

**OPEN**



**OnDemand &**



# Collaboration

INTERNET®



2023

**COMMUNITY**  
exchange



**Ohio Supercomputer Center**

An OH·TECH Consortium Member



University at Buffalo

Center for Computational Research



# Agenda

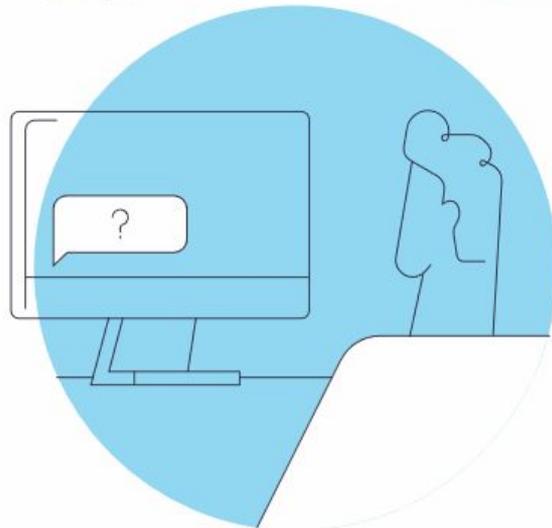
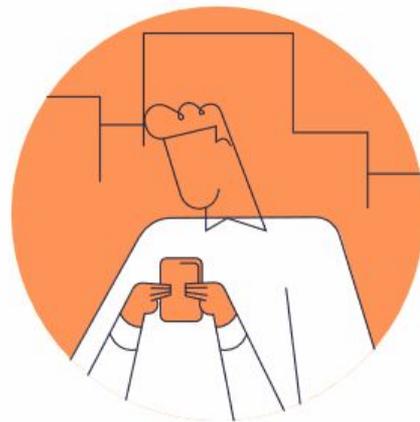
1. Intro
2. Overview of Open OnDemand
3. Overview of CloudyCluster and Omnibond Research Solutions
4. Discussion of the initial collaboration
5. Discussion of the next project
6. General Discussion around collaborations.
7. Demo (Alan has to run to another session)

INTERNET<sup>®</sup>

2023  
COMMUNITY  
exchange

# Overview for 2023 Internet2 Community Exchange

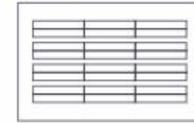
Alan Chalker, Ph.D.



Ohio Supercomputer Center

# Run Open OnDemand

Access your organization's supercomputers through the web to compute from anywhere, on any device.



## Zero installation

Run Open OnDemand entirely in your browser. No client software installation required.

## Easy to use

Start computing immediately. A simple interface makes Open OnDemand easy to learn and use.

## Compatible with any device

Launch on any device with a browser—even a mobile phone or tablet.

[openondemand.org/run](https://openondemand.org/run)

# Install Open OnDemand

Administer remote web access to your supercomputers to transform the way users work and learn.



## Low barrier to entry

Empower users of all skill levels by offering an alternative to command-line interface.

## Free and open source

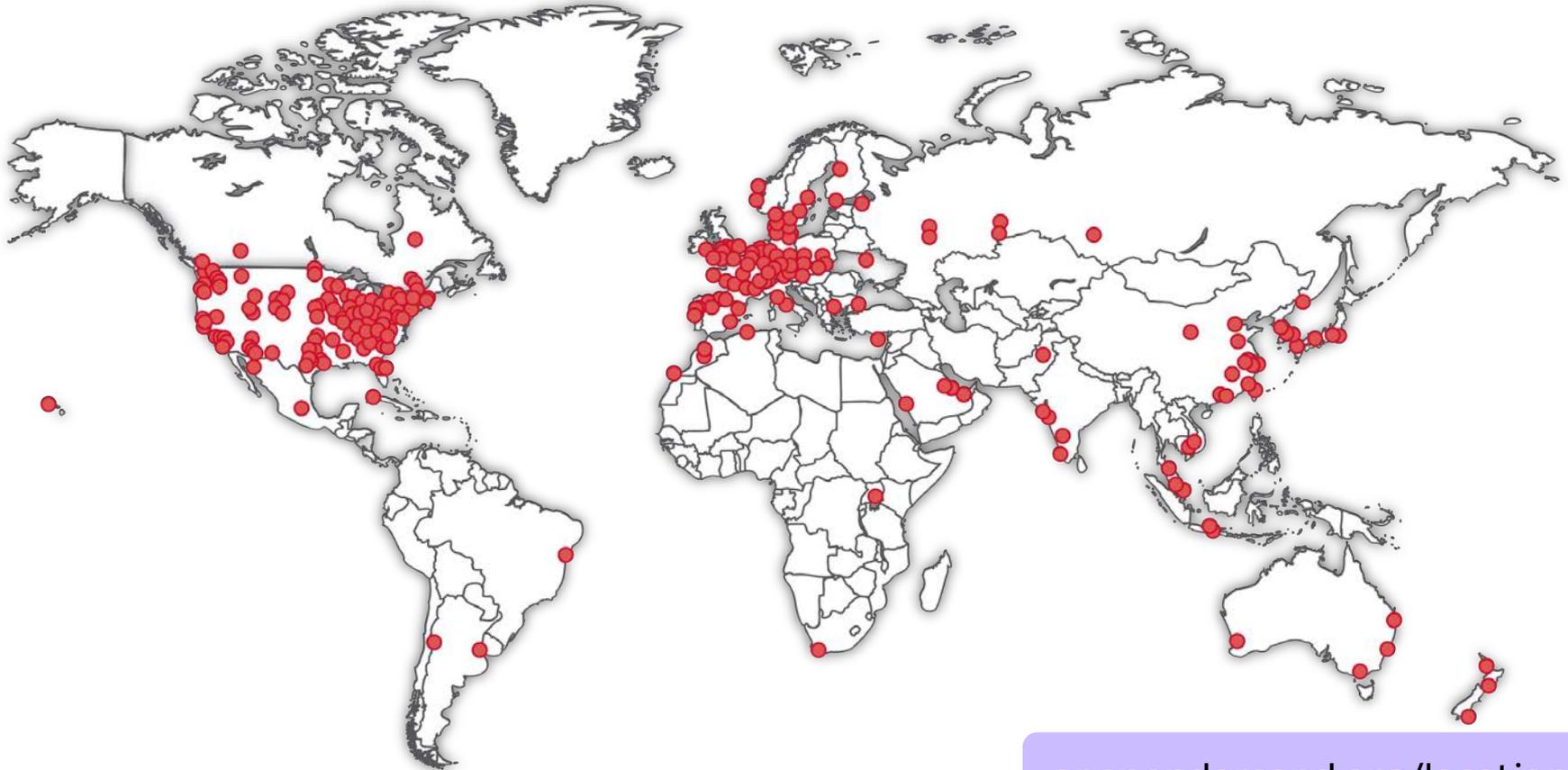
Install Open OnDemand for free, and gather knowledge from our large open-source community.

## Configurable and flexible

Create and deploy your own applications to meet your users' unique needs.

[openondemand.org/install](https://openondemand.org/install)

# Deployed Worldwide



# Example Deployments



Don't see an organization?  
The more the merrier!  
Let us know any that belong on the list



# Community Events



## Tips and tricks calls

Hosted by the larger Open OnDemand community, tips and tricks webinars share best practices for setting up and using Open OnDemand. They take place on the first Thursday of every month at 1 p.m. ET.

