networks with more neurons and connections) combined with large datasets are increasingly the top performers in benchmark tasks for vision, speech, and Natural Language Processing. One needs to train a deep neural network from a large (>>1TB) corpus of data (typically imagery, video, audio, or text). Such training procedures often require customization of the neural network architecture, learning criteria, and dataset pre-processing. In addition to the computational expense demanded by the learning algorithms, the need for rapid prototyping and ease of development is extremely high.

**Current Approach: The** largest applications so far are to image recognition and scientific studies of unsupervised learning with 10 million images and up to 11 billion parameters on a 64 GPU HPC Infiniband cluster. Both supervised (using existing classified images) and unsupervised applications investigated.

**Futures:** Large datasets of 100TB or more may be necessary in order to exploit the representational power of the larger models. Training a self-driving car could take 100 million images at megapixel resolution. Deep Learning shares many characteristics with the broader field of machine learning. The paramount requirements are high computational throughput for mostly dense linear algebra operations, and extremely high productivity for researcher exploration. One needs integration of high performance libraries with high level (python) prototyping environments.

### Organizing large-scale, unstructured collections of consumer photos

*David Crandall, Indiana University*

**Application:** Produce 3D reconstructions of scenes using collections of millions to billions of consumer images, where neither the scene structure nor the camera positions are known a priori. Use resulting 3d models to allow efficient and effective browsing of large-scale photo collections by geographic position. Geolocate new images by matching to 3d models. Perform object recognition on each image. 3d reconstruction can be posed as a robust non-linear least squares optimization problem in which observed (noisy) correspondences between images are constraints and unknowns are 6-d camera pose of each image and 3-d position of each point in the scene.

**Current Approach:** Hadoop cluster with 480 cores processing data of initial applications. Note over 500 billion images on Facebook and over 5 billion on Flickr with over 500 million images added to social media sites each day.

**Futures:** Need many analytics including feature extraction, feature matching, and large-scale probabilistic inference, which appear in many or most computer vision and image processing problems, including recognition, stereo resolution, and image denoising. Need to visualize large-scale 3-d reconstructions, and navigate large-scale collections of images that have been aligned to maps.

### Truthy: Information diffusion research from Twitter Data

*Filippo Menczer, Alessandro Flammini, Emilio Ferrara, Indiana University*

**Application:** Understanding how communication spreads on socio-technical networks. Detecting potentially harmful information spread at the early stage (e.g., deceiving messages, orchestrated campaigns, untrustworthy information, etc.)

**Current Approach:** 1) Acquisition and storage of a large volume (30 TB a year compressed) of continuous streaming data from Twitter (~100 million messages per day, ~500GB data/day increasing over time); (2) near real-time analysis of such data, for anomaly detection, stream clustering, signal classification and online-learning; (3) data retrieval, big data visualization, data-interactive Web interfaces, public API for data querying. Use Python/SciPy/NumPy/MPI for data analysis. Information diffusion, clustering, and dynamic network visualization capabilities already exist.

**Futures:** Truthy plans to expand incorporating Google+ and Facebook. Need to move towards Hadoop/IndexedHBase & HDFS distributed storage. Use Redis as a in-memory database as a buffer for real-time analysis. Need streaming clustering, anomaly detection and online learning.

### Crowd Sourcing in the Humanities as Source for Big and Dynamic Data

*Sebastian Drude, Max-Planck-Institute for Psycholinguistics, Nijmegen The Netherlands*

**Application:** Capture information (manually entered, recorded multimedia, reaction times, pictures, sensor information) from many individuals and their devices and so characterize wide ranging individual, social, cultural and linguistic variation among several dimensions (space, social space, time).

**Current Approach:** Use typically XML technology, traditional relational databases, and besides pictures not much multi-media yet.

**Futures:** Crowd sourcing has been barely started to be used on a larger scale but with the availability of mobile devices, now there is a huge potential for collecting much data from many individuals, also making use of sensors in mobile devices. This has not been explored on a large scale so far; existing projects of crowd sourcing are usually of a limited scale and web-based. Privacy issues may be involved (A/V from individuals), anonymization may be necessary but not always possible. Data management and curation critical. Size could be hundreds of terabytes with multimedia.

### CINET: Cyberinfrastructure for Network (Graph) Science and Analytics

*Madhav Marathe or Keith Bisset, Virginia Tech*

**Application:** CINET provides a common web-based platform for accessing various (i) network and graph analysis tools such as SNAP, NetworkX, Galib, etc. (ii) real-world and synthetic networks, (iii) computing resources and (iv) data management systems to the end-user in a seamless manner.

**Current Approach:** CINET uses an Infiniband connected high performance computing cluster with 720 cores to provide HPC as a service. It is being used for research and education.

**Futures:** As the repository grows, we expect a rapid growth to lead to over 1000-5000 networks and methods in about a year. As more fields use graphs of increasing size, parallel algorithms will be important. Data manipulation and bookkeeping of the derived data for users is a challenge there are no well-defined and effective models and tools for management of various graph data in a unified fashion.

### NIST Information Access Division analytic technology performance measurement, evaluations, and standards

*John Garofolo, NIST*

**Application:** Develop performance metrics, measurement methods, and community evaluations to ground and accelerate the development of advanced analytic technologies in the areas of speech and language processing, video and multimedia processing, biometric image processing, and heterogeneous data processing as well as the interaction of analytics with users. Typically employ one of two processing models: 1) Push test data out to test participants and analyze the output of participant systems, 2) Push algorithm test harness interfaces out to participants and bring in their algorithms and test them on internal computing clusters.

