ARISTOTLE
CLOUD FEDERATION

CC*DNI DIBBs: Data Analysis and Management Building Blocks for Multi-Campus Cyberinfrastructure through Cloud Federation

Monthly Report 3/31/2017

Report 18 of 18

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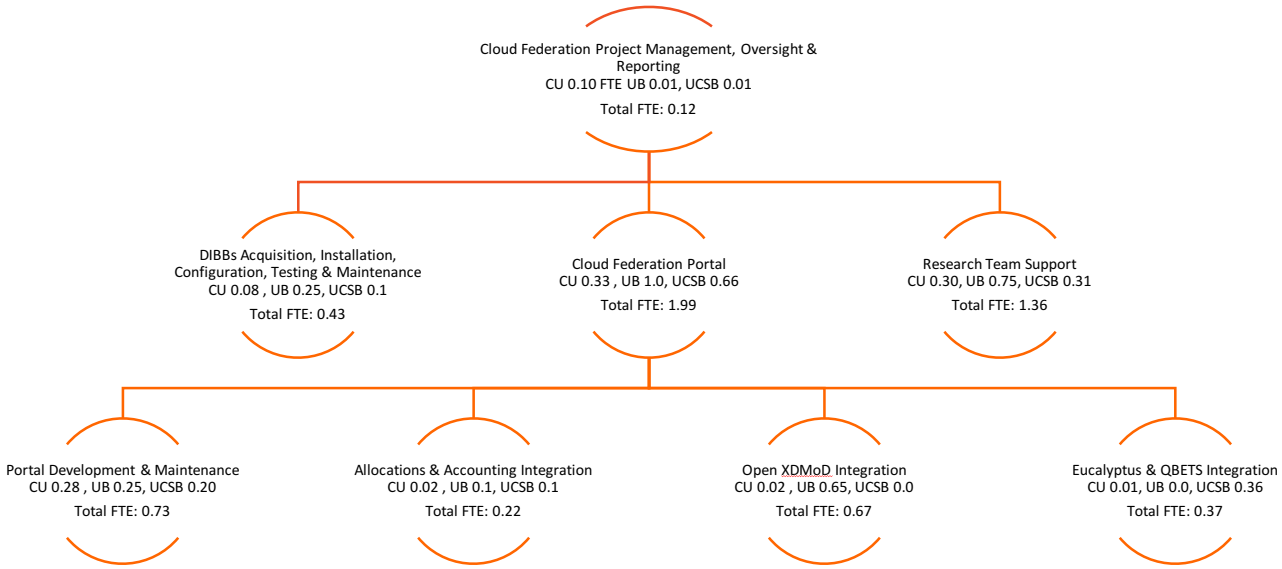
This is the eighteenth required monthly report of the Aristotle Cloud Federation team. We report on plans and activities for each area of the project Work Breakdown Structure (WBS).



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1.0 Cloud Federation Project Management, Oversight & Reporting Report

1.1 Subcontracts
All subcontracts are in place. Nothing new to report.

1.2 Project Change Request
No new project change requests were made this month.

1.3 Project Execution Plan
The Project Execution Plan (PEP) was approved by NSF on 12/18/2015. We are operating as planned and continuously updating our PEP on a monthly basis.

1.4 PI Meetings
No meetings this month.

1.5 Status Calls
2/28/2017 and 3/14/2017 project status call topics:

- Planning is underway for the April 25th 18-month review. Amy Walton participated in this month's Aristotle Science Team Advisory Committee (STAC) meeting and provided information on the review. She also complemented the team for organizing and leading the first NSF Data Infrastructure Building Blocks PI Workshop (DIBBs17) which was regarded as highly successful by NSF as well as the workshop participants.
- All project reports (annual, quarterly, monthly, and supplemental) will be available online for the 18-month NSF review committee at https://federatedcloud.org/reports/. STAC meeting minutes will also be available at: https://federatedcloud.org/science/advisorycommittee.php.
- The Blue Waters Workload Analysis carried out by the UB XMS (XD Net Metric Services) team at the request of NSF from July 2016-July 2017 delayed the Aristotle federated XDMoD target release date from 12/2016 to 7/2017.
- UCSB is troubleshooting a problem with slow snapshotting. Snapshotting a 400GB volume in the UCSB cloud took hours and sometimes resulted in error. While the snapshot error was fixed in the official Eucalyptus 4.4 release, slow performance was attributed to uploading the snapshot to object store. Cornell implemented a workaround for its single availability zone by setting *<cloud>.storage.shouldtransfersnapshots* to false so snapshots are not uploaded to object store. However, uploading to the Ceph cluster in the UCSB cloud is significantly slower than Cornell's (8.3MB/s vs. 50MB/s). UCSB and Cornell are comparing notes on their configurations of the Eucalyptus cloud and Ceph cluster to see what could attribute to the differences in performance.
- RT help desk accounts are being set up for UCSB and UB (central RT is at Cornell).
- Different software capabilities at the 3 sites is a plus; it will provide Aristotle users with more diverse resources to choose from, e.g., finance software at UB, MATLAB cluster software at Cornell, etc.
- Launch of the new MATLAB capability at Cornell has occurred. Users can now fire up 28 MATLAB Distributed Computing Server (MDCS) workers. This capability will be expanded in the future.