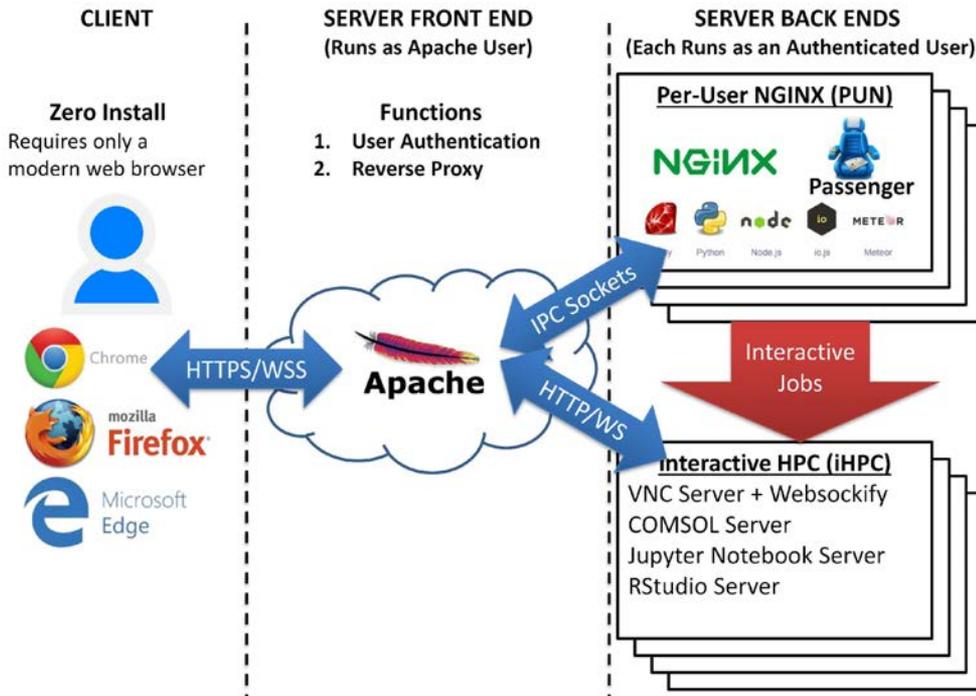


## Open office hours

Hosted by our development team, Zoom open office hours are the perfect opportunity to ask questions or make a suggestion. They are held on the second Tuesday of every month from 11:15 a.m. to 12:45 p.m. ET.

[openondemand.org/events](https://openondemand.org/events)

# Architecture



## Requirements

RedHat/CentOS/Rocky/Ubuntu  
 Software Collections repos  
 Lsof  
 Sudo  
 Nmap-ncat  
 TurboVNC  
 websockify

# Enabled Utilities & Apps

Abaqus

ANSYS

COMSOL

Coot

CSD

Galaxy

Grace

Grafana

Grid Engine

IDL

Jupyter

Kubernetes

LSE

Lumerical

Mathematica

MATLAB

Meshroom

NAGIOS

Octave

Open XDMoD

Ovito

Paraview

PBS Professional

QGIS

RELION

RStudio

SAS

Shiny

Slurm

Spark

STATA

Tensorboard

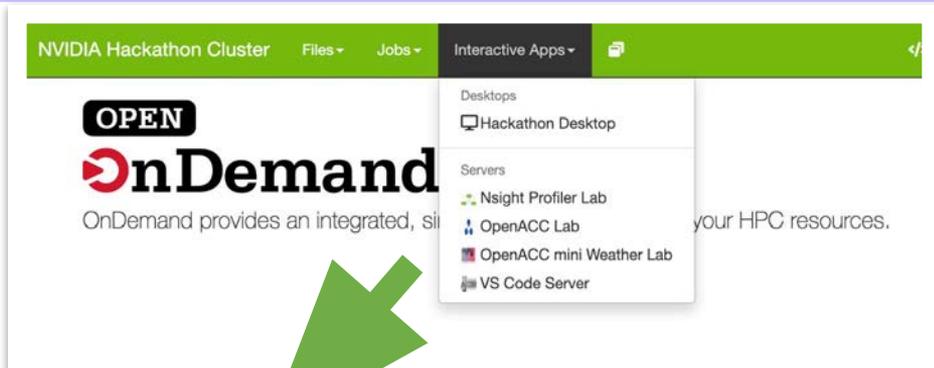
Torque

VISIT

Visual Studio Code

VMD

# Desktop Example



## Hackathon Desktop version: v0.2.2

This app will launch an interactive desktop on one or more compute nodes. You will have full access to the resources these nodes provide. This is analogous to an interactive batch job.

### Number of hours

### Number of nodes

### Bc Num Gpus

I would like to receive an email when the session starts

Launch

\* The Hackathon Desktop session data for this session can be accessed under the [data root directory](#).

## Hackathon Desktop (7475)

1 node | 8 cores | Running

Host: >\_dgg@f81

Delete

Created at: 2020-11-17 13:54:54 PST

Time Remaining: 59 minutes

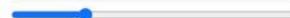
Session ID: f681b932-3804-491e-ad1d-988dcf6ad9ef

### Compression



0 (low) to 9 (high)

### Image Quality



0 (low) to 9 (high)

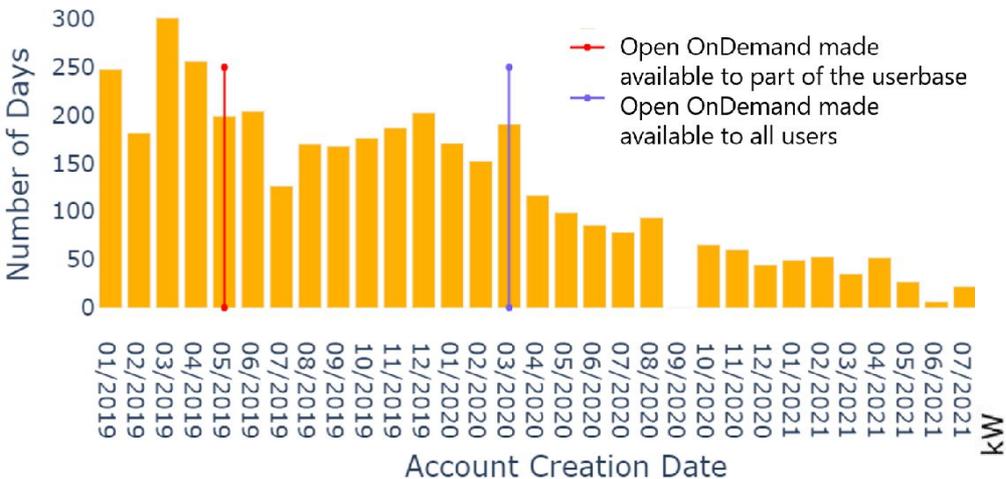
Launch Hackathon Desktop

View Only (Share-able Link)



# Idaho National Lab

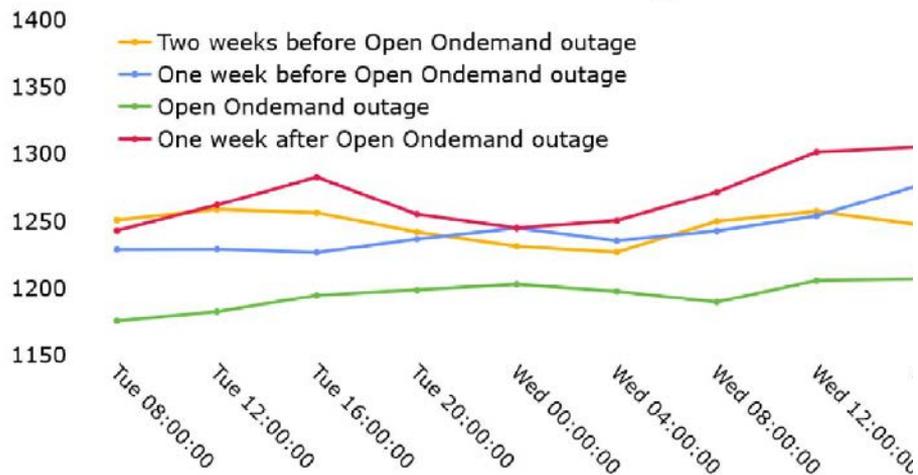
Average Number of Days Between Account Creation to First Job Submission



**19 times shorter**  
 In days between account creation and first job submission

**3.7% drop**  
 In power used during an unscheduled Open OnDemand outage

Datacenter Power Usage



[openondemand.org/idaho](https://openondemand.org/idaho)

# Example Case Studies



## WEB PORTALS

Open OnDemand aids engineering school's supercomputing curriculum

■ Research Landscape ▲ Invention/Discovery

In 2018, the Milwaukee School of Engineering (MSOE) unveiled a major addition to its campus: the Dwight and Dian Diercks Computational Science Hall, featuring Rosie the supercomputer. The facility opened in the wake of the launch of MSOE's bachelor's degree in computer science, with a curriculum focused on the growing field of artificial intelligence.