**Current Approach:** Large annotated corpora of unstructured/semi-structured text, audio, video, images, multimedia, and heterogeneous collections of the above including ground truth annotations for training, developmental testing, and summative evaluations. The test corpora exceed 900M Web pages occupying 30 TB of storage, 100M tweets, 100M ground-truthed biometric images, several hundred thousand partially ground-truthed video clips, and terabytes of smaller fully ground-truthed test collections.

**Futures:** Even larger data collections are being planned for future evaluations of analytics involving multiple data streams and very heterogeneous data. As well as larger datasets, future includes testing of streaming algorithms with multiple heterogeneous data. Use of clouds being explored.

## The Ecosystem for Research

### DataNet Federation Consortium DFC

*Reagan Moore, University of North Carolina at Chapel Hill*

**Application:** Promote collaborative and interdisciplinary research through federation of data management systems across federal repositories, national academic research initiatives, institutional repositories, and international collaborations. The collaboration environment runs at scale: petabytes of data, hundreds of millions of files, hundreds of millions of metadata attributes, tens of thousands of users, and a thousand storage resources.

**Current Approach:** Currently 25 science and engineering domains have projects that rely on the iRODS (Integrated Rule Oriented Data System) policy-based data management system including major NSF projects such as Ocean Observatories Initiative (sensor archiving); Temporal Dynamics of Learning Center (Cognitive science data grid); the iPlant Collaborative (plant genomics); Drexel engineering digital library; Odum Institute for social science research (data grid federation with Dataverse). iRODS currently manages petabytes of data, hundreds of millions of files, hundreds of millions of metadata attributes, tens of thousands of users, and a thousand storage resources. It interoperates with workflow systems (NCSA Cyberintegrator, Kepler, Taverna), cloud and more traditional storage models and different transport protocols. The full description has a diagram of the iRODS architecture.

### The ‘Discinnet process’, metadata <-> big data global experiment

*P. Journeau, Discinnet Labs*

**Application:** Discinnet has developed a web 2.0 collaborative platform and research prototype as a pilot installation now becoming deployed to be appropriated and tested by researchers from a growing number and diversity of research fields through communities belonging a diversity of domains.

Its goal is to reach a wide enough sample of active research fields represented as clusters–researchers projected and aggregating within a manifold of mostly shared experimental dimensions–to test general, hence potentially interdisciplinary, epistemological models throughout the present decade.

**Current Approach:** Currently 35 clusters started with close to 100 awaiting more resources and potentially much more open for creation, administration and animation by research communities. Examples range from optics, cosmology, materials, microalgae, health to applied math, computation, rubber and other chemical products/issues.

**Futures:** Discinnet itself would not be Bigdata but rather will generate metadata when applied to a cluster that involves Bigdata. In interdisciplinary integration of several fields, the process would reconcile metadata from many complexity levels.

### Semantic Graph-search on Scientific Chemical and Text-based Data

*Talapady Bhat, NIST*

**Application:** Establish social media-based infrastructure, terminology and semantic data-graphs to annotate and present technology information using ‘root’ and rule-based methods used primarily by some Indo-European languages like Sanskrit and Latin.

**Current approach:** Many reports, including a recent one on Material Genome Project finds that exclusive top-down solutions to facilitate data sharing and integration are not desirable for federated multi-disciplinary efforts. However, a bottom-up approach can be chaotic. For this reason, there is need for a balanced blend of the two approaches to support easy-to-use techniques to metadata creation, integration and sharing. This challenge is very similar to the challenge faced by language developer at the beginning. One of the successful effort used by many prominent languages is that of ‘roots’ and rules that form the framework for creating on-demand words for communication. In this approach a top-down method is used to establish a limited number of highly re-usable words called ‘roots’ by surveying the existing best practices in building terminology. These ‘roots’ are combined using few ‘rules’ to create terms on-demand by a bottom-up step.

Y(uj) (join), O (creator, God, brain), Ga (motion, initiation) –leads to ‘Yoga’ in Sanskrit, English

Geno (genos)-cide–race based killing – Latin, English

Bio-technology –English, Latin

Red-light, red-laser-light –English.

A press release by the American Institute of Physics on this approach is at <http://www.eurekalert.org/pub_releases/2013-07/aiop-ffm071813.php>

Our efforts to develop automated and rule and root-based methods (Chem-BLAST -. <http://xpdb.nist.gov/chemblast/pdb.pl> ) to identify and use best-practice, discriminating terms in generating semantic data-graphs for science started almost a decade back with a chemical structure database. This database has millions of structures obtained from the Protein Data Bank and the PubChem used world-wide. Subsequently we extended our efforts to build root-based terms to text-based data of cell-images. In this work we use few simple rules to define and extend terms based on best-practice as decided by weaning through millions of popular use-cases chosen from over hundred biological ontologies.

Currently we are working on extending this method to publications of interest to Material Genome, Open-Gov and NIST-wide publication archive - NIKE. - <http://xpdb.nist.gov/nike/term.pl>. These efforts are a component of Research Data Alliance Working Group on Metadata <https://www.rd-alliance.org/filedepot_download/694/160> & <https://rd-alliance.org/poster-session-rda-2nd-plenary-meeting.html>

**Futures:** Create a cloud infrastructure for social media of scientific information where many scientists from various parts of the world can participate and deposit results of their experiment. Some of the issues that one has to resolve prior to establishing a scientific social media are: a) How to minimize challenges related to establishing re-usable, inter-disciplinary, scalable, on-demand, use-case and user-friendly vocabulary? b) How to adopt a existing or create new on-demand ‘data-graph’ to place an information in an intuitive way such that it would easily integrate with existing ‘data-graphs’ in a federated environment without knowing too much about the data management? c) How to find relevant scientific data without spending too much time on the internet? Start with resources like the Open Government movement, Material genome Initiative and Protein Databank. This effort includes many local and networked resources. Developing an infrastructure to automatically integrate information from all these resources using data-graphs is a challenge that we are trying to solve. Good database tools and servers for data-graph manipulation are needed.

