The Design of a Community Science Cloud: The Open Science Data Cloud Perspective

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Abstract

In this paper we describe the design, and implementation of the Open Science Data Cloud, or OSDC. The goal of the OSDC is to provide petabyte-scale data cloud infrastructure and related services for scientists working with large quantities of data. Currently, the OSDC consists of more than 2000 cores and 2 PB of storage distributed across four data centers connected by 10G networks. We discuss some of the lessons learned during the past three years of operation and describe the software stacks used in the OSDC. We also describe some of the research projects in biology, the earth sciences, and social sciences enabled by the OSDC.

Keywords: data intensive computing, cloud computing, science clouds, open data

1 Introduction

The Open Science Data Cloud or OSDC (www.opensciencedatacloud.org) is a petabyte-scale science cloud managed and operated by the Open Cloud Consortium (OCC) that has been in operation for approximately three years. The OCC is a not-for-profit that develops and operates cloud computing infrastructure for the research community.

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The OSDC allows scientists to manage, analyze, share and archive their datasets, even if they are large. Datasets can be downloaded from the OSDC by anyone. Small amounts of computing infrastructure are available without cost so that any researcher can compute over the data managed by the OSDC. Larger amounts of computing infrastructure are made available to researchers at cost. In addition, larger amounts of computing resources are also made available to research projects through a selection process so that interested projects can use the OSDC to manage and analyze their data.

The OSDC is not only designed to provide a long term persistent home for scientific data, but also to provide a platform or “instrument” for data intensive science so that new types of data intensive algorithms can be developed, tested, and used over large amounts of heterogeneous scientific data.

The OSDC is a distributed facility that spans four data centers connected by 10G networks. Two data centers are in Chicago, one is at the Livermore Valley Open Campus (LVOC), and one is at the AMPATH facility in Miami.

2 Science Clouds

Although NIST has provided a definition of a cloud [1], it is probably most helpful for the purposes here to think of a cloud as a warehouse scale computing facility [2] that provides services. Usually, these services are self-provisioned. The services may be infrastructure services, such as compute and storage resources, or software services, such as data analysis services. We will use the term Cloud Service Provider (CSP) to refer to the provider of these services.

There are quite a few commercial CSPs and a growing number of CSPs focused on serving the needs of scientists. Table 1 shows some of the important differences between commercial CSPs and those serving the needs of researchers.

![Figure 1: Tukey provides the link between the users and services provided by the OSDC. From the user’s perspective they log into the Tukey Console (a web application) and have immediate access to the services listed. This is accomplished by the web application interfacing with the middleware authorizing users and performing API translations between various cloud software stacks for virtual machine provisioning and determining usage.](image)

CSOC. Essentially, the OSDC systems group operates what you might call a Cloud Services Operation Center (CSOC) to manage and operate the OSDC data centers, cloud services, and related administrative services, as well as to support OSDC researchers using the OSDC. A CSOC is roughly analogous to a Network Operations Center (NOC). Much as NOCs enable the operations of the high performance research networks that have served an important role in today’s cyberinfrastructure, CSOCs have the potential to play an analogous role for high perfor-
3 Open Science Data Cloud

3.1 Open Cloud Consortium

The Open Cloud Consortium (OCC) is a 501(c)(3) not-for-profit supporting the scientific community by operating cloud infrastructure to support scientific, medical, health care, and environmental research. OCC members include universities, such as the University of Chicago and Northwestern University; NASA; and foreign partners, such as AIST. Table 2 contains a summary of the resources currently operated by the OCC (we will be more than doubling these resources in 2013).

The Open Science Data Cloud (OSDC) is one of the projects managed by the OCC.

### Table 1: Some of the differences between Commercial CSPs and Science CSP serving the research community.

|                           | Commercial CSP                               | Science CSP                                         |
|---------------------------|---------------------------------------------|-----------------------------------------------------|
| Point of view             | Make a profit by providing services.         | Democratize access to data. Support data driven discovery. Provide long term archiving of data. |
| Computing and storage     | scale out computing and object based storage | also support data intensive computing and high performance storage |
| Flows                     | lots of small web flows                      | also large incoming and outgoing data flows          |
| Accounting                | essential                                    | essential                                            |
| Lock in                   | lock in is good                              | important to support moving data and computation between CSPs |

3.2 OSDC Approach

The OSDC currently manages about a PB of data for the researchers that it supports and operates a PB-scale Eucalyptus, OpenStack, and Hadoop-based infrastructure so that researchers can compute over their data. It provides tools so that researchers can upload and analyze datasets, integrate their data with data from research collaborators, and integrate their data with public data for analysis.