2.0 DIBBs Acquisition, Installation, Configuration, Testing & Maintenance Report

2.1 Hardware Acquisition

- UB received their 10Gb network switches and is configuring them with UB Campus switches to provide 10Gb cloud connection to the public network.
- Cornell's year 2 hardware is on back order due to a worldwide SSD shortage; we expect it to arrive in early April. This hardware will allow Cornell to build their production Eucalyptus 4.4 cloud with Ceph storage.
- UCSB ordered their year 2 hardware from HPE and Dell and resolved failed hardware components on Eucalyptus NC and Ceph OSD servers. Specific details on UCSB hardware will be available soon.

2.2 Software Installation, Configuration, and Testing

- UB is investigating Ceph configurations and will purchase hardware using the remainder of year 2 funding (supplemented with UB Center for Computational Research funds). With the impending removal of support for SANs in future versions of Eucalyptus, all Aristotle sites plan to migrate to Ceph.
- Cornell upgraded their test cloud to the official Eucalyptus 4.4 release and continued to develop and test configuration scripts for Globus single sign-on. Users can now log into their Aristotle accounts on the Eucalyptus Console via Globus Auth. Once logged in, they can access cloud resources as well as generate AWS-style access and secret keys to be used with command line tools or AWS API calls. Cornell is writing instructions for deploying these scripts and will work with UB and UCSB to configure their clouds to support Globus single sign-on so that Aristotle users can access all 3 clouds in the federations using their Globus credentials. Cornell is also installing and testing XDMoD on both the test and the production cloud.
- UCSB is planning their upgrade to Eucalyptus 4.4 and installing XDMoD.

The infrastructure planning table was updated this month:

	Cornell (CU)	Buffalo (UB)	Santa Barbara (UCSB)
Cloud URL	https://euca4.cac.cornell.edu	https://console.ccr-cbls-2.ccr.buffalo.edu/	https://console.aristotle.ucsb.edu
Cloud Status	Production	Production	Production
Euca Version	4.2.2	4.3.1	4.3
Globus	Yes	Planned	Planned
InCommon	Yes	Yes	Yes
Hardware Vendor	Dell	Dell/Ace	Dell
# Cores	*168	**256	140
RAM/Core	4GB/6GB	up to 8GB	up to 9GB

Storage	SAN (226TB)	SAN (336TB)	Ceph (288TB)
10Gb Interconnect	Yes	Yes	Yes
Largest Instance Type	28 core/192GB RAM	24 core/192GB RAM	16 core/16GB RAM
	* 168 additional cores augmenting the existing Red Cloud (376 total cores)	** 256 additional cores augmenting the existing Lake Effect Cloud (424 total cores)	

2.3 Potential Tools

- **CloudLaunch** - nothing new to report.
- **HPE Helion Eucalyptus -** version 4.4 was released and implementation plans are underway at all 3 sites.
- **Supercloud -** nothing new to report.

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3.0 Cloud Federation Portal Report

Content updates to the project are ongoing: https://federatedcloud.org.

We continue to monitor the usage graph (https://federatedcloud.org/using/federationstatus.php) to ensure data is being collected consistently from all sites. We are investigating software solutions.