### Light source beamlines

*Eli Dart, LBNL*

**Application:** Samples are exposed to X-rays from light sources in a variety of configurations depending on the experiment. Detectors (essentially high-speed digital cameras) collect the data. The data are then analyzed to reconstruct a view of the sample or process being studied.

**Current Approach:** A variety of commercial and open source software is used for data analysis – examples including Octopus for Tomographic Reconstruction, Avizo (http://vsg3d.com) and FIJI (a distribution of ImageJ) for Visualization and Analysis. Data transfer is accomplished using physical transport of portable media (severely limits performance) or using high-performance GridFTP, managed by Globus Online or workflow systems such as SPADE.

**Futures:** Camera resolution is continually increasing. Data transfer to large-scale computing facilities is becoming necessary because of the computational power required to conduct the analysis on time scales useful to the experiment. Large number of beamlines (e.g. 39 at LBNL ALS) means that aggregate data load is likely to increase significantly over the coming years and need for a generalized infrastructure for analyzing gigabytes per second of data from many beamline detectors at multiple facilities.

## Astronomy and Physics

### Catalina Real-Time Transient Survey (CRTS): a digital, panoramic, synoptic sky survey

*S. G. Djorgovski, Caltech*

**Application:** The survey explores the variable universe in the visible light regime, on time scales ranging from minutes to years, by searching for variable and transient sources. It discovers a broad variety of astrophysical objects and phenomena, including various types of cosmic explosions (e.g., Supernovae), variable stars, phenomena associated with accretion to massive black holes (active galactic nuclei) and their relativistic jets, high proper motion stars, etc. The data are collected from 3 telescopes (2 in Arizona and 1 in Australia), with additional ones expected in the near future (in Chile).

**Current Approach:** The survey generates up to ~ 0.1 TB on a clear night with a total of ~100 TB in current data holdings. The data are preprocessed at the telescope, and transferred to Univ. of Arizona and Caltech, for further analysis, distribution, and archiving. The data are processed in real time, and detected transient events are published electronically through a variety of dissemination mechanisms, with no proprietary withholding period (CRTS has a completely open data policy). Further data analysis includes classification of the detected transient events, additional observations using other telescopes, scientific interpretation, and publishing. In this process, it makes a heavy use of the archival data (several PB’s) from a wide variety of geographically distributed resources connected through the Virtual Observatory (VO) framework.

**Futures:** CRTS is a scientific and methodological testbed and precursor of larger surveys to come, notably the Large Synoptic Survey Telescope (LSST), expected to operate in 2020’s and selected as the highest-priority ground-based instrument in the 2010 Astronomy and Astrophysics Decadal Survey. LSST will gather about 30 TB per night. The schematic architecture for a cyber-infrastructure for time domain astronomy illustrated by a figure in full description.

### DOE Extreme Data from Cosmological Sky Survey and Simulations

*Salman Habib, Argonne National Laboratory; Andrew Connolly, University of Washington*

**Application:** A cosmology discovery tool that integrates simulations and observation to clarify the nature of dark matter, dark energy, and inflation, some of the most exciting, perplexing, and challenging questions facing modern physics including the properties of fundamental particles affecting the early universe. The simulations will generate comparable data sizes to observation.

**Futures:** Data sizes are Dark Energy Survey (DES) 4 PB in 2015; Zwicky Transient Factory (ZTF) 1 PB/year in 2015; Large Synoptic Sky Survey (LSST see CRTS description) 7 PB/year in 2019; Simulations > 10 PB in 2017. Huge amounts of supercomputer time (over 200M hours) will be used.

### Large Survey Data for Cosmology

*Peter Nugent LBNL*

**Application:** For DES (Dark Energy Survey) the data are sent from the mountaintop via a microwave link to La Serena, Chile. From there, an optical link forwards them to the NCSA as well as NERSC for storage and "reduction”. Here galaxies and stars in both the individual and stacked images are identified, catalogued, and finally their properties measured and stored in a database.

**Current Approach:** Subtraction pipelines are run using extant imaging data to find new optical transients through machine learning algorithms. Linux cluster, Oracle RDBMS server, Postgres PSQL, large memory machines, standard Linux interactive hosts, GPFS. For simulations, HPC resources. Standard astrophysics reduction software as well as Perl/Python wrapper scripts, Linux Cluster scheduling.

**Futures:** Techniques for handling Cholesky decompostion for thousands of simulations with matrices of order 1M on a side and parallel image storage would be important. LSST will generate 60PB of imaging data and 15PB of catalog data and a correspondingly large (or larger) amount of simulation data. Over 20TB of data per night.

### Particle Physics: Analysis of LHC Large Hadron Collider Data: Discovery of Higgs particle

*Michael Ernst BNL, Lothar Bauerdick FNAL, Geoffrey Fox, Indiana University; Eli Dart, LBNL*

**Application:** Study CERN LHC (Large Hadron Collider) Accelerator and Monte Carlo producing events describing particle-apparatus interaction. Processed information defines physics properties of events (lists of particles with type and momenta). These events are analyzed to find new effects; both new particles (Higgs) and present evidence that conjectured particles (Supersymmetry) have not been detected. LHC has a few major experiments including ATLAS and CMS. These experiments have global participants (for example CMS has 3600 participants from 183 institutions in 38 countries), and so the data at all levels is transported and accessed across continents.