Alumnus Dwight Diercks, who along with his wife Dian donated \$34 million for the facility, has worked for the technology company NVIDIA since 1994 and today serves as its senior vice president of software engineering. MSOE worked closely with the company on assembling the necessary hardware and software for the supercomputer, which features NVIDIA graphics processing units (GPUs).

NVIDIA recommended that MSOE adopt Open OnDemand, an open-source high performance computing portal developed by the Ohio Supercomputer Center (OSCC). Open OnDemand is used by researchers and college students around the world to access supercomputing resources anywhere from any device.

Derek Riley, a professor and program director for electrical engineering and computer science

at MSOE, reports that most of the jobs run on Rosie use the Open OnDemand portal. MSOE established the supercomputer primarily as a teaching tool for undergraduates studying machine learning and data science, and Open OnDemand has made it easy for them to directly access Rosie, Riley said. Students can avoid time-consuming technical setups and instead gain more experience using the supercomputer to answer a variety of scientific and engineering questions.

"It can't be overstated how important it is for students to focus on the problems we want them to learn," he said.

MSOE's approach to supercomputing also reflects the work environment that many students will find themselves in after graduation, as most employers have engineering teams that handle the more technical aspects of supercomputer setup and maintenance while the data scientists conduct analyses, Riley said.

Not only has Open OnDemand been beneficial for undergraduates to use, but MSOE's own system administrators have found it easy to learn and manage, Riley said.

"We've had a really great experience using it—we've been really happy with it," he said. "We've been able to use it primarily out of the box, and it's the main entry point for students and faculty to the cluster."

Read and share online: [oscc.edu/h27/msoe](https://oscc.edu/h27/msoe)

Above: Rosie the supercomputer supports the Milwaukee School of Engineering's computer science program. Image: © 2018 MSOE and OSCC. All rights reserved.

"In order to learn from millions and millions of chemical structures, we need a lot of computational power," Ning said.

The Ohio Supercomputer Center (OSC) is integral to the project. Each model requires the use of one graphical processing unit (GPU) and 96 GB of RAM for the data generated, Ning noted.

Alumnus Dwight Diercks, who along with his wife Dian donated \$34 million for the facility, has worked for the technology company NVIDIA since 1994 and today serves as its senior vice president of software engineering. MSOE worked closely with the company on assembling the necessary hardware and software for the supercomputer, which features NVIDIA graphics processing units (GPUs).

## ARTIFICIAL INTELLIGENCE

Accelerating drug discovery with AI

■ BIOLOGICAL SCIENCES ▲ INVENTION/DISCOVERY

Xia Ning has a large portfolio of research projects at The Ohio State University that focus on understanding how artificial intelligence can be used to solve issues in health care.

Discovering new drugs to treat disease is one of Ning's goals. Traditional research methods, which call for lengthy trials with animal models, have disadvantages.

"To find a single drug is costly and time consuming," said Ning, an associate professor who holds joint appointments in Ohio State's College of Medicine and College of Engineering.

Ning is drawing on her expertise in computer science and biomedical informatics to create a new path to drug discovery. Her lab examines millions of small molecules and uses that information to create novel models that could be good candidates for drugs.

"We're looking at millions and millions of molecules, and we need a lot of computational power," Ning said.

The Ohio Supercomputer Center (OSC) is integral to the project. Each model requires the use of one graphical processing unit (GPU) and 96 GB of RAM for the data generated, Ning noted.

Compared to the conventional central processing units (CPUs) researchers may use in their labs, GPUs offer a significant boost in computing power. OSC features GPUs across its systems to allow clients to efficiently process large amounts of data, and consistently upgrades its hardware to ensure access to the most cutting-edge technologies.

Those computing resources have helped Ning reach important milestones in her drug discovery work. Research findings from the project have been accepted for publication in the prestigious journal Nature Machine Intelligence and also have attracted new grant funding to the lab.

Ning has been a heavy user of high performance computing centers since her days as a faculty member at Indiana University. She joined Ohio State in 2016.

"The first thing I did here was look for similar resources," Ning recalled. "I didn't think about having my own cluster—that would have taken me a lot of effort."

In addition to OSC's capabilities and technical support, Ning appreciates its availability to her lab members. OSC offers Open OnDemand, an interface funded by the National Science Foundation that allows users to remotely access the Center resources online from any device.

"OSC provides a very nice Open OnDemand tool that we can access through the web," Ning said. "I believe all of my students are using it. It's very easy for us to use, and we don't need to worry about maintenance or software installation."

Ning also employs OSC for teaching Python programming in her biomedical course. The Center creates a class project through which her students can quickly access computational resources and see results immediately through the OSC web portal, she said.

Over the next year, Ning will continue to work with OSC on the drug discovery project, as well as on research on predicting peptides that could be used for vaccine development.

"As long as we're doing research," Ning said, "we'll rely on OSC." \*

Website: [u.osu.edu/hing.104](https://u.osu.edu/hing.104)

● active compounds  
● selective compounds  
● x-selective compounds

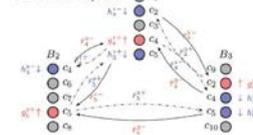
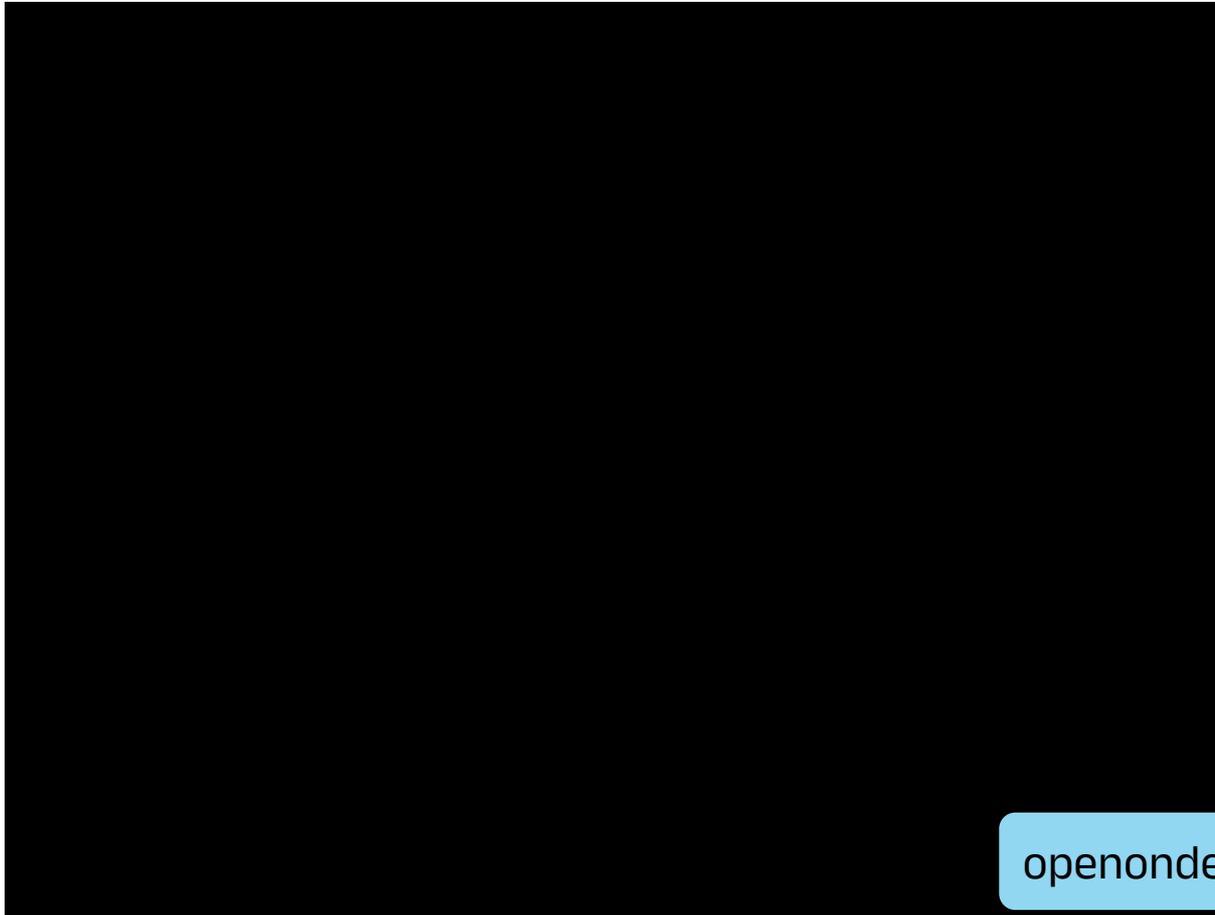