Changes were made to the portal planning table this month:

Portal Framework			
Phase 1	**Phase 2**	**Phase 3**	**Phase 4**
10/2015 – 3/2016	**4/2016 – 12/2016**	**1/2017 - End**	**1/2017 - End**
Gather portal requirements, including software requirements, metrics, allocations, and accounting. Install web site software.	Implement content/functionality as shown in following sections. Add page hit tracking with Google Analytics, as well as writing any site downloads to the database.	Implement content/functionality as shown in following sections. Add additional information/tools as needed, such as selecting where to run based on software/hardware needs and availability.	Release portal template via GitHub. Update periodically.

Documentation			
Phase 1	**Phase 2**	**Phase 3**	**Phase 4**
10/2015 – 3/2016	**4/2016 – 10/2016**	**11/2016 – End**	**1/2017 - End**
Basic user docs, focused on getting started. Draw from existing materials. Available through CU doc pages.	Update materials to be federation-specific and move to portal access.	Add more advanced topics as needed and after implementation in Science Use Cases, including documents on "Best Practices" and "Lessons Learned." Check and update docs periodically, based on ongoing collection of user feedback	Release documents via GitHub. Update periodically.
Training			
Phase 1	**Phase 2**	**Phase 3**	**Phase 4**
10/2015 – 3/2016	**4/2016 – 12/2017**	**4/2017 – 12/2017**	**1/2018 - End**
Cross-training expertise across the Aristotle team via calls and science group visits.	Hold training for local researchers. Offer Webinar for remote researchers. Use recording/materials to provide asynchronous training on the portal.	Add more advanced topics as needed. Check and update materials periodically, based on training feedback and new functionality.	Release training materials via GitHub. Update periodically.
User Authorization and Keys			
Phase 1	**Phase 2**	**Phase 3**	**Phase 4**
10/2015 – 1/2016	**2/2016 – 5/2016**	**6/2016 – 3/2017**	**4/2017 – End**
Plan how to achieve seamless login and key transfer from portal to Euca dashboard.	Login to the portal using InCommon.	Beta testing Euca 4.4 with Euca console supporting Globus Auth. Will deploy and transition to Euca 4.4 on new Ceph-based cloud.	Move seamlessly to Euca console after portal Globus Auth login.
Euca Tools			
Phase 1	**Phase 2**	**Phase 3**	**Phase 4**
10/2015 – 3/2016	**4/2016 – 12/2016**	**1/2017 – End**	**1/2017 – End**
Establish requirements, plan implementation.	No longer relevant since Globus Auth will let us interface with Euca web console	N/A	N/A
Allocations and Accounting			
Phase 1	**Phase 2**	**Phase 3**	**Phase 4**
10/2015 – 3/2017	**3/2017 –5/2017**	**6/2017 – 10/2017**	**6/2017 – End**
Plan requirements and use cases for allocations and account data collection across the	Display usage and CPU hours by account or project on the portal. Integration hooks for	Automate project (account) creation by researcher, via the portal.	Report on usage by account, if the researcher has multiple funding sources. Release

federation. Design database schema for Users, Projects and collections of CPU usage and Storage Usage of the federated cloud.	user and project creation/deletion and synchronization across sites.		database schema via GitHub.
Metrics and Usage			
Phase 1	**Phase 2**	**Phase 3**	**Phase 4**
10/2015 – 7/2016	**7/2016 – 9/2016**	**10/2016 – 3/2017**	**10/2017 - End**
Buffalo team utilize Cornell scripts to design a REST API for basic cloud data and deploy at 3 sites and publish usage data to project portal (completed). Buffalo currently standardizing the API by using UTC across the sites and refactoring the code efficiency. Buffalo also completed a redesign of the XDMoD data warehouse to support cloud metrics and is switching XDMoD to use this implementation.	Provide documentation for installing XDMoD and SUPReMM at individual sites. Install Open XDMoD/SUPReMM at individual sites and begin data collection. This includes installation of SUPReMM and the data collection piece at the federation sites. Begin integration with federated authentication providers. Open XDMoD (v.6.5.0) has been released and is available at http://open.xdmod.org/. Note: this version does not support cloud metrics but will give sites an opportunity to get infrastructure in place for a future version that does.	Federated data collection will ship data from XDMoD instances at the individual sites to a master XDMoD instance at UB where overall cloud data will be displayed. This is in alpha testing at UB with completion planned for 3/2017. Federated XDMoD is being updated to support the new cloud schema.	A prototype cloud realm using Euca data is planned for 10/2017. When completed, federated data from all 3 sites will be available at the master XDMoD instance. Release materials via GitHub. Update periodically.

