ARISTOTLE
CLOUD FEDERATION

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

Program Year 6: Quarterly Report 1
(No-Cost Extension Year Ending 9/30/2021)

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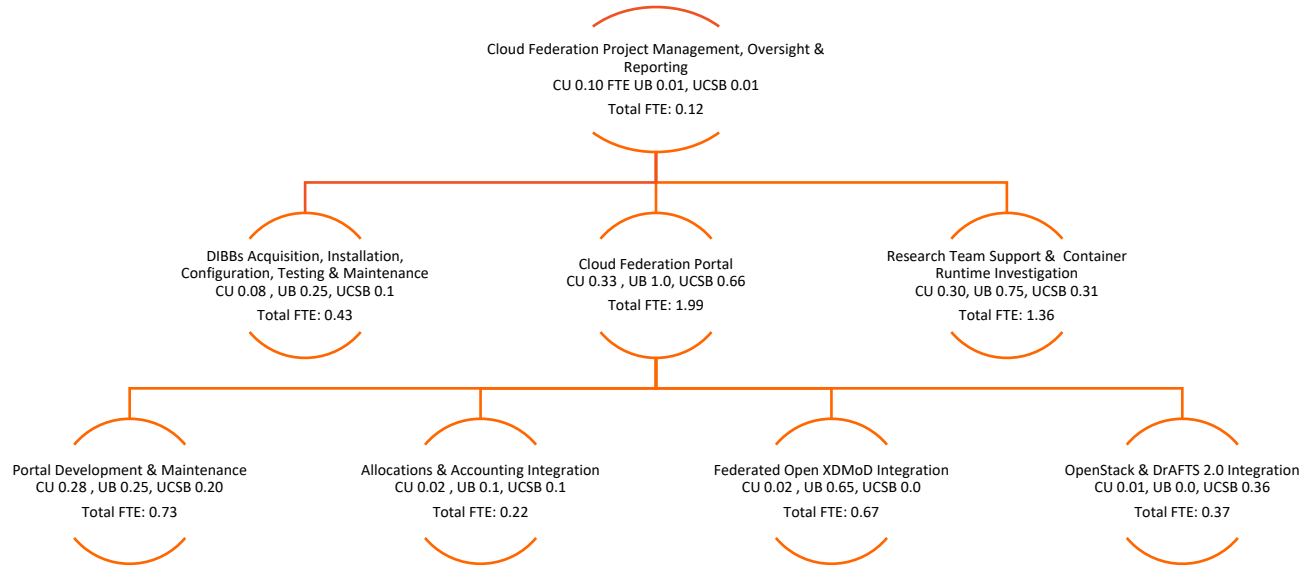
This is the Program Year 6: Quarterly Report 1 (PY6 Q1) of the Aristotle Cloud Federation team. This report is part of a one-year No-Cost Extension. We report on plans and activities for each area of the project Work Breakdown Structure (WBS).



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1.0 Cloud Federation Project Management, Oversight & Reporting

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

1.2 Project Change Request
A one-year No-Cost Extension was approved by NSF for 10/1/2020 to 9/30/2021 without additional funds. We will complete all remaining project and supplemental work during the NCE period. The final Financial Report, Technical Report, and Project Outcomes Report will be submitted by the specified 1/28/2022 due date.

1.3 Project Execution Plan
The Project Execution Plan (PEP) was approved by NSF on 12/18/2015. We are operating as planned.

1.4 PI/Partner Virtual Meetings
- After discussions with multiple vendors (including Red Hat), UB's Aristotle infrastructure team requested and NSF approved the use of $64,000 of the Aristotle subaward 1161820-1-73295 to hire an external consultant to perform a one-time deployment, migration, and support of a new OpenStack private cloud and to help migrate current workloads to it. UB plans to move to a non-vendor specific version of OpenStack so that they are in a better position to support it on their own without costly vendor lock-in. This approach will also provide services to provision Kubernetes and increase the use of open source tools. A private cloud is available via this consulting firm for additional flexibility. Staffing shortages and Covid-19 restrictions have made it increasingly difficult to bring in new staff, particularly someone with this skill set.