Figure: Advanced AI and large-scale computing enabling multi-purpose drug discovery.

OSCC SUPERCOMPUTER CENTER

# Any Device, Anywhere



[openondemand.org/anydevice](https://openondemand.org/anydevice)



Research Computing Solutions  
Overview for:



Boyd Wilson, CEO



# Leadership Team

**Omnibond**

a customer-focused  
software engineering and  
support company

- Over 40 years combined experience in facilitating and supporting academic and corporate research in using the tools and technologies of advanced computing
- Experience at the working and technical, project and executive management levels at Clemson, Purdue and Miami Universities and the National Center for Supercomputing Applications located at UIUC
- Expertise in software development, systems integration, operations, applications support, data transmission, identity and access management, customer relations and research facilitation and engagement
- Founded ACI-REF <http://www.aciref.org> and CaRCC <http://carcc.org>
- Over three decades of funded projects from NSF, DoD, DoE, NSA, NIST and DARPA
-  Presidential Fellow & CSTAAC Committee Member

- Identity & Security Management
  - NetIQ Identity Manager Connectors
  - Thousands of customers, sold through Novell/Micro Focus/OpenText, since early 2000's
  - OmniPasskey Passwordless MFA Shibboleth Plug-in
- Computer Vision & AI
  - TrafficVision - AI based Automated Incident Detection (AID) & Data from existing cameras on roadways
  - BayTracker - Retail Vehicle Tracking and Timing
  - Port Observer - Drayage Queuing, AIS, Dashboard for Ports
- Cloud HPC and Storage Orchestration
  - CloudyCluster
  - OrangeFS
  - Eureka Project
  - Custom Cloud <-> On-Prem Integration

A laptop screen is shown in the background, displaying a dashboard with a line graph and a pie chart. The line graph has several data points connected by a dark line, and the pie chart is divided into several segments. The text 'Software Products' is overlaid on the right side of the screen in a large, white, sans-serif font.

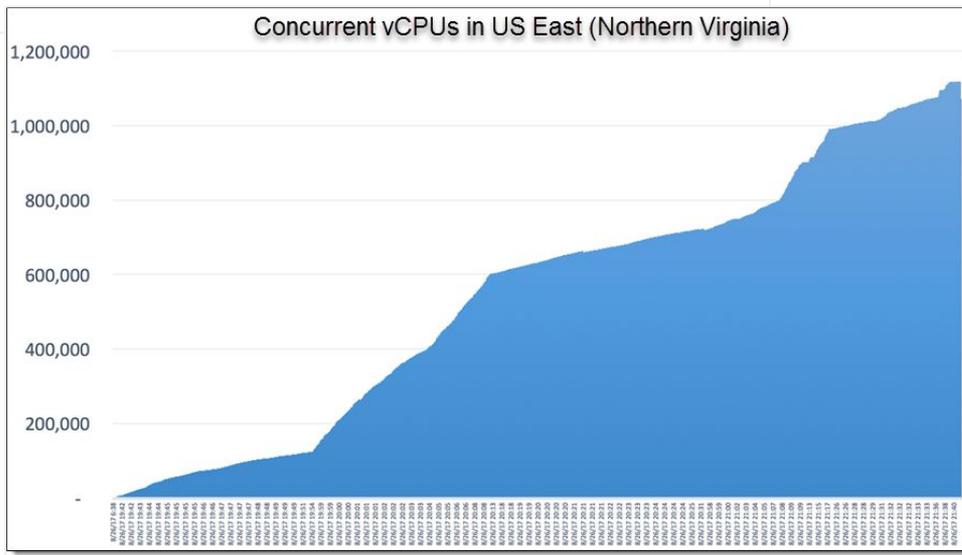
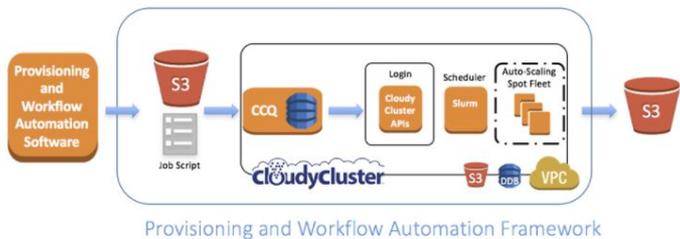
# Software Products

**Omnibond**  
a customer-focused  
software engineering and  
support company

# Scaling on AWS

AWS News Blog

## Natural Language Processing at Clemson University – 1.1 Million vCPUs & EC2 Spot Instances



Data Intensive Computing Ecosystems (DICE)  
School of Computing, Clemson University

<https://aws.amazon.com/blogs/aws/natural-language-processing-at-clemson-university-1-1-million-vcpus-ec2-spot-instances/>

# Scaling

## Google HPC Blog Post

### Cloud against the storm: Clemson's 2.1 million VCPU experiment

<https://cloud.google.com/blog/topics/hpc/clemson-experiment-uses-2-1-million-vcpus-on-google-cloud>

Kevin Kissell, Technical Director,  
Office of the CTO



THE NEXT PLATFORM

### Urgent HPC can Burst Affordably to the Cloud

<https://www.nextplatform.com/2020/01/08/urgent-hpc-can-burst-affordably-to-the-cloud/>



GCP CPU Core Ramp and Count



- 133,573 GCP Instances at peak
- 2,138,000 vCPUs at peak
- 6,022,964 vCPU hours

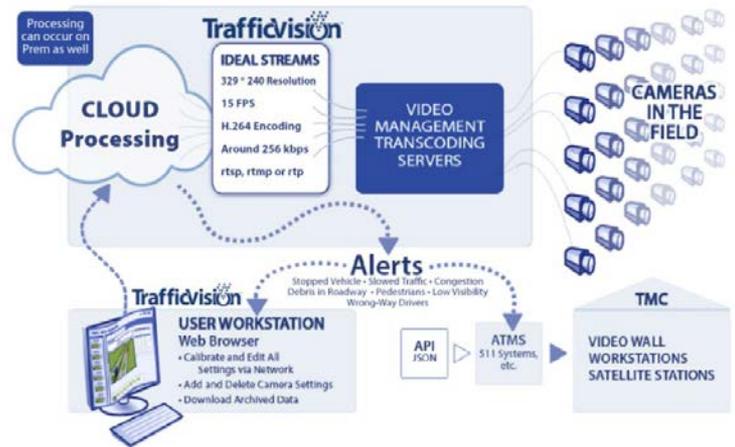
Processed 2,479,396 hours (~256TB) of video data