The approach adopted by the not-for-profit OSDC is modest: 1) Use a community of users and data curators to identify data to add to OSDC. This data is managed by the OSDC-Root cluster. Data is made available via a high performance storage system (currently GlusterFS). 2) Use permanent IDs to identify this data and associate metadata with these IDs. 3) Support permissions so that colleagues can access this data prior to its public release and to support
| Resource               | Type                          | Size                                      |
|------------------------|-------------------------------|-------------------------------------------|
| OSDC-Adler & Sullivan  | OpenStack & Eucalyptus based utility cloud | 1248 cores and 1.2PB disk                 |
| OSDC-Root              | Storage cloud                 | approximately 1 PB of disk                |
| OCC-Y                  | Hadoop data cloud             | 928 cores and 1.0 PB disk                 |
| OCC-Matsu              | Hadoop data cloud             | approximately 120 cores and 100 TB        |

Table 2: Summary of resources operated by the OCC.

analysis of access-controlled data. 4) Support both file-based descriptors and APIs to access the data. 5) Make available computing images via infrastructure as a service that contain the software tools and applications commonly used by a community. 6) Provide mechanisms to both import and export data and the associated computing environment so that researchers can easily move their computing infrastructures between science clouds. 7) Identify a sustainable level of investment in computing infrastructure and operations and invest this amount each year. 8) Provide general support for a limited number of applications. 9) Encourage OSDC users and community of users to develop and support their own tools and applications.

4 Research Communities Served

The OCC’s Open Science Data Cloud (OSDC) currently serves multiple disciplines that use big data, including the earth sciences, biological sciences, social sciences, and digital humanities. In addition, the OSDC provides backup for a variety of multiple terabyte size datasets, including the Sloan Digital Sky Survey, modENCODE, and ENCODE.1

4.1 Biological Sciences

The OSDC hosts over 400 TB for the biological sciences community, including the 1000 Genomes dataset, many of the datasets available from NIH’s NCBI, and the Protein Data Bank.

The OSDC provides biologists working with big data several benefits. First, the OSDC make it easy to store and share data, which is particularly beneficial for large collaborations in which many different research groups are analyzing the same data using different techniques. With the OSDC, different groups can analyze large biological datasets without the necessity of each group downloading the data.

Second, the OSDC makes available previously published data as OSDC public datasets and also makes available OSDC managed virtual machine images that include the analysis tools and pipelines used by the different research groups. In practice, that has significantly reduced the time required for a research group to analyze or reanalyze data. This approach is also quite helpful for those groups that do not want to code and maintain their own pipelines.

1Many of these datasets are available from opensciencedatacloud.org/publicdata.
Third, by supporting the integrated storage of both raw and analysed data in OSDC, it has been easier for biologists to combine different datasets for integrative analysis.

As mentioned, the OSDC has served as a back up facility for a number of research projects. For example, the OSDC was able to recover data for the modENCODE after an unusual failure at their Data Coordinating Center (DCC) and their back up site. Beginning later this year, the OSDC will be a backup site with cloud enabled computation for the ENCODE Project, which over four years is expected to produce over 500 TB of data.

An OSDC project called Bionimbus (www.bionimbus.org) has developed a cloud-based infrastructure for managing, analyzing, archiving, and sharing large genomic datasets. Bionimbus is used by a number of projects, including modENCODE and the T2D-Genes consortia. There are also secure, private Bionimbus clouds that are designed to hold controlled data, such as human genomic data.

4.2 Earth Sciences

Project Matsu (matsu.opencloudconsortium.org) is a joint research project with the NASA that is developing cloud based infrastructure for processing satellite image data. With support from the OSDC, scientists from NASA’s EO-1 mission have ported the processing of Level 0 and Level 1 data from EO-1’s ALI and Hyperion instruments to the OSDC-Sullivan Cloud. We are also using OSDC-Root to archive data on a go forward basis in the OSDC. We currently have over three years worth of data from EO-1 in the OSDC (approximately 30 TB). Project Matsu is also developing analytics for detecting fire and floods and distributing this information to interested parties.

4.3 Digital humanities

The OSDC supports Bookworm (arxiv.culturomics.org), which is being developed by Harvard’s Cultural Observatory and offers a way to interact with digitized book content and full text search. Bookworm uses ngrams extracted from books in the public domain and integrates library metadata, including genre, author information, publication place and date.

4.4 Social Sciences

The OSDC hosts a variety of datasets available from the social sciences, including the U.S. Census, Current Population Survey, General Social Survey, and a wide variety of datasets from the Inter-University Consortium for Political and So-
cial Research (ICPSR), the world's largest repository for social science data.