1.5 Project Planning Virtual Meetings/Status Calls

9/22/2020 status call:

- Working with the XSEDE CRI group, we demonstrated a multi-platform solution which uses the Nix package manager in an MPI-capable Docker container that is converted to Singularity. It provides consistent installations, dependencies, and environments in each image that are reproducible and portable across infrastructures. We demonstrated the utility of these containers with cluster benchmark runs in a self-scaling cluster using the Slurm scheduler deployed in the Jetstream and Aristotle Red Cloud OpenStack clouds. Our paper—"Self-Scaling Clusters and Reproducible Containers to Enable Scientific Computing," P.Z. Vaillancourt, J.E. Coulter, R. Knepper & B. Barker—is available on *arXiv*. See https://arxiv.org/pdf/2006.14784.pdf.
- Andreas Boschke, Aristotle infrastructure team lead at UCSB, and Jeff Oakes, Letters and Science IT, provided virtual machine image development and cloud training for a new Aristotle cloud use case in computational communications. UCSB researchers have developed an interface for communications research (iCORe) to access, explore, and analyze the Global Database of Events, Language, and Tone (GDELT). It provides fast access to GDELT data and replicability through transparent query and analysis protocols. Their paper—"iCoRe: The GDELT Interface for the Advancement of Communication Research," F.R. Hopp, J. Schaffer, J.T. Fisher & R. Weber—was published in *Computational Communications Research* and credits the Aristotle project. See https://computationalcommunication.org/ccr/article/view/27/2. The researchers continue to use the Aristotle cloud and recently published "Dynamic Transactions Between News Frames and

Sociopolitical Events: An Integrative, Hidden Markov Model Approach" in the *Journal of Communication*.

9/29/2020 status call:

- The need for "platform independence" (retargeting applications to other platforms), the issue of practical portability between XSEDE resources and clouds, and reproducibility across platforms were discussed. Researchers can achieve research results faster if they can readily move their scientific workflows around to other platforms.

10/13/2020 status call:

- Cornell's Exotanium team (http://exotanium.io/) is installing the latest version of X-Containers (https://www.x-containers.org/) on an instance that the Aristotle team prepared for them. We will benchmark X-Containers next. A comparison of different container runtimes—Docker, Singularity, and X-Containers—is the ultimate goal of our research.
- We're developing virtual cluster stacks on Aristotle Red Cloud using Singularity for multiple users.

11/6/2020 status call:

- Work continued on paring down the Aristotle portal to form a template that will be made available on GitHub with a pointer from our "Build Your Own Federation" page. The template will enable other institutions to build cloud federations more quickly.
- Dartmouth's cloud deployment has been delayed due to Covid-19 interruptions.
- Aristotle containerization and benchmarking work is proceeding as planned. We're regularly updating our "lessons learned" doc so we can share our experiences with the CI community via a technical report.
- We documented how to get an OpenFOAM Docker container running on Red Cloud with various use cases. This documentation is based on Aristotle REU student Priyanka Dilip's research project. See: https://www.cac.cornell.edu/wiki/index.php?title=OpenFOAM.
- The containerization team has implemented 3 multi-node methods in the cloud: Terraform with Kubernetes in Google Cloud, Terraform in Ansible in Google Cloud and Azure, and a self-scaling Slurm cluster on Red Cloud and Jetstream (in collaboration with Eric Coulter). The Terraform approaches use Docker and the self-scaling cluster uses Singularity. We plan to assess Kubernetes next.
- We also plan to make the repository for Aristotle REU student Jeffrey Lantz's code public. Lantz created a Terraform-Kubernetes MPI-capable tool and used High Performance LINPAC benchmarks to compare the cost efficiency of an updated Terraform-Ansible tool vs. his Terraform Kubernetes tool. He found that the Terraform-Kubernetes tool is faster and less costly to deploy as a cloud computing cluster.