3.1 Software Requirements & Portal Platform

No activity this month.

3.2 Integrating Open XDMoD and DrAFTS into the Portal

Modifications to the XDMoD schema to support cloud data have been finalized. Improvements to the Eucalyptus log scraper have been made to improve coverage of desired events such as detaching a volume from an instance. Preliminary modifications to the XDMoD ETLv2 process are underway to support ingesting cloud data.

Planning for completion and cloud beta implementation of Open XDMoD is detailed in the table below with an August target.

		Feb		March				April				May				June				July				August			
Task	**Order**	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
Update cloud schema docs	1																										
Implement static dimension tables	2																										
Document JSON import schema	3																										
Documentation Updated	3M		X																								
Define file-based API	4																										
ETL config file references	7																										
Subquery support	8																										
Improve start/end/number handling	9																										
Action date chunk handling	11																										
ActionState	12																										
ETL Required Additions	12M										X																
XDMoD cloud event mapper	13																										
Updates to StructuredFile ingestor	14																										
Build single record ingestor	15																										
Build directory crawler	16																										
Aggregator	17																										
Testing	18																										
Eucalypus Data Ingested	18M															X											
Migrate from modw.jobfact	21																										
Implement realm & metrics	22																										
Implement drilldowns	23																										
Testing	24																										
Cloud Beta (Accounting)	24M																								X		
Summarization Infrastructure	25																										
Develop summarization tools	26																										
Summary docs in mongodb	27																										
Ingest summaries into XDMoD	28																										
Display perf data via existing Job Viewer	29																										
Cloud Beta (Performance)	29M																								X		

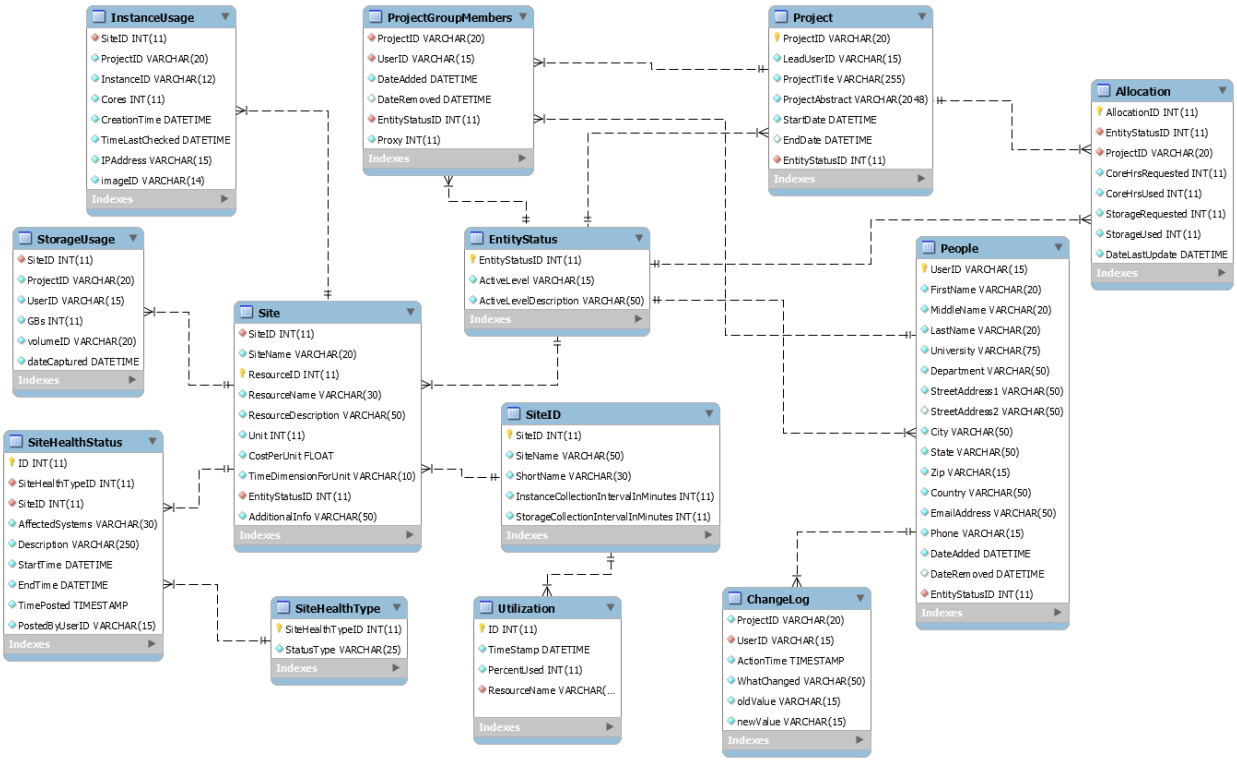
ETLv2 Housekeeping
Cloud Data
Cloud Realm
SUPReMM
Milestone