**Current Approach:** The LHC experiments are pioneers of a distributed Big Data science infrastructure, and several aspects of the LHC experiments’ workflow highlight issues that other disciplines will need to solve. These include automation of data distribution, high performance data transfer, and large-scale high-throughput computing. Grid analysis with 350,000 cores running “continuously” over 2 million jobs per day arranged in 3 tiers (CERN, “Continents/Countries”. “Universities”). Uses “Distributed High Throughput Computing” (Pleasing parallel) architecture with facilities integrated across the world by WLCG (LHC Computing Grid) and Open Science Grid in the US. 15 Petabytes data gathered each year from Accelerator data and Analysis with 200PB total. Specifically in 2012 ATLAS had at Brookhaven National Laboratory (BNL) 8PB Tier1 tape; BNL over 10PB Tier1 disk and US Tier2 centers 12PB disk cache. CMS has similar data sizes. Note over half resources used for Monte Carlo simulations as opposed to data analysis.

**Futures:** In the past the particle physics community has been able to rely on industry to deliver exponential increases in performance per unit cost over time, as described by Moore's Law. However the available performance will be much more difficult to exploit in the future since technology limitations, in particular regarding power consumption, have led to profound changes in the architecture of modern CPU chips. In the past software could run unchanged on successive processor generations and achieve performance gains that follow Moore's Law thanks to the regular increase in clock rate that continued until 2006. The era of scaling HEP sequential applications is now over. Changes in CPU architectures imply significantly more software parallelism as well as exploitation of specialized floating point capabilities. The structure and performance of HEP data processing software needs to be changed such that it can continue to be adapted and further developed in order to run efficiently on new hardware. This represents a major paradigm-shift in HEP software design and implies large scale re-engineering of data structures and algorithms. Parallelism needs to be added at all levels at the same time, the event level, the algorithm level, and the sub-algorithm level. Components at all levels in the software stack need to interoperate and therefore the goal is to standardize as much as possible on basic design patterns and on the choice of a concurrency model. This will also help to ensure efficient and balanced use of resources.

### Belle II High Energy Physics Experiment

*David Asner & Malachi Schram, PNNL*

**Application** The Belle experiment is a particle physics experiment with more than 400 physicists and engineers investigating CP-violation effects with B meson production at the High Energy Accelerator KEKB e+ e- accelerator in Tsukuba, Japan. In particular look at numerous decay modes at the Upsilon(4S) resonance to search for new phenomena beyond the Standard Model of Particle Physics. This accelerator has the largest intensity of any in the world but events simpler than those from LHC and so analysis is less complicated but similar in style compared to the CERN accelerator.

**Futures:** An upgraded experiment Belle II and accelerator SuperKEKB will start operation in 2015 with a factor of 50 increased data with total integrated RAW data ~120PB and physics data ~15PB and ~100PB MC samples. Move to a distributed computing model requiring continuous RAW data transfer of ~20Gbps at designed luminosity between Japan and US. Will need Open Science Grid, Geant4, DIRAC, FTS, Belle II framework software.

### EISCAT 3D incoherent scatter radar system

*Yin Chen, Cardiff University; Ingemar Häggström, Ingrid Mann, Craig Heinselman, EISCAT Science Association*

**Application:** EISCAT, the European Incoherent Scatter Scientific Association, conducts research on the lower, middle and upper atmosphere and ionosphere using the incoherent scatter radar technique. This technique is the most powerful ground-based tool for these research applications. EISCAT studies instabilities in the ionosphere, as well as investigating the structure and dynamics of the middle atmosphere. It is also a diagnostic instrument in ionospheric modification experiments with addition of a separate Heating facility. Currently EISCAT operates 3 of the 10 major incoherent radar scattering instruments worldwide with its facilities in in the Scandinavian sector, north of the Arctic Circle.

**Current Approach:** The current running old EISCAT radar generates terabytes per year rates and does not present special challenges.

**Futures:** The design of the next generation radar, EISCAT\_3D, will consist of a core site with a transmitting and receiving radar arrays and four sites with receiving antenna arrays at some 100 km from the core. The fully operational 5-site system will generate several thousand times data of current EISCAT system with 40 PB/year in 2022 and is expected to operate for 30 years. EISCAT 3D data e-Infrastructure plans to use the high performance computers for central site data processing and high throughput computers for mirror sites data processing. Downloading the full data is not time critical, but operations require real-time information about certain pre-defined events to be sent from the sites to the operation center and a real-time link from the operation center to the sites to set the mode of radar operation on with immediate action. See figure in full description.

### ENVRI, Common Operations of Environmental Research Infrastructure

*Yin Chen, Cardiff University*

**Application:** ENVRI Research Infrastructures (ENV RIs) addresses European distributed, long-term, remote controlled observational networks focused on understanding processes, trends, thresholds, interactions and feedbacks and increasing the predictive power to address future environmental challenges. ENVRI includes **ICOS** is a European distributed infrastructure dedicated to the monitoring of greenhouse gases (GHG) through its atmospheric, ecosystem and ocean networks; EURO-Argo is the European contribution to Argo, which is a global ocean observing system; **EISCAT-3D** separately described is a European new-generation incoherent-scatter research radar for upper atmospheric science; **LifeWatch** separately described is an e-science Infrastructure for biodiversity and ecosystem research; **EPOS** is a European Research Infrastructure on earthquakes, volcanoes, surface dynamics and tectonics; **EMSO** is a European network of seafloor observatories for the long-term monitoring of environmental processes related to ecosystems, climate change and geo-hazards; **IAGOS** Aircraft for global observing system; **SIOS** Svalbard arctic Earth observing system

**Current Approach:** ENVRI develops a Reference Model (ENVRI RM) as a common ontological framework and standard for the description and characterization of computational and storage infrastructures in order to achieve seamless interoperability between the heterogeneous resources of different infrastructures. The ENVRI RM serves as a common language for community communication, providing a uniform framework into which the infrastructure’s components can be classified and compared, also serving to identify common solutions to common problems. Note data sizes in a given infrastructure vary from gigabytes to petabytes per year.