12/1/20 status call:

- Aristotle researchers presented a new edge computing technology, "NanoLambda: Implementing Functions as a Service at All Resource Scales for the Internet of Things," G. George, F. Bakir, R. Wolski and C. Krintz at the *Fifth ACM/IEEE Symposium on Edge Computing (SEC 2020)* in November. See: https://federatedcloud.org/papers/nanolambda-sec20.pdf.

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12/4/20 status call:

- Cornell Aristotle computation consultants continued to update the implementing containers lessons learned doc and are reviewing and improving the container repositories and READMEs. Networking steps and how to open files will be one area of focus.
- We are implementing multi-node MATLAB on Aristotle Red Cloud. Users are currently connecting from their desktops to 28 workers on 1 node; they would like to expand to 56 workers on 2 nodes, and beyond using MATLAB's dashboard and orchestration tools.
- We discussed our plans to produce a technical report on the features of different runtime environments (Aristotle Red Cloud, Google Cloud, Stampede2) and the use of Kubernetes as an orchestration methodology.

2.0 Container Runtime Investigation

The Cornell Aristotle team has been working on running and documenting containers with different runtimes for comparison. The team has regular calls with Exotanium staff on how to get the X-Container runtime working on OpenStack clouds. Other members of the team have prototyped application containers with Docker and Singularity to run on Aristotle and Stampede2. In addition, the team is working to establish a scope and focus for multi-container jobs that allow parallel computing for applications which require greater scale; they are using WRF as the example application.

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

3.1 Hardware Acquisition

- Cornell had no acquisitions this quarter.
- UCSB had no acquisitions this quarter.
- UB will receive new infrastructure (servers, switches, and PDUs) to support production and development clouds and a data transfer node (DTN) with a 100GB interface to allow for data and images to be more easily transferred.

3.2 Installation, Configuration, and Testing

- Cornell has been moving forward with the new OpenStack 16.1 infrastructure using Red Hat's Director method. We will look closely at the cloud computing platform options UB has investigated and will assess what is the best platform to move forward with based on ease of deployment, user migration, open source tool availability, and long-term support costs.
- UCSB has received and next quarter will be installing 6 cloud nodes for an additional 288 cores and 4608TB RAM along with 4 storage nodes for an additional 768TB Ceph storage (raw) and some GPUs. Additional racks are needed. This installation was delayed because of the need to shift resources to support campus learning systems.
- UB will be hiring a consulting firm to install a non-vendor specific OpenStack platform, migrate users, and deliver ongoing support.
- Dartmouth's cloud installation is on hold due to Covid-19 impacts (also experiencing campus learning demands).

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3.3 Federated Identity Management

Researchers use single sign-on at any member site.

3.4 Cloud Status by Site

The chart below shows each site's production cloud status.

	Cornell	Buffalo	UCSB
Cloud URL	https://redcloud.cac.cornell.edu	https://lakeeffect.ccr.buffalo.edu/ (access only to federation)	https://openstack.aristotle.ucsb.edu/
Status	Production	Production	Production
Software Stack	OpenStack	OpenStack	OpenStack
Hardware Vendors	Dell	Dell, Ace	Dell, HPE, DXC
DIBBs Purchased Cores	*616	**792	***740
RAM/Core	8GB	up to 8GB	9GB Dell, 10GB HPE
Storage	Ceph (1.6PB)	Ceph (768TB)	Ceph (720TB)
10gb Interconnect	Yes	Yes	Yes
Largest Instance Type	28core/192GB RAM	24core/192GB RAM	48core/119GB RAM
Globus File Transfer	Yes	In Progress	In Progress
Globus OAuth 2.0	Yes	Yes	Yes
Total Cores (DIBBs purchased cores + existing cores) = 2776	* 616 additional cores augmenting the existing Red Cloud (1316 total cores).	** 792 total cores (UB Lake Effect Cloud and CCR cloud will be one pool after upgrade).	***740 cores in UCSB Aristotle cloud (956 total cores, Aristotle is separate from UCSB campus cloud)

4.0 Cloud Federation Portal Report

Content updates to the project portal are ongoing (https://federatedcloud.org). In particular, we updated the following user documentation:

- Docker on Aristotle: https://github.com/federatedcloud/Aristotle-Docs/wiki/Docker
- Nix on Aristotle: https://github.com/federatedcloud/Aristotle-Docs/wiki/Nix
- Shared File Systems: https://github.com/federatedcloud/Aristotle-Docs/wiki/Shared-File-Systems
- OpenStack Basics: https://github.com/federatedcloud/Aristotle-Docs/wiki/OpenStack-Basics
- Linux Instances: https://github.com/federatedcloud/Aristotle-Docs/wiki/Linux-Instances

4.1 Software Requirements & Portal Platform

No software changes were made to the portal platform this quarter.

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4.2 Integrating DrAFTS into the Portal

The DrAFTS 2.0 system is collecting data correctly, but we do not yet have the CSS set up to display it according to the portal specification. The CSS is the last piece to be completed. Hopefully, we can get that done in January.

4.3 Integrating Open XDMoD into the Portal

4.3.1 Application Kernels (AK) Containerization in the Cloud

AK containers are used in all Aristotle OpenStack instances within the XDMoD performance monitoring module.

4.3.2 XDMoD Cloud Integration

We upgraded all 3 sites to Federated Open XDMoD 9.0 (the latest release).
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4.4 Allocations & Accounting

The database schema was shared with the broader community via GitHub.

5.0 Research Team Support

5.1 Science Use Case Team Updates

Use Case 1: A Cloud-Based Framework for Visualization & Analysis of Big Geospatial Data

Aristotle use case scientist and UB CS professor Varun Chandola and colleagues continued developing the OUTSTEPS Community Platform (https://www.community-outsteps.org) hosted on the Aristotle Cloud. Currently, over 20 members representing universities, government agencies, and non-profit organizations use the platform to interact and share data with each other. As a next step, we plan to couple OUTSTEPS with the webGlobe analysis engine to allow users to run data analysis jobs on the various data sets hosted on the platform.

Use Case 2: Global Market Efficiency Impact

Dominik Roesch, working with Jonathan Brogaard and Matthew Ringgenberg, revised their "Does Floor Trading Matter" paper (https://papers.ssrn.com/sol3/papers.cfm?abstract_id=3609007). The paper describes the impact of the closure of the New York Stock Exchange Floor due to Covid-19. Working with UB graduate student Yihe Yu, Roesch also completed the code to implement the Least Absolute Shrinkage and Selection Operator (LASSO) method and is currently profiling the code. In addition, Roesch is working with Jonathan Brogaard on an investigation of cum-ex trading which took advantage of a loop hole in tax law and rapidly exchanged stock with and the without dividends between three parties. At least two of these parties then claimed tax rebates on taxes only paid once, pocketing $60 billion in a massive tax evasion scheme.

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Use Case 3: Application of the Weather Research and Forecasting (WRF) Model for Climate-Relevant Simulations on the Cloud

New simulations by Sara C. Pryor and collaborators: Derechos are fast-moving, damaging deeply convective systems, associated with tornadoes, wind gusts, very heavy precipitation and hail. These events have traditionally been very difficult to simulate even with the advanced Weather Research and Forecasting (WRF) model due to the physical complexity and multi-scale nature of these phenomena and resulting high compute demands. Thus, little work has been performed to assess model fidelity for these transient events and/or identify optimal WRF configurations. There is an increasing demand for multi-member ensembles to better characterize uncertainty in climate projections that arises in part from internal climate variability and/or to explore model response and changing fidelity to simulation settings with the ultimate goal of defining 'best practice'. We have commenced developing a simulation ensemble of a historically important derecho that impacted the US Northeast that occurred during June 2012. Thus far we have developed an 8-member ensemble of a derecho that impacted Washington, DC 29-30 June 2012. Figure 1 shows output from a single hour within the 8-day simulation that illustrates the member-to-member variation in derived RADAR composite reflectivity from WRF simulations that arise due to changes in microphysics package, lateral boundary conditions, model resolution and the timing of the start of the simulation.