4.5 Information sciences

Finally, the OSDC has a variety of datasets that are useful to researchers developing big data algorithms, systems for processing big data, and applications for moving big datasets. These datasets include the Common Crawl, the results of focused crawls, the Enron datasets, datasets provided by the City of Chicago, etc.

In addition, the OCC runs the OCC-Y cluster for eight computer science departments in the U.S. that were formerly supported by the Yahoo-NSF M45 Project, including Carnegie Mellon University and the University of California at Berkeley. The OCC-Y Cluster was donated by Yahoo! to the OCC to support big data research.

5 Tukey

The current components of the OSDC can be roughly partitioned into two major categories: services for users, and backend components that enable data intensive computing.

The OSDC user services include the ability to provision virtual machines, access usage and billing information, share files, and access to a key service and public datasets. All of the OSDC user services are tied together by Tukey, an application we have developed to provide a centralized and intuitive web interface for accessing public and private cloud services. Figure 1 provides a high level overview of how Tukey provides OSDC user services.

Tukey powers the OSDC web-based user interface. Tukey is composed of a customizable web application and middleware that enables uniform access to the cloud services by the Tukey Console web application.

5.1 Tukey Console

The Tukey Console is a web application based on Django and utilizes the Tukey middleware to provide easy access to cloud services for users. The project began as an extension of Horizon, OpenStack's Dashboard. However, the need to support different authentication methods and other cloud software stacks required forking from the Horizon project. The core functionality of the web application is virtual machine provisioning with usage and billing information. We have also developed optional modules to provide web interfaces to other OSDC capabilities. These include file sharing management (Section 5.2) and public data set management (Section 5.3). Since all components of the application communicate through sockets, they can be moved to separate servers and use encrypted channels on our private network.

5.2 Tukey Middleware

The middleware portion of Tukey provides the ability to authenticate users and interface with various cloud software stacks. It consists of HTTP based proxies for authentication and API translations that sit between the Tukey web application and the cloud software stacks. This design allows it to be extensible to use other forms of authorization and cloud software stacks. Currently, the software can handle authentication via Shibboleth or OpenID and can interface with OpenStack and Eucalyptus based clouds. After receiving either a Shibboleth or OpenID identifier, the proxy looks for the cloud credentials associated with the identifier in the user database.
These credentials are securely provided to the API translation proxies. The translation proxies take in requests based on the OpenStack API and then issue commands to each cloud based on mappings outlined in configuration files for each cloud. The result of each request is then transformed according to the rules of the configuration file, tagged with the cloud name and aggregated into a JSON response that matches the format of the OpenStack API.

6 OSDC User Services

6.1 Dataset IDs

As part of our efforts to provide persistent, long-term access to scientific data we have developed a cloud service that provides IDs to datasets based upon ARK Keys [3]. We obtained a registered Name Assigning Authority Number (NAAN) and have begun assigning ARKs to the data in the OSDC. Currently, the key service can resolve persistent identifiers and provide metadata based on ARK inflections. The service can also be used with other persistent identifiers, which we may add in the future.

6.2 File Sharing and Permissions

One of the goals of the OSDC is to offer a platform where researchers can easily collaborate on big data projects. In addition to hosting large public datasets we also allow our users to share private datasets with specific users or groups of their choosing. Toward this goal, we have developed a functional prototype for distributed file sharing, with access control based on users, groups, and file-collection objects. Users have the ability to create and modify groups. A file-collection object can be a file, a collection of files, or a collection of collections. This hierarchical structure provides a foundation for users to manage projects and associated datasets. In the prototype implementation, users share files by adding them to a designated directory. This directory is monitored by a daemon process that propagates file information to a database. Users then utilize the OSDC web interface to grant permissions to users or groups on file-collection objects. The system serves the files using the WebDAV protocol while referencing the database backend. Users can access shared files on the OSDC by mounting the WebDAV file system with their own credentials.

6.3 Public Datasets

The OSDC currently hosts more than 600 TB of public datasets from a number of disciplines as discussed in Section 4. One of Tukey’s modules allows a data curator to manage the dataset and the associated metadata. This information is then published online so users can browse and search the datasets. The datasets are stored on a GlusterFS share, described in Section 7.1, so OSDC users have immediate access to all of the public datasets. The data is freely available for download, including over high performance networks via StarLight (www.startap.net)

6.4 Billing and Accounting

One of the lessons learned from early OSDC operations is that even basic billing and accounting are effective limiting bad behavior and providing incentives to properly share resources. We currently bill based on core hours and storage usage. For OSDC-Adler and OSDC-Sullivan, we poll every minute to see the number and types of virtual machine a user has provisioned and then
use this information to calculate the core hours. Storage is checked per user once a day. We plan to roll out similar billing and accounting on the Hadoop clusters. Our billing cycle is monthly and users can check their current usage via the OSDC web interface.