**Futures:** ENVRI’s common environment will empower the users of the collaborating environmental research infrastructures and enable multidisciplinary scientists to access, study and correlate data from multiple domains for "system level" research. It provides Bigdata requirements coming from interdisciplinary research.

As shown in Figure 1 in full description, analysis of the computational characteristics of the 6 ESFRI Environmental Research infrastructure, 5 common subsystems has been identified. The definition of them are given in the ENVRI Reference Model, www.envri.eu/rm:

* **Data acquisition:** collects raw data from sensor arrays, various instruments, or human observers, and brings the measurements (data streams) into the system.
* **Data curation**: facilitates quality control and preservation of scientific data. It is typically operated at a data centre.
* **Data access:**  enables discovery and retrieval of data housed in data resources managed by a *data curation* *subsystem*.
* **Data processing:** aggregates the data from various resources and provides computational capabilities and capacities for conducting data analysis and scientific experiments.
* **Community support:**  manages, controls and tracks users' activities and supports users to conduct their roles in communities.

As shown in Figure 2 of full description, the 5 sub-system map well to the architectures of the ESFRI Environmental Research Infrastructures.

### Radar Data Analysis for CReSIS Remote Sensing of Ice Sheets

*Geoffrey Fox, Indiana University*

**Application:** This data feeds into intergovernmental Panel on Climate Change (IPCC) and uses custom radars to measures ice sheet bed depths and (annual) snow layers at the North and South poles and mountainous regions.

**Current Approach:** The initial analysis is currently Matlab signal processing that produces a set of radar images. These cannot be transported from field over Internet and are typically copied to removable few TB disks in the field and flown “home” for detailed analysis. Image understanding tools with some human oversight find the image features (layers) that are stored in a database front-ended by a Geographical Information System. The ice sheet bed depths are used in simulations of glacier flow. The data is taken in “field trips” that each currently gather 50-100 TB of data over a few week period.

**Futures:** An order of magnitude more data (petabyte per mission) is projected with improved instrumentation. Demands of processing increasing field data in an environment with more data but still constrained power budget, suggests low power/performance architectures such as GPU systems.

The full descriptions gives workflows for different parts of problem and pictures of operation.

### UAVSAR Data Processing, Data Product Delivery, and Data Services

*Andrea Donnellan and Jay Parker, NASA JPL*

**Application:** Synthetic Aperture Radar (SAR) can identify landscape changes caused by seismic activity, landslides, deforestation, vegetation changes and flooding. This is for example used to support earthquake science as well as disaster management. This use case supports the storage, application of image processing and visualization of this geo-located data with angular specification.

**Current Approach:** Data from planes and satellites is processed on NASA computers before being stored after substantial data communication. The data is made public as soon as processed and requires significant curation due to instrumental glitches. The current data size is ~150TB.

**Futures:** The data size would increase dramatically if Earth Radar Mission launched. Clouds are suitable hosts but are not used today in production.

### NASA LARC/GSFC iRODS Federation Testbed

*Brandi Quam, NASA Langley Research Center*

**Application:** NASA Center for Climate Simulation (NCCS) and NASA Atmospheric Science Data Center (ASDC) have complementary data sets, each containing vast amounts of data that is not easily shared and queried. Climate researchers, weather forecasters, instrument teams, and other scientists need to access data from across multiple datasets in order to compare sensor measurements from various instruments, compare sensor measurements to model outputs, calibrate instruments, look for correlations across multiple parameters, etc.

**Current Approach:** The data includes MERRA (described separately) and NASA Clouds and Earth's Radiant Energy System (CERES) EBAF(Energy Balanced And Filled)-TOA(Top of Atmosphere) Product which is about 420MB and Data from the EBAF-Surface Product which is about 690MB. Data grows with each version update (about every six months). To analyze, visualize and otherwise process data from heterogeneous datasets is currently a time consuming effort that requires scientists to separately access, search for, and download data from multiple servers and often the data is duplicated without an understanding of the authoritative source. Often times accessing data is greater than scientific analysis time. Current datasets are hosted on modest size (144 to 576 cores) Infiniband clusters.

**Futures:** The improved access will be enabled through the use of iRODS that enables parallel downloads of datasets from selected replica servers that can be geographically dispersed, but still accessible by users worldwide. iRODS operation will be enhanced with semantically organized metadata, and managed via a highly precise Earth Science ontology. Cloud solutions will also be explored.

### MERRA Analytic Services MERRA/AS

*John L. Schnase & Daniel Q. Duffy , NASA Goddard Space Flight Center*

**Application:** This application produces global temporally and spatially consistent syntheses of 26 key climate variables by combining numerical simulations with observational data. Three-dimensional results are produced every 6-hours extending from 1979-present. This supports important applications like Intergovernmental Panel on Climate Change (IPCC) research and the NASA/Department of Interior RECOVER wildfire decision support system; these applications typically involve integration of MERRA with other datasets. The full description has a typical MERRA/AS output.

