Open Geospatial Consortium

Publication Date: 2014-05-20

Approval Date: 2014-04-30

Submission Date: 2013-11-05

Reference number of this document: OGC 11-145

External identifier of this OGC® document: http://www.opengis.net/doc/WP/cyber-arch-geosciences

Category: OGC® White Paper

Editors: George Percivall, OGC
See List on next page

Cyberarchitecture for Geosciences White Paper

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Document type: **OGC® White Paper**
Document subtype: **not applicable**
Document stage: **Approved for Public Release**
Document language: **English**

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Introduction

The National Science Foundation (NSF) is developing "EarthCube" - Towards a National Data Infrastructure for Earth System Science[1]. In a new partnership between GEO and the NSF Office of Cyberinfrastructure, NSF seeks transformative concepts and approaches to create a sustained, integrated data management infrastructure spanning the Geosciences. Meeting the challenges in geoscience research requires innovation and paradigm shifts in cyberinfrastructure. Information technology must advance to meet the emerging approaches to science. A cyber-architecture identifies repeatable patterns, reusable components, and open standards that provide starting point for innovative developments.

This white paper was written by Open Geospatial Consortium (OGC) members and associates to contribute to development of the NSF EarthCube. This document does not represent an official position of the OGC. However, the discussions in this document could very well lead to NSF developments and subsequent OGC documents. Recipients of this document are invited to reply to the authors' with notification of any relevant patent rights of which they are aware and to provide supporting documentation.

Cyberarchitecture for Geoscience

Cyberarchitecture represents a paradigm shift in scientific research that facilitates collaboration across disciplines and across great distances, and enables breakthroughs to be reached more quickly and efficiently. Geospatial cyberarchitecture is a specific type of CI that synergistically integrates the capabilities of CI, geographic information systems, and spatial analysis for geospatial problem solving and decision-making [Wright 2011a]. The deluge of data from sensor networks, satellites, and cell phones cannot be understood or analyzed unless it can be properly managed for interoperability. The complexity of geographic space in which these entities are embedded (e.g., at multiple spatial dimensions and scales) poses significant computational and intellectual challenges in distributed spatial data mining and analysis, the geospatial semantic web, and spatial information infrastructures. This paper describes elements of cyberarchitecture that are vital to advancement of the geosciences. The elements listed here include proven technology that can now be applied to geosciences as well as trends in the GeoWeb that will be enhanced by results of geoscience implementations.

Key Elements of Cyberarchitecture for Geosciences

- Location-based data management, fusion and presentation
- Semantic and linked data for bridging gaps between geoscience communities
- Data publication and long-term preservation services
- Provenance and uncertainty reporting for data/model evaluation and use
- Increasing geoscience observations from sensors and citizens
- Environmental models and simulations of many different types
- Geoscience workflows through mashups of web services
- Federated resource management
- Flexibility to operate over different distributed computing platforms
- Cyberarchitecture based on prototype-driven standards

Location-based data management, fusion and presentation

A participatory cyberenvironment enables collaborations that span disciplines, laboratories, organizations and national boundaries, and involves working with heterogeneous resources such as sensors, software components, databases, scientific instruments and models, and people. It is also an integration and presentation platform for knowledge network that requires rich contextual information, including social, geospatial, provenance, and semantic contexts.

Geoscience data is almost always location based. This feature should help define the focus of geoscience CI architecture design. For example, for presenting (visualizing) data on a global scale, the architecture should allow seamless integration of sub-systems that are geo-politically accepted. That is actually a federated CI

[1] http://www.nsf.gov/geo/earthcube/

system of regional CI systems. This feature on data visualization should be reflected in data management and workflow automation and therefore impose specific requirements in the CI architecture.

> "With the advent of the geospatial web or "geoweb" and community efforts such as Open Geospatial Consortium to promote geo-information and solution interoperability, geospatial context is playing an increasingly important role in knowledge network presentation and integration, which is critical for a participatory Cyberenvironment." [Liu 2007]

The ability to discover, access, integrate, analyze, and present geospatial data across a distributed computing environment has tremendous scientific value. Indeed, with the growing connectedness of our world —through data-collecting instruments, data centers, supercomputers, departmental machines, and personal devices — we expect a wide range of information to be instantly accessible from anywhere [Lee 2008].