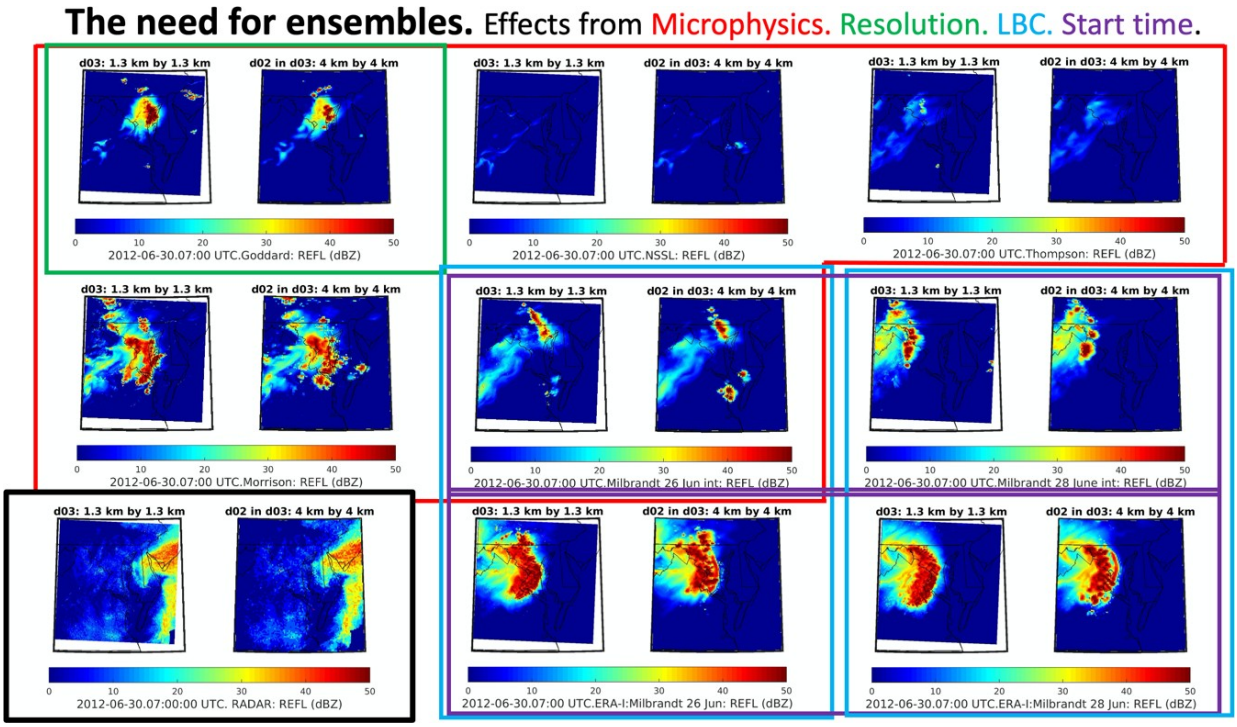

Fig. 1. *Composite RADAR reflectivity on 2012-06-30 at 0700 UTC from NWS dual polarization RADAR observations sampled on a 1.3 by 1.3 km and 4 by 4 km grid (bottom left, outlined in black) and in WRF output for an eight- member ensemble. The 8 panels each show output for one ensemble member run at two resolutions 1.33 km grid spacing (left) and 4 km grid spacing (right). The ensemble contains 5 members that differ only in their microphysics scheme (outlined in red), two sets of two members that use the same microphysics scheme but different simulation start time (outlined in purple) and two sets of two simulations that use the same microphysics scheme but a different reanalysis for the lateral boundary conditions (outlined in cyan). All model configurations exhibited too slow a propagation of the derecho and there are marked differences in terms thunderstorm intensity and associated wind gusts, hail and precipitation.*

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Analysis of prior simulations:

Journal manuscripts in review this quarter:

- Aird J.A., Barthelmie R.J., Shepherd T.J. and Pryor S.C.: WRF-simulated Low-Level Jets over Iowa: Characterization and sensitivity studies. *Wind Energy Science Discussions* https://doi.org/10.5194/wes-2020-113, in review, 2020.