**Current Approach:** MapReduce is used to process a current total of 480TB. The current system is hosted on a 36 node Infiniband cluster

**Futures:** Clouds are being investigated. The data is growing by one TB a month.

### Atmospheric Turbulence - Event Discovery and Predictive Analytics

*Michael Seablom, NASA HQ*

**Application:** This builds datamining on top of reanalysis products including the North American Regional Reanalysis (NARR) and the Modern-Era Retrospective-Analysis for Research (MERRA) from NASA where latter described earlier. The analytics correlate aircraft reports of turbulence (either from pilot reports or from automated aircraft measurements of eddy dissipation rates) with recently completed atmospheric re-analyses. This is of value to aviation industry and to weather forecasters. There are no standards for re-analysis products complicating system where MapReduce is being investigated. The reanalysis data is hundreds of terabytes and slowly updated whereas turbulence is smaller in size and implemented as a streaming service. A typical turbulent wave image is in full description.

**Current Approach:** Current 200TB dataset can be analyzed with MapReduce or the like using SciDB or other scientific database.

**Futures:** The dataset will reach 500TB in 5 years.The initial turbulence case can be extended to other ocean/atmosphere phenomena but the analytics would be different in each case.

### Climate Studies using the Community Earth System Model at DOE’s NERSC center

*Warren Washington, NCAR*

**Application: We need to** understand and quantify contributions of natural and anthropogenic-induced patterns of climate variability and change in the 20th and 21st centuries by means of simulations with the Community Earth System Model (CESM). The results of supercomputer simulations across the world need to be stored and compared.

**Current Approach:** The Earth Systems Grid (ESG) enables world wide access to Peta/Exa-scale climate science data with multiple petabytes of data at dozens of federated sites worldwide. The ESG is recognized as the leading infrastructure for the management and access of large distributed data volumes for climate change research. It supports the Coupled Model Intercomparison Project (CMIP), whose protocols enable the periodic assessments carried out by the Intergovernmental Panel on Climate Change (IPCC).

**Futures:** Rapid growth of data with 30 PB produced at NERSC (assuming 15 end-to-end climate change experiments) in 2017 and many times more this worldwide.

### DOE-BER Subsurface Biogeochemistry Scientific Focus Area

*Deb Agarwal, LBNL*

**Application:** Development of a Genome-Enabled Watershed Simulation Capability (GEWaSC) that will provide a predictive framework for understanding how genomic information stored in a subsurface microbiome, affects biogeochemical watershed functioning; how watershed-scale processes affect microbial functioning; and how these interactions co-evolve.

**Current Approach:** Current modeling capabilities can represent processes occurring over an impressive range of scales (ranging from a single bacterial cell to that of a contaminant plume). Data crosses all scales from genomics of the microbes in the soil to watershed hydro-biogeochemistry. Data are generated by the different research areas and include simulation data, field data (hydrological, geochemical, geophysical), ‘omics data, and observations from laboratory experiments.

**Futures:** Little effort to date has been devoted to developing a framework for systematically connecting scales, as is needed to identify key controls and to simulate important feedbacks. GEWaSC will develop a simulation framework that formally scales from genomes to watersheds and will synthesize diverse and disparate field, laboratory, and simulation datasets across different semantic, spatial, and temporal scales.

### DOE-BER AmeriFlux and FLUXNET Networks

*Deb Agarwal, LBNL*

**Application:** AmeriFlux and FLUXNET are US and world collections respectively of sensors that observe trace gas fluxes (CO2, water vapor) across a broad spectrum of times (hours, days, seasons, years, and decades) and space. Moreover, such datasets provide the crucial linkages among organisms, ecosystems, and process-scale studies—at climate-relevant scales of landscapes, regions, and continents—for incorporation into biogeochemical and climate models.

**Current Approach:** Software includesEddyPro, Custom analysis software, R, python, neural networks, Matlab. There are ~150 towers in AmeriFlux and over 500 towers distributed globally collecting flux measurements.

**Futures:** Field experiment data taking would be improved by access to existing data and automated entry of new data via mobile devices. Need to support interdisciplinary studies integrating diverse data sources.

## Energy

### Consumption forecasting in Smart Grids

*Yogesh Simmhan, University of Southern California*

**Application:** Predict energy consumption for customers, transformers, sub-stations and the electrical grid service area using smart meters providing measurements every 15-mins at the granularity of individual consumers within the service area of smart power utilities. Combine Head-end of smart meters (distributed), Utility databases (Customer Information, Network topology; centralized), US Census data (distributed), NOAA weather data (distributed), Micro-grid building information system (centralized), Micro-grid sensor network (distributed). This generalizes to real-time data-driven analytics for time series from cyber physical systems

**Current Approach:** GIS based visualization. Data is around 4 TB a year for a city with 1.4M sensors in Los Angeles. Uses R/Matlab, Weka, Hadoop software. Significant privacy issues requiring anonymization by aggregation. Combine real time and historic data with machine learning for predicting consumption.

**Futures:** Wide spread deployment of Smart Grids with new analytics integrating diverse data and supporting curtailment requests. Mobile applications for client interactions.

# Use Case Requirements

## General Requirements

[some description goes here….]

**Data Sources Requirements (DSR)**

DSR-1: Needs to support reliable real time, asynchronize, streaming, and batch processing to collect data from centralized, distributed, and cloud data sources, sensors, or instruments

DSR-2: Needs to support slow, bursty and high throughput data transmission between data sources and computing clusters.

DSR-3: Needs to support diversified data content ranging from structured and unstructured text, document, graph, web, geospatial, compressed, timed, spatial, multimedia, simulation, and instrumental data.

**Transformation Provider Requirements (TPR)**

TPR-1: Needs to support diversified compute intensive, analytic processing and machines learning techniques

TPR-2: Needs to support batch and real time analytic processing

TPR-3: Needs to support processing large diversified data content and modeling

TPR\_4: Needs to support processing data in motion (streaming, fetching new content, tracking, etc.)