- **Semantic and linked data for bridging gaps between geoscience communities**

The geosciences branch into diverse communities, which are usually weakly connected. Each of these communities uses distinct terminologies, data models, environmental simulations, etc. A cyberarchitecture to support geoscientists must provide all means to overcome these barriers. Linked Data principles for spatial and environmental relationships must play a role in this endeavor.

The GeoWeb is based on a set of standards for geospatial information. The information standards are of many types ranging from syntactic to semantic. Use of the GeoWeb standards will aid EarthCube in responding to this ACCI Finding:

> "A lack of standards in application programming interfaces, data models and formats, and interoperability of programming models makes the integration of different pieces of software representing different models and different phases of the workflow challenging." [ACCI 2011]

Similar to standards for units of measure, information standards are fundamental to the progress of science. Use of internationally accepted standards allows scientists to reliably access and review data and information gathered by other scientists in order to advance the knowledge of our world. Geospatial information standards provide the basis for communicating data, information and hypothesis about the geosciences [Khalsa 2010].

Yet heterogeneity will continue to exist and be useful, requiring introduction of mediators (also termed brokers) as has been proposed to implement interoperability in a number of geospatial issues, particularly discovery services [Nativi 2009]. This approach addresses shortcomings of catalog services by identifying three additional functionalities: Messaging providing support for asynchronous communication patterns; Distribution addressing the communication between one consumer and multiple producers; Mediation addressing the mismatches between heterogeneous consumers and providers.

- **Data Publication and long-term preservation services**

The CI must support publication and long-term preservation not only of data references, but of access to the data as well. The overall objective is simple: make it possible for authors to create online publications that enable readers to access, analyze, and display the data discussed in the publication [Domenico 2011]. Currently available (formal and community) standard web services have made it possible to create rudimentary examples of such data interactive documents.

The assumption that future scientists will be able to use data collected over long time periods and to integrate data from disparate sources to create new datasets is dependent upon interoperability of the data, software (including both data base and analytic software), and hardware. Coordination in standards development and the use of commonly accepted standards are needed to promote data interoperability, so that data collected in different countries, in different time periods, using different software and hardware configurations, and across different disciplines can be integrated. (ICSU 2004)

Data curation is especially important in geoscience due to the long-term temporal features in many geoscience phenomena. Other sciences, such as climate change, biodiversity, phenology, can truly benefit from well-curated geoscience data. Proper data curation needs careful design and inclusion in the system from the beginning, which means extra investment for seeing potential returns many years later.

- **Provenance and uncertainty reporting for data/model evaluation and use**

As an infrastructure for science, EarthCube must address the issues of uncertainty quantification and reporting with an emphasis on experimentation. Quality science requires transparency. This certainly includes the characterization of sensors, reporting and visualization of uncertainty, appropriate lineage information (used data, parameters and models), as for example requested in ISO metadata, but also additional information in order to ensure reproducibility of presented science results.

This need has been studied for the ocean observing community with recommendations that apply to all geosciences. Just as there are now tools for the development of text-based web content, we need to develop tools for observation web services that fuel our earth observing systems. Data Centers could ingest data from OGC Sensor Observation Services with minimal impact on the providers operations (no additional software to be written, no additional data service required). These data can be pulled into an archive, parsing metadata on the fly and populating its data bases for discoverability. Since the data and provenance are fully-described and integrated as a service, the records are archive-ready. Use of SensorML would guide manufacturers of environmental sensors to generate fully-described sensor descriptions in a standards-based XML encoding [Fredericks 2010].

In many cases key simulation codes grow organically as a new research code is added to an existing body of code, resulting in unsustainable applications that cannot be easily verified, where error propagation from one part of the code to others may not be well understood [ACCI 2011]. Developments in UnCertML and the UnCertWeb project have lead to methods to characterize uncertainty propagation through algorithmic transforms.