Journal manuscripts published this quarter:

- Letson F., Shepherd T.J., Barthelmie R.J. and Pryor S.C. (2020): WRF Modelling of Deep Convection and Hail for Wind Power Applications. *Journal of Applied Meteorology and Climatology* **59** (10): 1717– 1733, https://doi.org/10.1175/JAMC-D-20-0033.1.
- Pryor S.C., Shepherd T., Volker P., Hahmann A., and Barthelmie R.J. (2020): Diagnosing systematic differences in predicted wind turbine array-array interactions. *Journal of Physics: Conference Series* **1618** 062023 doi:10.1088/1742-6596/1618/6/062023, https://iopscience.iop.org/article/10.1088/1742-6596/1618/6/062023/pdf.
- Aird J., Barthelmie R.J., Shepherd T.J. and Pryor S.C. (2020): WRF-simulated springtime low-level jets over Iowa: Implications for wind energy. *Journal of Physics: Conference Series* **1618** 062020 doi:10.1088/1742-6596/1618/6/062020, https://iopscience.iop.org/article/10.1088/1742-6596/1618/6/062020.
- Barthelmie R.J., Shepherd T.J. and Pryor S.C. (2020): Increasing turbine dimensions: Impact on shear and power. *Journal of Physics: Conference Series* **1618** 062024 doi:10.1088/1742-6596/1618/6/062024, https://iopscience.iop.org/article/10.1088/1742-6596/1618/6/062024.

Use Case 4: Transient Detection in Radio Astronomy Search Data

A Singularity container packaging our pulsar and single pulse search pipeline is now ready. We have secured a trial XSEDE allocation for deploying our Singularity container on Bridges and for running pulsar/FRB searches on large data volumes. At present, we are evaluating performance and deriving scaling laws for different pipeline modules to push towards a full XSEDE research allocation.

Relevant links:

- GitHub repo containing both the Dockerfile and Singularity definition file: https://github.com/federatedcloud/pulsar-pipeline-container
- Docker Hub image: https://hub.docker.com/r/cornellcac/pulsar-pipeline
- Singularity Hub image: https://singularity-hub.org/collections/4541

Use Case 5: Water Resource Management Using OpenMORDM

Cornell cloud engineer Bennett Wineholt met with Bernardo Trinidade to discuss how to profile MPI Borg codes:

- Linking remora mpi profiling to Borg code is nontrivial and currently segfaults; Bennett may dig deeper on this with similar mpi code on Red Cloud
- Borg already has timing instrumentation which logs send recv eval and wait times on all threads, but wait time may not be all network communication; it is also waiting for workers to finish.

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Bernardo will pursue an overhead vs. useful work summary per run with these numbers. We already have total runtime for our other performance metric.
- A decision is needed on job size to run and the platforms to run on—one cloud platform and one HPC platform; TheCube HPC cluster at Cornell has 16-core nodes, Aristotle Red Cloud has 28 or 14 2-core nodes, and Azure has 16 core nodes if we pursue Azure credits.

In addition, we also need to decide what factors to normalize before measurement? Options are:
- Core count normalized based on price performance from the cloud perspective (core-minutes so that faster runtime per core is better).
- Function evaluation time normalized to isolate hardware differences (so the percentage of network overhead is the primary metric).

Once we come to consensus on metrics and the platforms to run on, we can right-size the mpi process and thread count as well as simulation size parameters such as scenarios per simulation, with a ballpark total simulation runtime of 30 hours for 8 x 16 core nodes (Azure H16r instances $1000 in credits). If we use larger nodes such as Stampede2 (HPC) vs Azure (Cloud) larger instances, the taller nodes are more efficient and can cut runtime by half (18 hours 8 x 48 core Azure D48a instances or $700 in credits)

Use Case 6: Mapping Transcriptome Data to Metabolic Models of Gut Microbiota

The technical part of the Angela Douglas Lab project has been completed. The manuscript on simulated metabolic interactions of Drosophila's gut microbes is being revised and resubmitted to *mSystems* based on reviewer comments. We will continue to use Aristotle for possible minor additions to the manuscript or adjustments to follow-up work on priority effects in gut microbes, but that work too is largely complete, other than perhaps adjusting parameters. Any updates to the paper's status will be included in future reports.