3.3 Allocations & Accounting

Development on accounting and allocations is proceeding. This month, we continued work on developing Stored Procedures for reporting usage data in report form.

At the same time, we are developing the portal dashboard which will display usage data on a project level to science team members.

There were no changes made to the database schema this month:



4.0 Research Team Support

4.1. General Update

- An Aristotle Science Team Advisory Committee meeting occurred March 20th (see meeting minutes in Section 4.3).
- Work on MPI continues. Advances this month include the use of s3fs for high-speed parallel writes for code output.
- An Aristotle REU supplemental proposal was completed and submitted for NSF review.

4.2 Science Use Case Team Updates

Use Case 1: A Cloud-Based Framework for Visualization & Analysis of Big Geospatial Data
Experiments are currently running to get scalability numbers for the change detection algorithm on the UB Lake Effect cloud. Additionally, we are finalizing the webGlobe website for the next month's demo and for future release to scientists.

Use Case 2: Global Market Efficiency Impact
Progress continued along the same vein as last month's report. The import of all TAQ data (one of the main databases used in finance, which contains intraday prices for US stocks) is now complete up until

2015. This data will be used to compute the first of four measures of efficiency. Up to 30 more stock pairs have been integrated into the research sample.

Use Case 3: High Fidelity Modeling and Analytics for Improved Understanding of Climate-Relevant Aerosol Properties

To our knowledge, WRF-Chem (i.e. the chemistry-enabled version of WRF) has never been successfully run on a cloud. This is particularly true for clouds such as Aristotle and Jetstream that are not configured out-of-the-box to operate with massively parallel computational codes, and are default to work on a single computational node. Consequently, we encountered a number of technical challenges in running the Weather Research and Forecasting (WRF-Chem) model on Aristotle. For these and other reasons, we are currently building capacity using the physics only version of WRF. This allows us to fully and comprehensively evaluate the simulations conducted on Aristotle and to work with a more stable and well documented version of WRF (i.e. the physics only version) while addressing very important questions of relevance to climate science.

Our modified science objectives for the near-term are to:
(1) Comprehensively evaluate the platform dependence of climate simulations. We will evaluate the reproducibility of climate simulations derived from operation of WRF on different platforms (on a cloud relative to a traditional HPC platform, i.e., the DOE NERSC Cray system Cori). This will be conducted under separate funding.
(2) Evaluate the fidelity of the climate simulations using a suite of remote sensing and in situ observations.
(3) Undertake a novel study of the impact of wind turbines on downstream climate using a module within WRF that simulates the momentum extraction and turbulence introduction downstream of major wind turbine deployments.

Progress: The WRF Preprocessing System (WPS) and WRF v3.8.1 were installed and compiled with parallel NetCDF on Aristotle. After the Cornell CAC team completed troubleshooting the network file server, benchmarking was completed in March. The WRF wind turbine input files have been prepared, along with the input meteorological files. We anticipate starting the production science case in April. The first case is a simulation of the year 2008, at 12 km resolution. This will serve as both a test run of the capabilities of running WRF on a cloud-based system, and as a means to assess the fidelity of the regional climate.

Future Plans: After running the 12 km simulation for the entire calendar year of 2008 over the U.S. east of the continental divide, we plan to re-run the simulation with a high-resolution nest of 4 km over the state of Iowa (a state with high wind energy penetration). This simulation will include all wind turbines in the state and will examine the degree to which the flow field is modified downstream (i.e., in the state of Illinois). This will address a key science question: how does this valuable renewable energy source reciprocally interact with the atmosphere?

Use Case 4: Transient Detection in Radio Astronomy Search Data

No updates this month.

Use Case 5: Water Resource Management Using OpenMORDM

The file system work for MPI jobs is nearly complete. We will then run benchmarks of Project Platypus (the Python version of OpenMORDM) to investigate scaling on science cases.