- **Increasing geoscience observations from sensors and citizens**

Sensor observations are indispensible source to enable the vision of understanding the Earth with EarthCube. They are capable of providing live or near-real time data to facilitate the timely monitoring of the Earth system. The EarthCube needs to adopt the Sensor Web concept and systems for supporting the discovery and access of sensor observations and ultimately providing bi-directional live connections between the sensors and the rest of Earth observing system of systems. The concept of Sensor Web carries different meanings due to the heterogeneous background of its developments and applications. Nevertheless, the consensuses are that Sensor Web will make ultimate and smart connections among sensors and between sensors and models in a service-oriented architecture (SOA). [Di 2011]

Beyond the standards based approach for Sensor Web Enablement, lies new technology for collecting observations that can inform science research. Volunteered geographic information (VGI) has become a major resource for understanding events observed and report by many people. With research into the provenance and quality, VGI may become a resource for studying some geo-phenomena. Geoscience provides foundation for environmental research, which naturally involves citizen efforts worldwide. However, collecting geo-based environmental sensitive data from volunteers' mobile devices, for example, is only meaningful when the data is integrated with research-end sensor data, satellite data, and scientific modeling data. The integration should be building into the infrastructure at the design phase to allow us benefit from Citizen Science.

Similarly the Internet of Things (IoT) is a technology that will enable access to many sensors and other information based on Machine-to-Machine communications scaling to and beyond current web-scale systems. For example, in Germany there is a public display of radiation readings, but the raw data was not generally available to the public. The institution in charge (Bundesamt für Strahlenschutz) may have let certain people access that data, but there was no publicly available download. The data has been made available via Pachube – an IoT pioneer – to approximately 1750 real-time radiation feeds. This is a real example of not only a shift in how governments are choosing to communicate and partner with their citizens, but of a new class of individual that has the ability and insight to leverage the Internet of Things to affect society in a significant and powerful way [Steinbach 2011].

- **Environmental models and simulations of many different types**

Environmental models and related techniques provide an important source of information and basis of research relevant to EarthCube. Many types of algorithms are included in discussions of "Models": global circulation models, geophysical models, ecology prediction models, data assimilation, ensemble techniques, information fusion, and data mining. Various "model web" or "integrated model" activities aim to develop clarity and interoperability to this important element of CI. Fundamental to developing geoscience knowledge based on predictive models is to well characterize the observations and simulations that make predictions of physical variables. It has been recommended that NSF should support standards development in both application specific data formats, and generic requirements for multi-scale, multi-model integration. [ACCI 2011].”

The many meanings of “model” need to be clarified in order that they may be used in a distributed, interoperable CI. Classification of models based on algorithm type has been suggested as two main categories: Data-Driven Model (DDM) and Physics-based Model (PBM). Classification based on user interaction is needed. Large institutional models are run on a routine basis by the institution with model results and provenance made accessible to user for “static interaction” similar to datasets. Cloud-based models allow “dynamic access” by users who can integrate multiple runs with varying inputs into their research methods. As an example of the later see the species presence prediction modeling based on dynamic interaction to the model using a Web Processing Service [Nativi 2011].

- **Geoscience workflows through mashups of web services**

“Scientific workflows, which provide for the expression, invocation, documentation, and exchange of mashups, are likely to become increasingly important as both experiments and simulations become increasingly complex and multidisciplinary” [ACCI 2011].

Processing of geoscience observations consist of data collected by satellite, surface and airborne sensors and processing capabilities distributed a many network accessible locations. OGC has developed standards that allow for geoscience processing mashups through web services:

> “The data are of multiple types including gridded and point coverages. Processing of these data occur at multiple points across the sensor observation-to-knowledge information flow, including on-board sensor processing, data re-formatting processing, and data analysis processing. Conducting the data flow through web services allows components to be distributed and coupled to form an end-to-end processing chain of services consisting of contributions from diverse and distributed service providers.” [Falke 2008]

Making data process workflow automation as part of the CI architecture is one way to control the data quality. As we all agree, sharing data is only the first step in this picture. Different users may get different results from the same data. Sharing data as well as data process workflow via workflow automation in Web services allows different users get the same results from the same data. Speaking from computer science perspective, workflow automation brings computational thinking to a whole new level.