- ~4 hours of runtime
- ~1M vCPU within an hour
- ~1.5M vCPU within 1.5 hours
- 2.13M vCPU within 3 hours

Total Cost: \$52,598.64 USD

Average cost of \$0.008 USD per vCPU hour

# Real-time HPC & AI TrafficVision



## Features

### Incident Detection

- Stopped Vehicle
- Slowed Traffic
- Debris in Roadway
- Low Visibility
- Pedestrians
- Wrong-Way Drivers\*

Alerts, Incident Images & Clips

### Real-Time Data Collection

- Speeds Per Lane / Per Direction
- Vehicle Counts Per Lane / Direction
- Lane Occupancy and Density
- Congestion Index
- Classification:  
\*\*Motorcycle / Car / Truck / Large Truck

Data CSV export & JSON API

## Customers



## Integration of OOD into CloudyCluster

- As part of the Cloudify Gateways program (Omnibond, OSC, U Buffalo, Va Tech)
- Full deployment automated as part of the CloudyCluster launch
- Working on project based UI initially to support data scientist project teams.
- The Collaboration Continues



Open OnDemand Deployments



CloudyCluster Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾

**OPEN**  
**OnDemand & CloudyCluster**

OnDemand provides an integrated, single access point for all of your HPC resources.

**Message of the Day**

With Open OnDemand you are able to leverage a graphical user interface, while accessing the power of High Performance Computing With CloudyCluster. Other benefits include:

- Startup Interactive Resources, like Jupyter Notebook and Virtual Desktops
- File access which resembles Windows, MacOS and Linux file managers
- Job Composer tool to help build your job script files

["Your browser is the supercomputer: On Demand is a no-tears shortcut to research-computing"](#) from Matt Windsor of University of Alabama at Birmingham. A key phrase: "No experience necessary"

This material is based upon work supported by the National Science Foundation under grant numbers 1534949 and 1835725, and under active development by a team from the Ohio Supercomputer Center, U. of Buffalo CCR, and Virginia Tech

# Relion & CRYO-EM

Working with the Cianfrocco Lab at University of Michigan to test data transfer and scalability to the Cloud for CRYO-EM projects using RELION

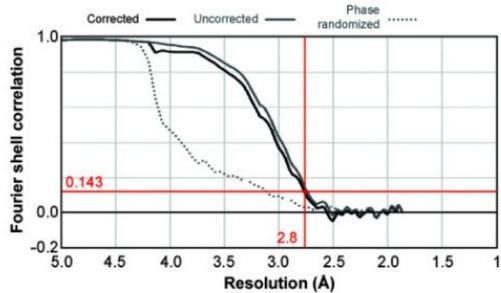
Also working with related Startups in the space that don't have access to large on prem clusters.

Initially Introduced as part of the Cloudify Program through the SGCI.

Cianfrocco is willing to consult with customers in conjunction with Omnibond and CloudyCluster

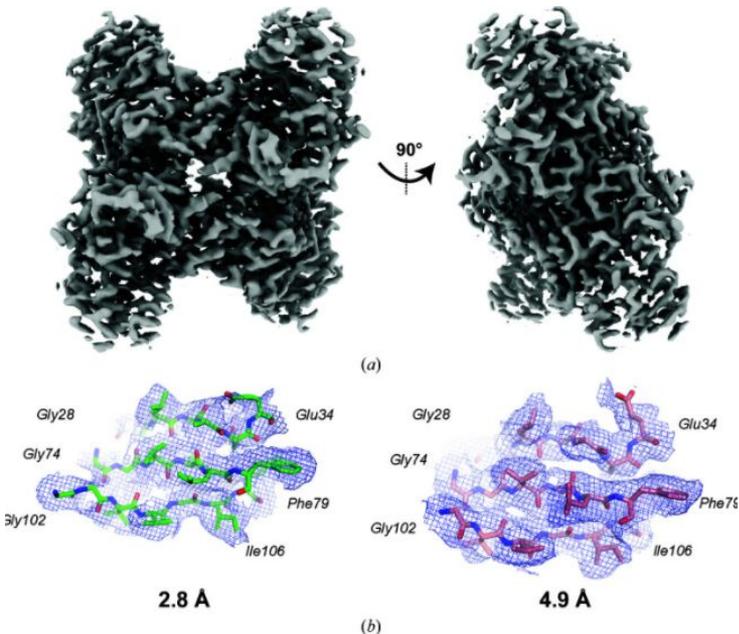
Another CRYO-EM project is in progress with the

ERN 



### High-resolution cryo-EM using beam-image shift at 200 keV

Jennifer N Cash<sup>1</sup>, Sarah Kearns<sup>1</sup>, Yilai Li<sup>1</sup>, Michael A Cianfrocco<sup>1</sup>



**Figure 5** Final aldolase reconstruction at 2.8 Å resolution. (a) Sharpened aldolase reconstruction at 2.8 Å resolution. (b) Example densities and models for aldolase at 2.8 and 4.9 Å resolution. (c) FSC curve for the final reconstruction.

# TAPIS - PEARC '22 Poster, Gateways '22 Paper



## Tapis

Unify, simplify, automate and secure your interactions with advanced computing infrastructure.

The Tapis Framework provides a hosted, unified web-based API for securely managing computational workloads across institutions so that experts can focus on their research instead of the technology needed to accomplish it.

## Projects Using Tapis

- A2CPS
- Bridging Barriers
- CyVerse
- DesignSafe
- Drug Discovery Portal
- ECCO
- Ike 'Wai (at the University of Hawaii Manoa)
- iReceptor
- iR+
- NeuroNex 3DEM
- Planet Texas 2050
- Science Gateways Community Institute
- Synergistic Discovery and Design Environment (SD2E)
- VDJSer
- UTRC

## Extending Tapis Workflow Management Framework with Elastic Google Cloud Distributed System using CloudyCluster by Omnibond

ERIC LAM, University of Hawaii, Manoa, USA

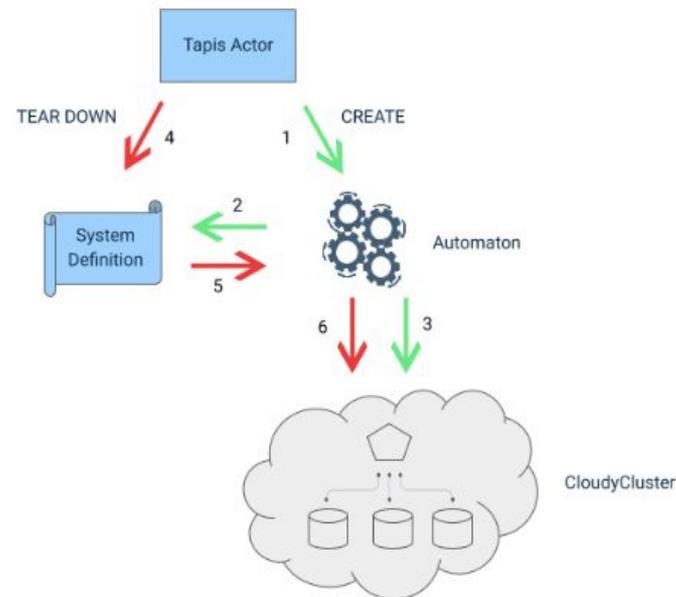
SEAN CLEVELAND, University of Hawaii - Information Technology Services - Cyberinfrastructure, USA