**Capability Provider Requirements (CPR)**

CPR-1: Needs to support legacy and advance software packages (subcomponent: SaaS)

CPR-2: Needs to support legacy and advance computing platforms (subcomponent: PaaS)

CPR-3: Needs to support legacy and advance distributed computing cluster, co-processors, I/O processing (subcomponent: IaaS)

CPR-4: Needs to support elastic data transmission (subcomponent: networking)

CPR-5: Needs to support legacy, large, and advance distributed data storage (subcomponent: storage)

CPR-6: Needs to support legacy and advance programming executable, applications, tools, utilities, and libraries

**Data Consumer Requirements (DCR)**

DCR-1: Needs to support fast search (~0.1 seconds) from processed data with high relevancy, accuracy, and high recall

DCR-2: Needs to support diversified output file formats for rendering and reporting

DCR-3: Needs to support visual layout for results presentation

DCR-4: Needs to support rich user interface for access using browser, visualization tools

DCR-5: Needs to support high resolution multi-dimension layer of data visualization

DCR-6: Needs to support streaming results to clients

**Security & Privacy Requirements (SPR)**

SPR-1: Needs to support protect and preserve security and privacy on sensitive data

SPR-2: Needs to support multi-level policy-driven, sandbox, access control, authentication on protected data

**Lifecycle Management Requirements (LMR)**

LMR-1: Needs to support data quality curation including pre-processing, format transformation

LMR-2: Needs to support dynamic updates on data, user profiles, and links

LMR-3: Needs to support data lifecycle and long-term preservation policy including data provenance

LMR-4: Needs to support data validation

LMR-5: Needs to support human annotation for data validation

LMR-6: Needs to support prevention of data loss or corruption

LMR-7: Needs to support multi-sites archival

LMR-8: Needs to support persistent identifier

**Other Requirements (OR)**

OR-1: Needs to support rich user interface from mobile platforms to access processed results

OR-2: Needs to support performance monitoring on analytic processing from mobile platforms

OR-3: Needs to support rich visual content search and rendering from mobile platforms