- **Federated Resource Management**

As noted above, a cyberinfrastructure (CI) for geosciences will be a *federation* of regional CI systems. Federations require some degree of *resource management*, depending on the federation's requirements. While resources may typically be thought of as data, storage, servers, or network bandwidth, resources can also include user identity, data access privileges, collaboration environments, and policy. In much the same way that common metadata schemas are necessary for *data interoperability*, analogous metadata schemas are necessary for resource interoperability, in general. Such schemas exist for basic hardware resources. Managing non-hardware resources, however, is strongly related to security, i.e., authentication, authorization, etc.

Different types of federation will require different types of federation security. Very loose, informal federations may be built using simple, low-security mash-ups, where data and services are openly available. Other federations may want at least password protection. Federations with more strict security requirements could require PKI certificates, Kerberos tickets, or some other form of strong authentication. Both passwords and certificates require some form of *Identity Management*. In the case of federated, regional CIs, having a different user ID and password for each institution is simply not scalable. Hence, the notions of *federated ID management* and *single sign-on (SSO)* have become essential.

Additional topics in this area include *delegation of trust* – where authority to act on one’s behalf is temporarily delegated to another user or site – and *virtual organizations (VOs)* that enable *role-based authorization* to be applied across a set of users from different institutions. Operational VO systems – running hundreds of VOs – are used by the European Grid Infrastructure, the Open Science Grid, the German D-Grid, and others, to support various experimental science user groups. Further discussion of these federated resource management issues, along with a survey of six existing and in-progress distributed computing infrastructures for geospatial remote sensing, is given in [Lee 2011].

- **Flexibility to operate over different distributed computing platforms**

EarthCube will need to provide seamless access to science information across distributed computing platforms. Some previous Cyberinfrastructure developments have been based on tightly coupled APIs. The GeoWeb demonstrates the success of interface and encoding standards that coexist easily with other interfaces and encodings in a rich and diverse ecosystem of choices and capabilities. This leads to something like a 'Multi-Style SOA.' Implementation as façades provides an inherently low adoption threshold.

Examples include the developments of a Linked Data Proxy to the OGC Sensor Observation Service (SOS), as part of general efforts on semantic enablement. SOS was originally developed and published as a "key-value pair" web service binding prior to the elaboration of REST bindings. Recently a RESTful proxy and data model for SOS has been developed and is under consideration [Janowicz 2011]. Such developments are typical of how application software evolves as the underlying software engineering and development platforms progress.

The cyberarchitecture must be flexible enough to operate on various distributed computing platforms, including cloud, cluster, and desktop environments, and should scale up or down as needed to meet the needs of the data size and analysis requirements.

- **Cyberarchitecture based on prototype-driven standards**

Systems of Systems – like EarthCube - deal with holistic solutions to implement resources interoperability and metadata sharing among disparate (i.e. heterogeneous and distributed) and autonomous systems. To address some of these interoperability challenges, the Earth science communities have been developing interoperability specifications by profiling international standards according to their specific domain needs. This has resulted in a somewhat fragmented multi-speed geosciences community, as for digital interoperability. The need to compare the on-going activities for disciplinary interoperability specifications and promote discussion forums on multi-disciplinary interoperability is clear. The Earth and Space Sciences Informatics (ESSI) sections of EGU and AGU have been a focus for these discussions [Nativi 2010].

Prototype-driven standards development and consensus endorsement process is a good match to the cautionary prescription given by the NSF ACCI report:

> "The identification of software standards that deserve to be supported is one of the roles that NSF's peer-review processes can facilitate. However, today's *ad hoc* and loosely coordinated approaches to software infrastructure allow unanticipated breakthroughs and chances for new ideas to arise and influence the entire cyber-ecosystem; this must not be lost in a well-meaning attempt to make the ecosystem more efficient through designation of approaches as preferred or deprecated." "A balance must be preserved between standardization for efficiency and flexibility for innovation" [ACCI 2011].