Use Case 7: Multi-Sourced Data Analytics to Improve Food Production & Security

Citrus Frost Prevention (Lindcove Research and Extension Center, Exeter, CA):
The Aristotle team from UCSB (practicing all advised and required Covid-19 safety protocols) visited the Lindcove citrus orchards to install new meteorological monitoring equipment for the Citrus Under Protective Screening (CUPS) facility. This facility (the largest in the nation) will be used to study the feasibility of using large-scale screen houses to prevent HLB citrus greening disease. With construction completed approximately 30 days ago, the growers decided that the risk of frost damage over the winter months was too great in such a new growing environment and, thus, have elected to plant trees inside the screen house in the Spring. However, they have asked the UCSB team to monitor the conditions over this coming frost season so that they can better understand and predict frost events once trees are introduced. UCSB installed several sensors both inside and immediately outside the facility and deployed an IoT system that provides both real time measurements and a prototype frost alerting system. The real time measurement visualization tool developed by Aristotle REU student Kerem Celik is linked to the CUPS main page: https://ucanr.edu/sites/Citrus@UCR/Citrus_Under_Protective_Screen_[CUPS]/Research_-_Publications/.

Growers are now using our IoT and data visualization technologies to monitor conditions both inside and outside the CUPS (in adjacent growing blocks) both to understand CUPS frost events that occur inside, but also as a real-time tool for the larger growing region. So successful has this prototype been that they are requesting deployment of the infrastructure through the entire Lindcove growing facility. They are also requesting additional features to be added to the analysis tool. In addition, UCSB managed to repurpose

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and integrate an older monitoring station in a different part of the Lindcove property that was originally deployed to monitor soil carbon sequestration. The team adapted the "Flux Tower" to the frost prevention and prediction application and integrated it into the real-time monitoring system.

While Covid-19 restrictions prevent frequent visits by the UCSB team, another is planned to enhance the real time alerting system and to extend the frost monitoring infrastructure to growing blocks not located near the CUPS screen house.

Other projects:
Edible Campus (the food security project) and the Sedgwick Reserve (wildlife management and land use project) remain closed to UCSB researchers due to Covid-19 restrictions in Santa Barbara county. The team is preparing new image processing capabilities for both sites that will be deployed once access is again possible.

6.0 Community Outreach and Education

6.1 Community Outreach

- The "New York zone" of Jetstream 2 (1,024 computer cores and 869TB storage) will be deployed in FY21/Q2 at Cornell. It will be used to explore the federation of clouds and to make OpenStack enhancements that will be shared with the rest of the project team and disseminated to the broader research community. Cornell will draw on our Aristotle experiences to create campus software so that campuses can set up their own clouds. We recently tested and deployed Slurm-based MPI clusters on Aristotle and Jetstream. The availability of the New York zone will help to facilitate faster development and dissemination of other cloud tools for research.
- We shared our work in containerizing scientific workflows for portability and multi-cloud deployment with the CI community at PEARC'20. Our paper, "Reproducible and Portable Workflows for Scientific Computing and HPC in the Cloud" and the presentation are now available at https://dl.acm.org/doi/10.1145/3311790.3396659.

6.2 Education

- Co-PI Rich Wolski's October talk on "Energy Efficiency for the Internet of Things" at the UCSB Institute for Energy Efficiency featured several Aristotle IoT technologies and use cases. It was recently posted here: https://www.youtube.com/watch?v=laLrP79ZDwQ.
- NSF REU student successes featured in *HPCwire (* https://www.hpcwire.com/off-the-wire/cornell-students-immersed-in-latest-cloud-technologies-thanks-to-nsf-research-experiences-for-undergraduates-program/) will also be featured in the upcoming 2021 CASC brochure.

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