COLE MCKNIGHT, Omnibond Systems, USA

BOYD WILSON, Omnibond Systems, USA

RICHARD CARDONE, Texas Advanced Computing Center, USA

JOE STUBBS, Texas Advanced Computing Center, USA

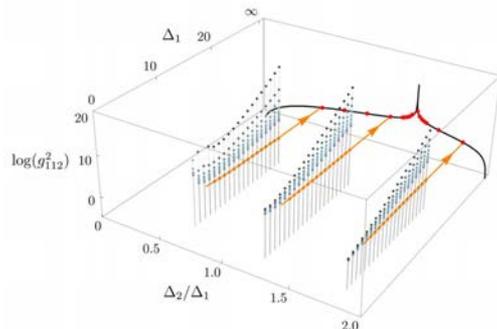


<https://github.com/omnibond/automaton>

# SDPB Solver MPI Tuning

## The Problem of Strong Coupling

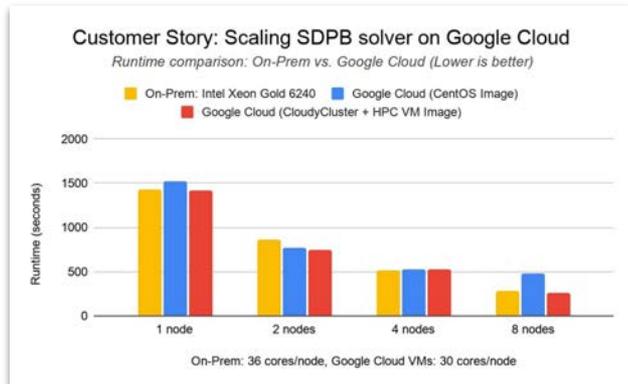
Quantum field theory (QFT) is a universal language for theoretical physics, describing the Standard Model of particle physics, early universe inflation, and condensed matter phenomena such as phase transitions, superconductors, and quantum Hall fluids. A triumph of 20th century physics was to understand weakly coupled QFTs. However, weakly interacting systems represent a tiny island in theory space and cannot capture many of the most interesting physical phenomena.



<https://bootstrapcollaboration.com/>

## Our Collaboration

Recently, members of our collaboration discovered new bootstrap techniques that apply in general dimensions. In the past few years we have applied these techniques to a wide variety of seemingly unrelated problems: to perform the world's most precise analysis of the 3d Ising model, to constrain strongly coupled theories of physics beyond the Standard Model, to aid in classifying superconformal field theories, to derive locality and black hole thermality in models of quantum gravity, and to prove irreversibility of renormalization group flows. We believe this is the beginning of a much larger enterprise, crossing traditional boundaries between string theory, condensed matter physics, and phenomenology, and making strong connections to modern mathematics and computer science.



<https://cloud.google.com/blog/topics/hpc/introducing-hpc-vm-images>

To expand the collaboration's computation capabilities, Walter Landry wanted to see how SDPB would scale on Google Cloud. Working with Omnibond's **CloudyCluster** and leveraging the HPC VM image, Landry achieved comparable performance and scaling to an on-premises cluster at Yale, based on Intel Xeon Gold 6240 processors and Infiniband FDR.

# Turn-Key Elastic HPC, HTC, & Storage in GCP

Create a familiar, secure & fully operational computational cluster in minutes, complete with:

**Encrypted Storage:** GCS, OrangeFS on PD

**Compute:** Job Driven Elastic Compute through CCQ (Preemptible, On-Demand, GPU)

**Schedulers:** Torque & SLURM with the CCQ Meta-Scheduler  
Supports Billing Labels per job/user  
Placement Groups, BulkAPI, Tier1 Networking  
Supports Multiple Custom Images

**End User Friendly UI:** Open OnDemand

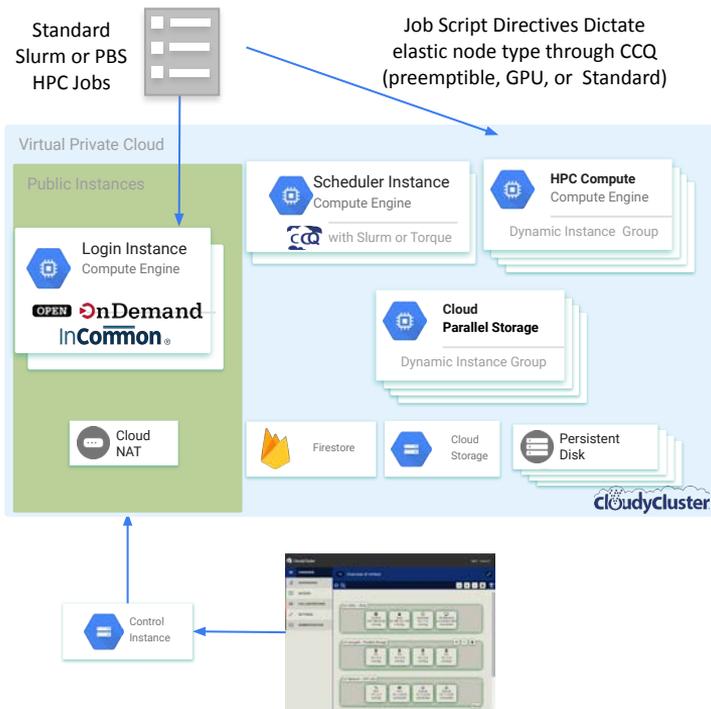
**Includes Familiar Software**

**HPC Libraries:** Boost, Cuda Toolkit, Docker, FFTW, FLTK, GCC, Gengetopt, GRIB2, GSL, HDF5, Intel MPI, Intel Runtimes, ImageMagick, JasPer, mpich, NetCDF, NumPy, Octave, OpenCV, OpenMPI, PROJ, R, Rmpi, SciPy, SWIG, WGRIB, UDUNITS, .NET Core, Singularity, Queue, Picard, xrootd, etc...

**HPC Software:** Ambertools, ANN, ATLAS, BLAS, Blast, Blender, Burrows-Wheeler Aligner, CESM, GROMACS, JupyterLab, LAMMPS, NCAR, NCL, NCO, nwchem, OpenFoam, papi, paraview, Quantum Espresso, SAMtools, WRF, Galaxy, Vtk, Su2, Dakota, Gatk, etc...

**ML Software:** Mlpack, NuPIC, Octave, OpenCV, PICARD, Queue, Scikit-learn, Tensorflow

**Sample Jobs:** Intel Cluster Checker, Mpi\_prime, wrf, etc...



# Turn-Key Elastic HPC, HTC, & Storage in AWS

Create a familiar, secure & fully operational computational cluster in minutes, complete with:

**Encrypted Storage:** EBS, OrangeFS on PD

**Compute:** Job Driven Elastic Compute through CCQ (Spot, On-Demand, GPU)

**Schedulers:** Torque & SLURM with the CCQ Meta-Scheduler

Supports Billing Tags per job/user

Placement Policies, Advanced Networking

Supports Multiple Custom Images

**End User Friendly UI:** Open OnDemand

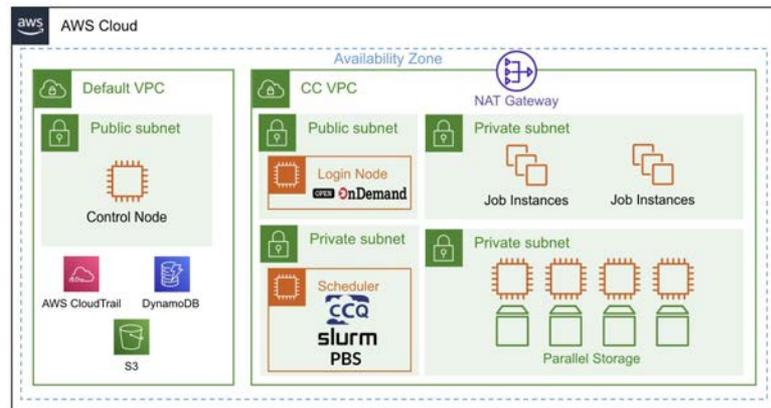
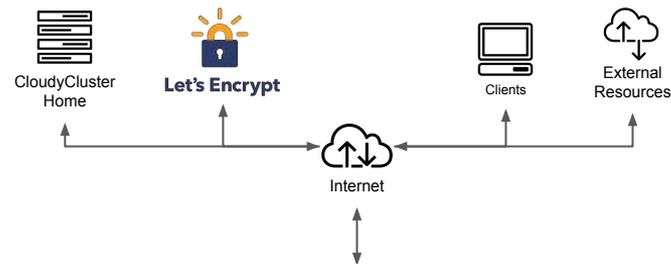
**Includes Familiar Software**

**HPC Libraries:** Boost, Cuda Toolkit, Docker, FFTW, FLTK, GCC, Gengetopt, GRIB2, GSL, HDF5, Intel MPI, Intel Runtimes, ImageMagick, JasPer, mpich, NetCDF, NumPy, Octave, OpenCV, OpenMPI, PROJ, R, Rmpi, SciPy, SWIG, WGRIB, UDUNITS, .NET Core, Singularity, Queue, Picard, xrootd, etc...