7 OSDC Backend Services

The OSDC is composed of compute clouds running OpenStack, Eucalyptus and Hadoop, with GlusterFS powering the storage on OpenStack and Eucalyptus. There are also storage racks that primarily host large GlusterFS shares. As discussed in the previous section, Tukey’s middleware links all of these systems to the OSDC web interface, diagrammed in Figure 3. This section discusses the design decisions and software used to make the OSDC a platform for scientific discovery.

7.1 High Performance Distributed Storage

A key component of the OSDC is providing file-based high performance access to large collections of data. Despite many advances in this realm, there are still a limited number of reliable open source file systems that can support these requirements. Our initial experiences with GlusterFS (version 3.1) were mixed; for example there was a bug in mirroring that caused some data loss and forced us to stop using mirroring. However, we now currently use version 3.3 and have observed improvements in stability and functionality. We are using GlusterFS on OSDC-Adler (156 TB), OSDC-Sullivan (38 TB), and OSDC-Root (459 TB) as the primary data stores. Since users have root access on their virtual machines we cannot allow them to mount the GlusterFS shares directly, as the current implementation of GlusterFS would allow them root access on the whole share. Therefore, the GlusterFS shares are exported to the virtual machine using Samba, which controls the permissions.

7.2 High Speed Data Transfers

The OSDC is a distributed facility connected by 10G networks so high speed transport protocols are important for enabling users to import data, export data, and to move data around flexibly in their analysis processes. For example, one project generates and preproceses their data on OSDC-Adler Eucalyptus cluster and then sends it to the OCC-Matsu Hadoop cluster for further analysis. Each time this is performed they have to move several terabytes. To ease the burden of large data transfers, we have developed UDR, a tool that provides the familiar interface of rsync while utilizing the high performance UDT protocol.

We monitored transfer speeds of a 108 GB and a 1.1 TB dataset, between OSDC nodes located in Chicago and LVOC with a round trip time of 104ms, using the protocols and encryption combinations shown in Table 3. In addition to measuring transfer speed, we calculate the the long distance to local ratio (LLR). LLR provides a measure of how close the transfer speed is of reaching the maximum throughput of the disks. The LLR is defined as the ratio between the transfer speed and the minimum of the source disk read speed and the target disk write speed. In our experiments the local source disk read speed was 3072 mbit/s and local target disk write speed was 1136 mbit/s, so the denominator for the LLR is 1136 mbit/s. The results of these transfers using UDR and rsync (version 3.0.7)
can be found in Table 3. The standard encryption used by the current version of rsync is 3des. However, only blowfish encryption is currently implemented in UDR, so results for both rsync using both 3des and blowfish are included. The results show that UDR achieves 87% and 41% faster speeds in the unencrypted and encrypted cases, respectively, than standard rsync while retaining the same familiar interface.

7.3 Automated Provisioning

Our first full rack installation of OpenStack was performed manually and took over a week to complete. As the OSDC scales, this would be unsustainable and limit our capabilities. To address this, we are using Chef (www.opscode.com/chef), along with PXE booting and IPMI, to fully automate provisioning with the goal of taking a full rack from bare metal to a compute or storage cloud in much less than a day. Our system starts with one PXE boot server, a Chef server, and a set of servers with IPMI configured. IPMI is triggered to boot the servers, which then pull a start-up image and boot options from the PXE boot server. The options define the location of a preseed file which the start-up sequence loads and uses as a guide to automate the installation of the generic Ubuntu Server. The installation uses the PXE boot server or a preconfigured proxy to install Ubuntu Server directly from the repositories to avoid any updates being required post-install. Then the installer runs a script specified at the end of the preseed file which sets up networking on the freshly installed system and adds another script to be run at boot. Upon rebooting, the next script double-checks the IPMI configuration, finishes partitioning the disk and sets up additional RAIDs as necessary, before downloading and installing the Chef client. The Chef client then checks in with the Chef server and runs the “recipes” listed for either a management node or a compute node. As a last step, a final clean up script runs to deliver us a fully functional OpenStack rack.
Table 3: Overall transfer speeds in mbit/s and the long distance to local ratio (LLR) between OSDC nodes in Chicago, IL and Livermore, CA, round trip time of 104 ms.