The transformative impact of standards on sharing and distribution of geospatial data has already been demonstrated in a variety of contexts. For example, the OGC Interoperability Program has conducted more than eight phases of OGC Web Services (OWS) testbeds with results now in operational Earth observation and geoscience systems. The OGC process is one element of the Governance process recommended for EarthCube in a companion white paper [Arctur 2011].

Architecting EarthCube

What is Architecting?

The preceding sections described elements of a Cyber-architecture suited to meet the needs of EarthCube. The processes and methods to build such a cyber-architecture are the topic of architecting. Three, non-exclusive approaches to architecting have been defined based on multiple projects [Rechtin 1991]

- Heuristics: Architectural rules of thumb for structuring that brings form to function
- Stakeholders: Process based on governance principles to meet the needs of stakeholders
- Normative: Use and advancement of standards and reference models to guide development

Rechtin's text provides a rich set of heuristics that were well honed during his time of leadership at Aerospace Corporation. A companion OGC white paper describes a Governance Process for evolutionary development of EarthCube [Arctur 2011]. The remainder of this paper suggests some starting points for the normative approach.

Science scenarios lead the way

In order to meet its objectives, the evolutionary development of EarthCube must be science driven. A companion OGC white paper defines sciences scenarios describing data-intensive, cross-disciplinary research that illustrate the need for an open, adaptable and integrative cyberinfrastructure [Welles 2011]. The scenarios cover a range of topics in the Geosciences, and target current and anticipated future problems faced by researchers and their support systems (research centers, libraries, data centers and archives and commercial service providers) working to address these challenges.

Cyberarchitecture and Scientific Epistemology

Development of EarthCube must build on the rapid advances in computers and computation that define new ways to determining how we know what we know about our world. Computation, along with theory and experiment, has become the "third pillar" of science and engineering. And making new scientific discoveries requires the computational ability to synthesize and analyze very large data sets, integrated across biological, physical, and social sciences and engineering, and across the science-technology interface. Hey *et al*. named this "data-intensive science" as the "fourth paradigm" [Hey 2009, Wright 2011a, Benioff 2005]. While we have attained high-performance computing at affordable cost and have made good progress on simulation tools, many challenges remain in effectively integrating multiple field observatories containing thousands of instruments, involving millions of users, and petabytes of data, built on a true data grid with the ability to analyze data on that grid with sophisticated data analysis [Wright 2011a, Hey 2009].

Starting places for Cyber-architecture

This paper has described some key CI aspects needed for EarthCube to meet its objectives along with an initial sketch of how this architecting can be done based on science leadership. Nothing like EarthCube exists today but some existing developments provide some starting points for describing the structures needed for the Cyberarchitecture of EarthCube. These documents can be used as resources for defining a cyber-architecture for EarthCube:

- The OGC Reference Model (ORM) describes the OGC Standards Baseline focusing on relationships between the baseline documents. The OGC Standards Baseline consists of the approved Abstract and Implementation Standards (interface, encoding, profile, application schema) and Best Practices. The ORM provides just an overview of the results of extensive development by hundreds of OGC member organizations and tens of thousands of individuals who have contributed to development of the OGC Standards Baseline [Percivall 2008].
- The GEOSS AIP Architecture defines a multi-viewpoint architecture for the exchange and dissemination of observational data and information in the Global Earth Observing System of Systems (GEOSS) [AIP 2010]. This architecture was developed and is used in the GEOSS Architecture Implementation Pilot (AIP). The Group on Earth Observations (GEO) is coordinating efforts to build GEOSS through a series of Tasks. GEO's Members include 80 Governments and the European Commission. In addition, 58 intergovernmental, international, and regional organizations with a mandate in Earth observation or related issues have been recognized as Participating Organizations.

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