**HPC Software:** Ambertools, ANN, ATLAS, BLAS, Blast, Blender, Burrows-Wheeler Aligner, CESM, GROMACS, JupyterLab, LAMMPS, NCAR, NCL, NCO, nwchem, OpenFoam, papi, paraview, Quantum Espresso, SAMtools, WRF, Galaxy, Vtk, Su2, Dakota, Gatk, etc...

**ML Software:** Mlpack, NuPIC, Octave, OpenCV, PICARD, Queue, Scikit-learn, Tensorflow

**Sample Jobs:** Intel Cluster Checker, Mpi\_prime, wrf, etc...



# The Meta-Scheduler Approach

## Scheduler Independent

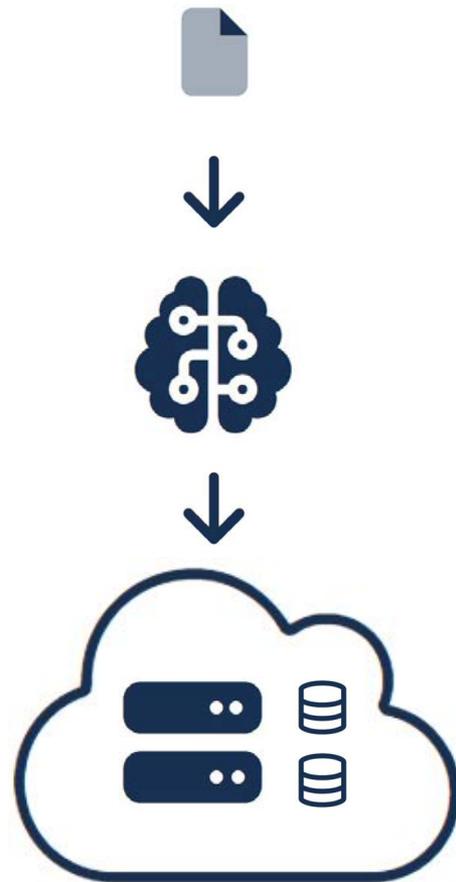
- Torque
- Slurm

## Allow for Meta-Scheduler Directives

- Instance Type, each job can have a different instance type and billing model.
- GPU
- Spot, Preemptible
- Billing Tags/Labels
- Volume Type
- Custom Images for Different Jobs

## Turns “Scheduler” into Dispatcher Handling:

- Instance and appropriate subnet provisioning
- Instance deletion



# Self Paced Learning (Ask for Free Credits for Lab)

← Omnibond: Creating an HPC Environment in Google Cloud with CloudyCluster

Start Lab 01:30:00

## Student Resources

- Job Scripts
- Using the CCQ Meta-scheduler
- Blog Articles
- Behind the Scenes Architecture of CloudyCluster v3 on GCP

## Omnibond: Creating an HPC Environment in Google Cloud with CloudyCluster

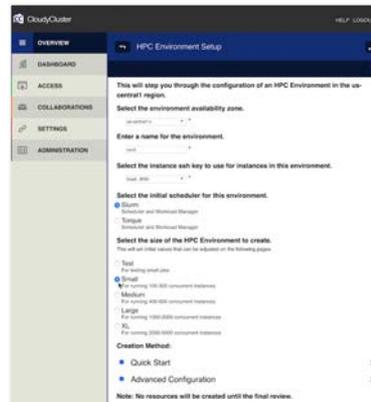
1 hour 30 minutes 5 Credits ☆☆☆☆☆

This lab was developed with our partner, [Omnibond](#). Your personal information may be shared with Omnibond, the lab sponsor, if you have opted-in to receive product updates, announcements, and offers in your Account Profile.

GSP862



[CloudyCluster Online Training](#)



## Learn How To:

- Setup GCP Account, Check Quotas, Configure IAM
- Launch a CloudyCluster instance from the GCP Marketplace
- Setup Admin user and credentials
- Choose the size of your environment (Test, SM, M, L, XL)
- Customize options for the environment -> Select Create
- CloudyCluster automatically creates a Private Network, Login, Scheduler (Slurm or PBS), and Parallel Storage all ready to run HPC jobs.
- Upload your data / Tweak your HPC job script
- Run your job and Download Results.

# Initial Collaboration Story In the Style of a Fireside Chat

# Cloudify Gateways

## Cloudify Program:

- **Solicitation:** Program from Science Gateways Community Institute (SGCI) to give out Google Cloud Credits for research projects to be “Cloudified”
- **Submissions:** Submissions over 3 years a batch per year
- **Total:** 15 Awardees over the 3 years
- **Awards:** Google Cloud Credits and Cloudify technical assistance from Omnibond

# Cloudify Gateways Proposal

“**Scientists accessing HPC resources today**, either at the campus or national level typically **need advanced knowledge of Linux**, familiarity with command-line interfaces and installation and configuration of custom client software. These additional requirements **create an accessibility gap** that for many scientists serves as **an impediment to adopting HPC** for their research. This accessibility gap is a long standing and recognized issue in HPC. **Removing, or even reducing this impediment to HPC use, will immediately increase the productiveness** of computationally intensive research. **Lowering the barrier** for access to HPC systems has long been the “**Holy Grail**” in the HPC community.”

...

“Open OnDemand (OOD) is an **innovative**, open-source, **web-based portal for accessing HPC services** that removes these intricacies, and in so doing reduces time to science for researchers by **facilitating their access to HPC resources**.”

...

“However, the **CloudyCluster team** is explicitly focused on providing an easy to use **Cloud-based HPC infrastructure**”

# OPEN OnDemand

Supercomputing. Seamlessly. Open, Interactive HPC Via the Web.

## About Open OnDemand

Provides an easy to install and use, web-based access to supercomputers, resulting in intuitive, innovative support for interactive supercomputing.

Features include:

- Plugin-free web experience
- Easy file management
- Command-line shell access
- Job management and monitoring
- Graphical desktop environments and applications

## Cloudify Project

- Need: Many HPC centers are evaluating the usage of cloud-based HPC resources
- Problem: OOD architecture based on traditional HPC resource managers and intra-node communication doesn't work in the cloud
- Solution: Combine the expertise of the OOD and CloudyCluster teams, with CCQ and Slurm running on the Google Cloud Platform
- Outcomes: A demo of OOD running on GCP and supporting an example HPC client workflow..