OR-4: Needs to support mobile device data acquisition

## Use Case Requirements Summary

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **UC** | **Data Source** | **Volume** | **Velocity** | **Variety** | **Transform.** | **Capability** | **Data User** | **Sec&Privacy** | **Lifecycle** | **Others** |
| General  Requirements | 3 |  |  |  | 4 | 6 | 6 | 2 | 8 | 4 |
| [**M0078**](http://bigdatawg.nist.gov/_uploadfiles/M0078_v1_8198680934.docx) | 3 |  |  |  | 2 | 4 | 1 | 1 | 1 | 1 |
| [**M0089**](http://bigdatawg.nist.gov/_uploadfiles/M0089_v1_7814086875.docx) | 4 |  |  |  | 3 | 4 | 1 | 1 | 1 | 1 |
| [**M0090**](http://bigdatawg.nist.gov/_uploadfiles/M0090_v1_7386661507.docx) | 2 |  |  |  | 4 | 2 | 1 | 1 | 1 | 1 |
| [**M0103**](http://bigdatawg.nist.gov/_uploadfiles/M0103_v1_9862181899.docx) | 1 |  |  |  | 2 | 1 | 1 | 1 | 1 | 1 |
| [**M0127**](http://bigdatawg.nist.gov/_uploadfiles/M0127_v1_8374144249.docx) | 2 |  |  |  | 5 | 3 | 1 | 1 | 2 | 1 |
| [**M0129**](http://bigdatawg.nist.gov/_uploadfiles/M0129_v1_8721988256.pdf) | 4 |  |  |  | 1 | 3 | 1 | 1 | 1 | 2 |
| [**M0136**](http://bigdatawg.nist.gov/_uploadfiles/M0136_v1_5489292512.docx) | 1 |  |  |  | 1 | 3 | 1 | 1 | 1 | 1 |
| [**M0147**](http://bigdatawg.nist.gov/_uploadfiles/M0147_v1_9011190023.docx) | 1 |  |  |  | 1 | 1 | 1 | 1 | 5 | 1 |
| [**M0148**](http://bigdatawg.nist.gov/_uploadfiles/M0148_v1_1457436047.docx) | 5 |  |  |  | 5 | 2 | 2 | 1 | 4 | 1 |
| [**M0155**](http://bigdatawg.nist.gov/_uploadfiles/M0155_v1_3537561150.docx) | 3 |  |  |  | 3 | 1 | 1 | 1 | 1 | 1 |
| [**M0157**](http://bigdatawg.nist.gov/_uploadfiles/M0157_v1_6396188402.docx) | 2 |  |  |  | 1 | 2 | 5 | 1 | 4 | 1 |
| [**M0158**](http://bigdatawg.nist.gov/_uploadfiles/M0158_v1_1209297717.docx) | 2 |  |  |  | 3 | 5 | 1 | 1 | 1 | 1 |
| [**M0160**](http://bigdatawg.nist.gov/_uploadfiles/M0160_v1_6667987957.docx) | 5 |  |  |  | 1 | 4 | 3 | 1 | 1 | 1 |
| [**M0161**](http://bigdatawg.nist.gov/_uploadfiles/M0161_v1_8712614971.docx) | 2 |  |  |  | 3 | 6 | 2 | 1 | 4 | 1 |
| [**M0162**](http://bigdatawg.nist.gov/_uploadfiles/M0162_v1_8977322730.docx) | 3 |  |  |  | 1 | 1 | 2 | 2 | 1 | 1 |
| [**M0164**](http://bigdatawg.nist.gov/_uploadfiles/M0164_v1_8073380462.docx) | 1 |  |  |  | 5 | 6 | 1 | 1 | 1 | 1 |
| [**M0165**](http://bigdatawg.nist.gov/_uploadfiles/M0165_v1_9206577703.docx) | 3 |  |  |  | 2 | 1 | 3 | 2 | 2 | 1 |
| [**M0166**](http://bigdatawg.nist.gov/_uploadfiles/M0166_v3_2675550648.DOCX) | 3 |  |  |  | 3 | 3 | 1 | 1 | 1 | 1 |
| [**M0167**](http://bigdatawg.nist.gov/_uploadfiles/M0167_v1_7320744610.docx) | 3 |  |  |  | 2 | 3 | 2 | 2 | 1 | 1 |
| [**M0170**](http://bigdatawg.nist.gov/_uploadfiles/M0170_v1_5720273656.docx) | 2 |  |  |  | 2 | 1 | 1 | 1 | 1 | 1 |
| [**M0171**](http://bigdatawg.nist.gov/_uploadfiles/M0171_v1_7185377580.docx) | 1 |  |  |  | 2 | 1 | 1 | 1 | 1 | 1 |
| [**M0172**](http://bigdatawg.nist.gov/_uploadfiles/M0172_v1_8972697421.docx) | 4 |  |  |  | 3 | 5 | 1 | 2 | 1 | 1 |
| [**M0173**](http://bigdatawg.nist.gov/_uploadfiles/M0173_v1_3577651730.docx) | 3 |  |  |  | 3 | 6 | 2 | 2 | 3 | 1 |
| [**M0176**](http://bigdatawg.nist.gov/_uploadfiles/M0176_v1_7714944584.docx) | 2 |  |  |  | 4 | 8 | 1 | 2 | 2 | 1 |
| [**M0177**](http://bigdatawg.nist.gov/_uploadfiles/M0177_v1_1133239355.docx) | 6 |  |  |  | 1 | 4 | 1 | 5 | 4 | 1 |
| [**M0182**](http://bigdatawg.nist.gov/_uploadfiles/M0182_v1_3824910269.docx) | 1 |  |  |  | 1 | 3 | 1 | 1 | 1 | 1 |
| [**M0183**](http://bigdatawg.nist.gov/_uploadfiles/M0183_v2_2632549904.docx) | 3 |  |  |  | 1 | 1 | 1 | 1 | 1 | 1 |
| [**M0184**](http://bigdatawg.nist.gov/_uploadfiles/M0184_v1_8925840651.docx) | 5 |  |  |  | 1 | 1 | 1 | 1 | 1 | 1 |
| [**M0185**](http://bigdatawg.nist.gov/_uploadfiles/M0185_v1_4843821869.docx) | 1 |  |  |  | 1 | 2 | 1 | 1 | 1 | 1 |
| [**M0186**](http://bigdatawg.nist.gov/_uploadfiles/M0186_v1_2893359960.docx) | 3 |  |  |  | 1 | 1 | 2 | 1 | 1 | 1 |
| [**M0190**](http://bigdatawg.nist.gov/_uploadfiles/M0190_v1_2052764107.docx) | 2 |  |  |  | 1 | 1 | 1 | 1 | 1 | 1 |
| [**M0209**](http://bigdatawg.nist.gov/_uploadfiles/M0209_v1_4702199454.docx) | 1 |  |  |  | 2 | 3 | 1 | 1 | 1 | 1 |
| [**M0210**](http://bigdatawg.nist.gov/_uploadfiles/M0210_v1_7474668890.docx) | 1 |  |  |  | 1 | 4 | 1 | 1 | 1 | 1 |
| [**M0211**](http://bigdatawg.nist.gov/_uploadfiles/M0211_v2_3994987602.docx) | 1 |  |  |  | 1 | 1 | 1 | 1 | 1 | 1 |
| [**M0213**](http://bigdatawg.nist.gov/_uploadfiles/M0213_v1_5447164009.docx) | 1 |  |  |  | 3 | 1 | 1 | 1 | 1 | 1 |
| [**M0214**](http://bigdatawg.nist.gov/_uploadfiles/M0214_v1_5406533104.docx) | 1 |  |  |  | 1 | 3 | 2 | 1 | 1 | 1 |
| [**M0215**](http://bigdatawg.nist.gov/_uploadfiles/M0215_v1_1579991796.docx) | 3 |  |  |  | 1 | 3 | 1 | 1 | 1 | 1 |
| [**M0219**](http://bigdatawg.nist.gov/_uploadfiles/M0219_v1_1106458060.docx) | 1 |  |  |  | 1 | 1 | 1 | 2 | 1 | 1 |
| [**M0222**](http://bigdatawg.nist.gov/_uploadfiles/M0222_v1_8823653701.docx) | 1 |  |  |  | 1 | 1 | 1 | 1 | 1 | 1 |
| [**M0223**](http://bigdatawg.nist.gov/_uploadfiles/M0223_v1_9531843932.docx) | 2 |  |  |  | 1 | 2 | 1 | 1 | 1 | 1 |

## Transformation Requirements

## Resource Requirements

## Data Usage Requirements

## Security & Privacy Requirements

## Lifecycle Management Requirements

## System Management and Other Requirements



# Service Abstractions (SAs) Requirements



## What is an SA?

## Service Abstractions Objectives

## Service Abstractions Management

## Types of Service Abstractions

### Data Service Abstraction

### Transport Service Abstraction

### Usage Service Abstraction

# Conclusions and Recommendations

# Reference

# Appendix A: Submitted Use Cases