Use Case 6: Mapping Transcriptome Data to Metabolic Models of Gut Microbiota
Computational development continues on the modeling. When the exploratory studies are completed, we will model a larger system.

Use Case 7: Multi-Sourced Data Analytics to Improve Food Production & Security
Agricultural Food Security Project: We are working on deploying version 3.0 of the sensor platform. The current version (which is attempting to use weather information to control the sensing rate) is able to survive to approximately 10:00 p.m. each evening before the battery expires. We have a new battery discharge model and it seems to be functioning properly. Readings from the following site http://169.231.235.16 which is hosted on Aristotle show the current soil moisture reading taken from the UCSB-developed sensor platform. Note that the time frame spans a 24-hour period. This is a substantial improvement over the previous version. The plan is to deploy this platform at several sites in the coming weeks to be able to track the full growing season. We will also continue to use this data to improve water usage.

Where's the Bear Project: We are beginning to work on a new version of the TensorFlow model that is trained "from scratch." While the current implementation uses transfer learning, the team hypothesizes that better accuracy can be achieved from a fully trained model. To do the training will require substantial Aristotle capacity which is currently on order.

4.3 Science Team Advisory Committee Meeting Minutes

Science Team Advisory Committee (STAC): 3/20/2017 Meeting Minutes
Adam Brazier, Aristotle science team lead

Invited to 3/20/2017 Science Team Advisory Committee Meeting *(attendees italicized)*

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NSF - *Amy Walton, NSF program manager*
- The 1st NSF Data Infrastructure Building Blocks PI Workshop (https://dibbs17.org) was led by Cornell as a supplement to the Aristotle award and was a tremendous success. There was high energy on the part of the 72 participants and the resulting data and insights produced will be invaluable to NSF as we plan for the future of research and data cyberinfrastructure. The final workshop report will be available by the end of March (see Section 5.1). Thank you all!
- Your 18-month review is scheduled for the morning of April 25th. Focus is on a working prototype and showing you are well on the way to success. The goal for these projects was to provide a robust and shared CI capability. Plan on 60-90 minutes of top level presentations/demos followed by an extensive questions/answer and discussion period through late lunch. Cover 5 areas: (1) rationale for the project, (2) CI approach used and how the prototype is doing, (3) project management, i.e., who is doing what and how it is being measured, (4) what are the next stages of the project, i.e., if we fund you for years 3 and 4, what are you going to accomplish? (note: this could include the possibility of adjusting milestones for new innovations or broader impacts), (5) when this award is completed, what will the community have that it doesn't have now? One week prior to April 25th, NSF should receive a reference package on the project with the PowerPoints, a copy of the execution plan, any report updates. This will be distributed by NSF to the panel. Hit the highlights. Explain what the prototype is, what is working, how what you have is helping the scientific community. Provide a well-organized package. Including some key application examples seems to work for some projects.

Infrastructure Update – *Adam Brazier (CU)*
- We're moving to Eucalyptus 4.4. We were successful in getting HPE to build OAuth2 support into 4.4 and testing it. This will provide us much more functionality. You will be able to login using your own institutions' authentication as well as InCommon. If you're using XSEDE resources, this is what they are using too, so it will be like one ticket access to potential resources.
- Year 2 hardware installations and purchases are underway. The University at Buffalo has added 112 cores and is upgrading their network. Cornell is adding Ceph storage since that was a greater need than more cores. UCSB, on the other hand, has ample storage, so they're adding cores since usage of their current cores is maxed out. Heterogeneous platforms and software at the various sites is a plus since it provides users with more alternatives to address their needs.

Portal Update – *Susan Mehringer, portal team lead (CU)*
- The Aristotle portal has been up for quite a while and is located at https://federatedcloud.org. If you have comments or suggestions, send them to help@federatedcloud.org. A status graph for all 3 sites is on the portal which shows the availability of cores. Monthly, quarterly, and annual reports are also available. They are password protected, so contact us via "help" if you'd like access.
- OAuth2 has been implemented on the portal, and will be used for all sections and functionality that require authentication.
- The next major step is to integrate allocations and accounting information into the portal, by project and by person. Information will include, e.g., project members, usage, allocations balance, and storage usage.