# Open OnDemand & CloudyCluster

## Extended Outcomes:

- **Open OnDemand - CloudyCluster Full Integration:** Because of this collaboration OOD is now an integral part of CloudyCluster and automatically launches when you bring up CloudyCluster
- **Expanded Coverage:** This full integration is now across Google Cloud and AWS
- **Expanded Use Cases:** Biomedical Startups

# Open Discussion

# Cloudfify Gateways from the SGCI & Google

## Open Discussion Starter Questions

- **How can you see other areas that would benefit from similar collaborations?**
- **Are there examples of similar collaborations that you have seen?**
- **Are there ways to help foster these?**

Next Phase of Collaboration

# Project Eureka - Unify Data Mgt & Computation



# EUReKA

see the [show](#)

# Eureka Goals

- Data Science, HPC, and HPC Adjacent
  - K8s, spark, etc...
  - Data Science Apps
  - Job Routing
- Storage
  - Staging
  - Dynamic scratch
  - Publish
- Project based UI in Open OnDemand
- Bridge to on-prem
- Easier for end users (cloud stuff still gets in the way for researchers)
- More modular
- Leverage more -> Provide more

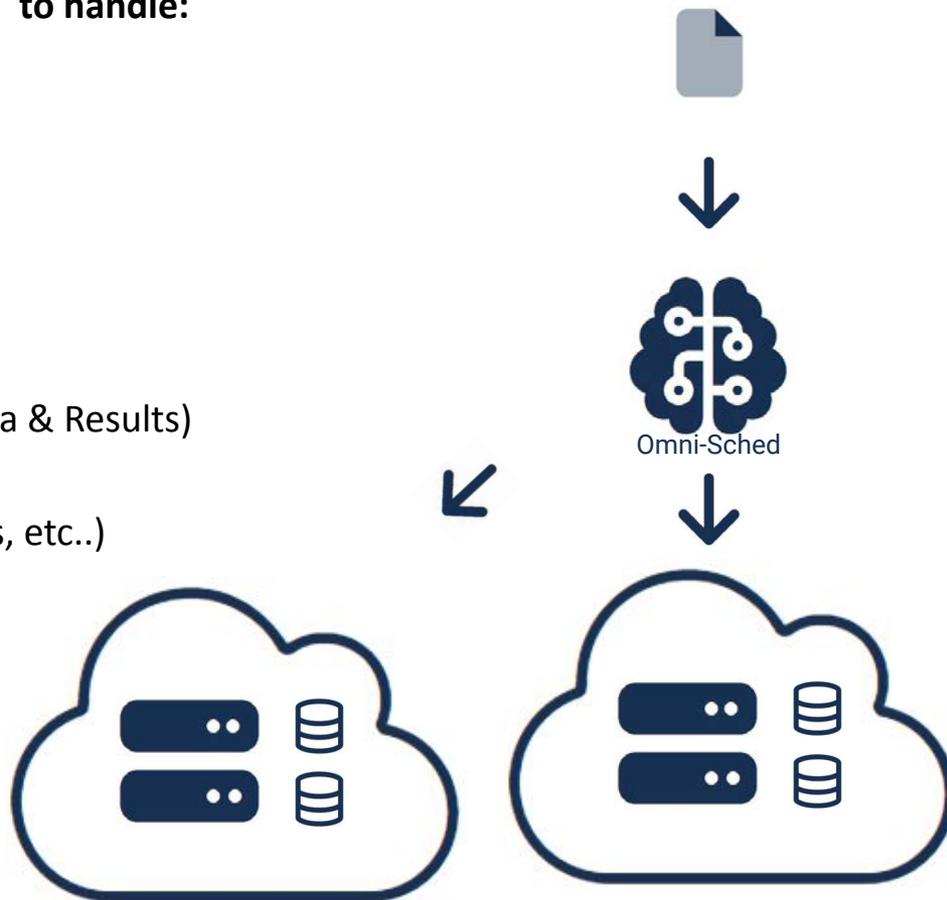


# The Omni-Scheduler Approach

Expand meta-scheduler concept (OmniSched) to handle:

- Cross Cloud - leverage TerraForm
- Enable On-Prem (TF -> kvm)
- Job routing between locations
- Dynamic Scratch
  - Driven by job Directives
- Data Staging
  - Driven by Job Directives (Input Data & Results)
- Beyond HPC
  - HPC adjacent (publishing, websites, etc..)
  - Enable Apache Spark
  - K8s
  - Etc...
- Scheduling Data Movements

With iRODS integration with OmniSched



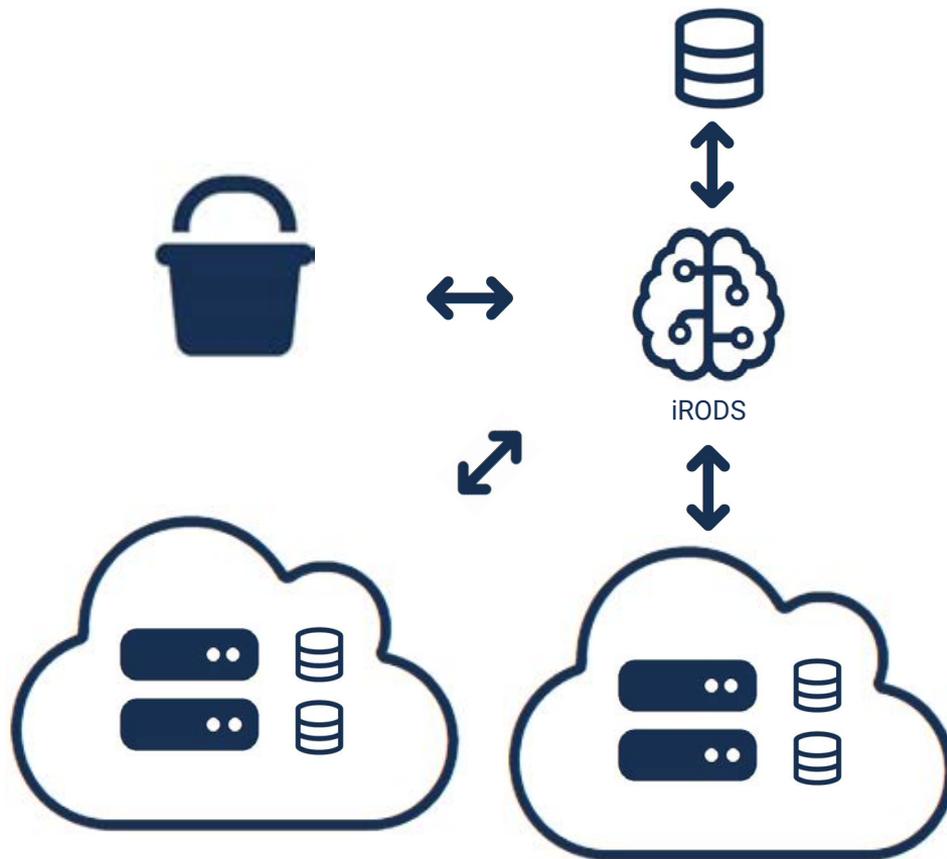
# The Integrated Data Management

## In addition to Job based directives

### Data Management Capabilities

- Replicate
- Archive
- Ingest
- Tier
- Publish

All configured in OOD with iRODS



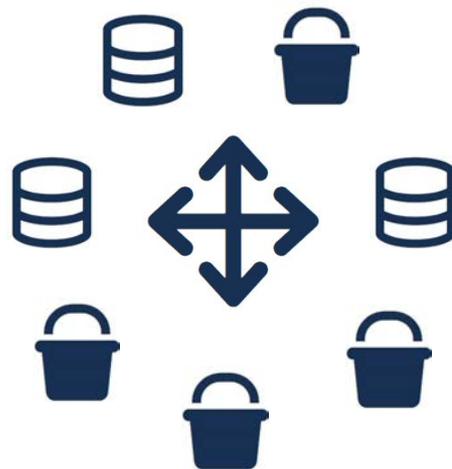
# Design Thinking UI

## Project

- **Data Science (and other) App Launcher**
- **Research Project Based Collaboration**

## Data

- **Cross System File Manager in OOD using iRODS**
- **Storage Resource Integration configured in OOD with iRODS**
- **Data Action Scheduling, configured in OOD with iRODS**



Demo