|                        | 108 GB Data Set | 1.1 TB Data Set |
|------------------------|-----------------|-----------------|
|                        | mbit/s | LLR  | mbit/s | LLR  |
| UDR (no encryption)    | 752     | 0.66 | 738     | 0.64 |
| rsync (no encryption)  | 401     | 0.35 | 405     | 0.36 |
| UDR (blowfish)         | 394     | 0.35 | 396     | 0.35 |
| rsync (blowfish)       | 280     | 0.25 | 281     | 0.25 |
| rsync (3des)           | 284     | 0.25 | 285     | 0.25 |

7.4 Monitoring Services

Once the systems are up and running, we perform two types of monitoring to automatically identify issues, provide alerts, and produce reports on the status and health of the systems. The first type of monitoring is cloud usage, such as how many instances each user is running. We have developed an in-house application for this purpose. The high level summary of the cloud status is made public on the OSDC website. The second type of monitoring is system and network status, for which we use the open source Nagios application (www.nagios.org).

The Nagios console is browser based and Nagios uses an agent, NRPE, to monitor the remote hosts in our environments and the services we wish to monitor on the remote hosts. The agent listens via TCP and communicates back to the master server after running checks on the remote servers that we configure using Nagios' text based configuration files. The master server, via the agent, asks for checks to be run and returns the values to the master server using binary plugins with arguments that designate the thresholds for “Warning” and “Critical” alerts. When those thresholds are crossed, Nagios sends alerts to the system administrators.

8 Sustainability Model

The OSDC is governed by a set of bylaws that are available on the web. Activities are organized into working groups. For example, the OSDC Working Group manages the Open Science Data Cloud. There is also an OCC Board of Directors and an OCC Advisory Committee.

The basic philosophy of the OSDC Working group is summarized by the following five rules:

1. Provide some services without charge to any interested researcher.
2. For larger groups and activities that require more OSDC resources, charge for these resources on a cost recovery basis.
3. Partner with university partners to gain research funding to tackle new projects and to develop new technology in order to further the mission of the OSDC.
4. Raise funding from donors and not-for-profits in order to provide more resources to more researchers.
5. Work to automate the operation of the OSDC as much as possible in order to reduce the costs of operations.
9 Commercial Clouds

Amazon Web Services (aws.amazon.com) provide a large and sophisticated set of infrastructure as a service (IaaS) capabilities, including computing (EC2) and storage (S3). The elastic (on-demand) nature of these services has made them popular for both business and scientific applications. Many applications have found that the eventual consistency model that Amazon’s SimpleDB supports to be adequate for their application requirements. Other providers such as Microsoft Azure and the Rackspace Cloud provide similar capabilities.

The OSDC is designed to interoperate with commercial clouds, such as provided by Amazon. In general, OSDC machine images can also run on AWS. The OSDC also supports high performance export of data from AWS with an in-house designed tool.

9.1 Why not just use Amazon?

A common question is whether researchers should just use public clouds, such as AWS, or in addition develop their own private and community cloud infrastructure. After three years of operation, it is clear that community science clouds such as the Open Science Data Cloud are complementary to public clouds such as AWS for the following reasons: First, science clouds such as the OSDC are designed to work with big data. They connect to high performance 10G and 100G networks, they support high performance storage, and they have support staff that are familiar with the problems arising when managing and transporting large datasets.

Second, for high end users, the OSDC is less expensive than using AWS, and for users with less demands, it is no more expensive. As a rough rule of thumb, when we operate an OSDC rack at approximately 80% efficiency or greater, it is less expensive than using Amazon for the same services. We are not arguing that every individual researcher should have their own cloud, but instead that it is less expensive for a community of researchers to have several well run community clouds that can interoperate with large scale commercial clouds, such as run by Amazon.

Third, many research products, including data products, are just too valuable to be entrusted exclusively to a commercial entity, which may over time, be bought, decide to close down a line of business, or go bankrupt. Not-for-profit community science clouds are a valuable complement to commercial clouds.

10 Conclusion

The OSDC provides research communities a high performance cloud infrastructure for data intensive science. Our design and implementation of the OSDC has been driven by the goal of providing both high performance and ease of use. The result is a number of projects utilizing the OSDC in biological sciences, earth science and digital humanities. Moving forward, we plan to expand both the infrastructure and services provided to meet the increasing data demands of scientific research. This expansion will be made possible by following our sustainability model. Additionally, we will continue to reevaluate the design and update the implementation of the OSDC based on user feedback, new technologies, lessons learned, and new data driven research projects.

\[2\text{Currently, a OSDC rack contains 39 servers, each with 8 cores and 8 TB of disk.}\]
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