Science Team Update - *Adam Brazier, science team lead (CU)*
- We're using Slack for communications which has been incredibly useful given the distributed nature of our project. If you are not a member of our Slack channel, email brazier@cornell.edu and ask to join. Our RT ticket tracking system is another valuable tool for science users (help@federatedcloud.org).
- Allocations are somewhat relaxed at this point; a formal allocations process will be implemented in the future.
- We're close to completing the development of a virtual cluster capability for MPI and OpenMP (we just need to improve the disc I/O speed). The intent is to provide virtual cluster access for modest size jobs (not thousands of cores). On-demand access to virtual clusters in the cloud vs. waiting in a queue for a very large-scale system will improve time to science for users with modest needs.
- We applied for and we're approved for 2 million virtual core hours on Jetstream.
- Science teams will be asked to provide science highlights for our upcoming 18-month NSF review. Lifka emphasized the importance of highlighting how the Aristotle project has helped (or will help) the science teams do things differently or better than in the past or, in some cases, with faster time to science.

Individual Science Team Updates

Use Case 1: A Cloud-Based Framework for Visualization and Analysis of Big Geospatial Data - *Varun Chandula update (UB)*
- We plan to add more analysis tools to our framework, add more simulation data, and make the system more robust.
- Next steps will include discussions about how to submit/track jobs which will be important in opening up the capability to the broader community.
- We can provide a demo for the 18-month review.

Use Case 2: Global Market Efficiency Impact - *Dominik Roesch (UB)*
- We've set up a framework for the analysis of high frequency trading data (20TB+) and will provide this capability to 3 PhD researchers this summer with the future goal of opening up this capability to researchers at other institutions in the future.

Use Case 3: High Fidelity Modeling and Analytics for Improved Understanding of Climate-Relevant Aerosol Properties - *Tristan Shepherd (CU)*
- We're had a productive collaboration with CAC and are very close to running WRF-Chem (a parallel version Cornell built for the cloud) on multi-year, high-resolution data across North American.

Use Case 4: Transient Detection in Radio Astronomy Search Data – *Adam Brazier (CU)*
- We're preparing for cloud usage and will do early runs on Jetstream. Cornell and a global team of astronomers previously uncovered the source of a "fast radio burst." We plan to expand the analysis of that data beyond the previously analyzed data to explore and, hopefully, produce new insights.

Use Case 5: Water Resource Management Using OpenMORDM – *Julianne Quinn (CU)*
- We're working to benchmark and test the scaling of OpenMORDM and its equivalent in the Python equivalent Project Platypus. Scientific output will commence when the MPI virtual cluster work is completed.

Use Case 6: Mapping Transcriptome Data to Metabolic Models of Gut Microbiota – *Brandon Barker (CU)*
- Several large instances were created (Windows and Linux) and used for modeling and genetic analysis. This resulted in a paper which will be published in the *Journal of Bacteriology* and a presentation that will be delivered at the *Data-Driven Biotechnology Conference* in Copenhagen (May 7-11, 2017).
- Computational development continues on the modeling, and usage is expected to ramp up when we're ready to model a larger system based on the initial exploration studies currently underway.

Use Case 7: Multi-Sourced Data Analytics to Improve Food Production – *Kate McCurdy (Sedgwick Reserve/UCSB)*
- Agricultural soil moisture monitoring and drought monitoring of oak trees will continue when soil sensor failures due to excessive moisture as remedied.
- The "Where's the Bear" project will continue when storm-impacted sensors are back up and running. This system is still using the Caffe framework and the Aristotle cloud to process all camera data from the field. The framework sorts images into species. We are still struggling with empty frames and frames with birds and will be honing this species recognition capability. We are using a citizen science site (Zooniverse) to pull data out of the Aristotle cloud and will be using volunteer crowdsourcing to verify the accuracy of the computer-generated data in the coming weeks. Ecology researchers are interested in using the first workflow to publish climate change impacts on wildlife. UCSB Computer Science is working with us to eventually launch our own repository site to manage the whole process of data acquisition, storage, and dissemination. Important note: this project has sparked a new scientific collaboration (not part of the original Aristotle proposal) with Sedgwick researchers who plan to perform latent species identification and analyze fishery health from images from SE Asia.

5.0 Outreach Activities

5.1 Community Outreach

- Cornell released the "Final Report: 1st NSF Data Infrastructure Building Blocks PI Workshop" on 3/28/2017. See https://dibbs17.org/report/DIBBs17FinalReport.pdf. This workshop was a supplemental award to the Aristotle project.