

# iRODS Open OnDemand Eureka

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



# Leadership Team

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

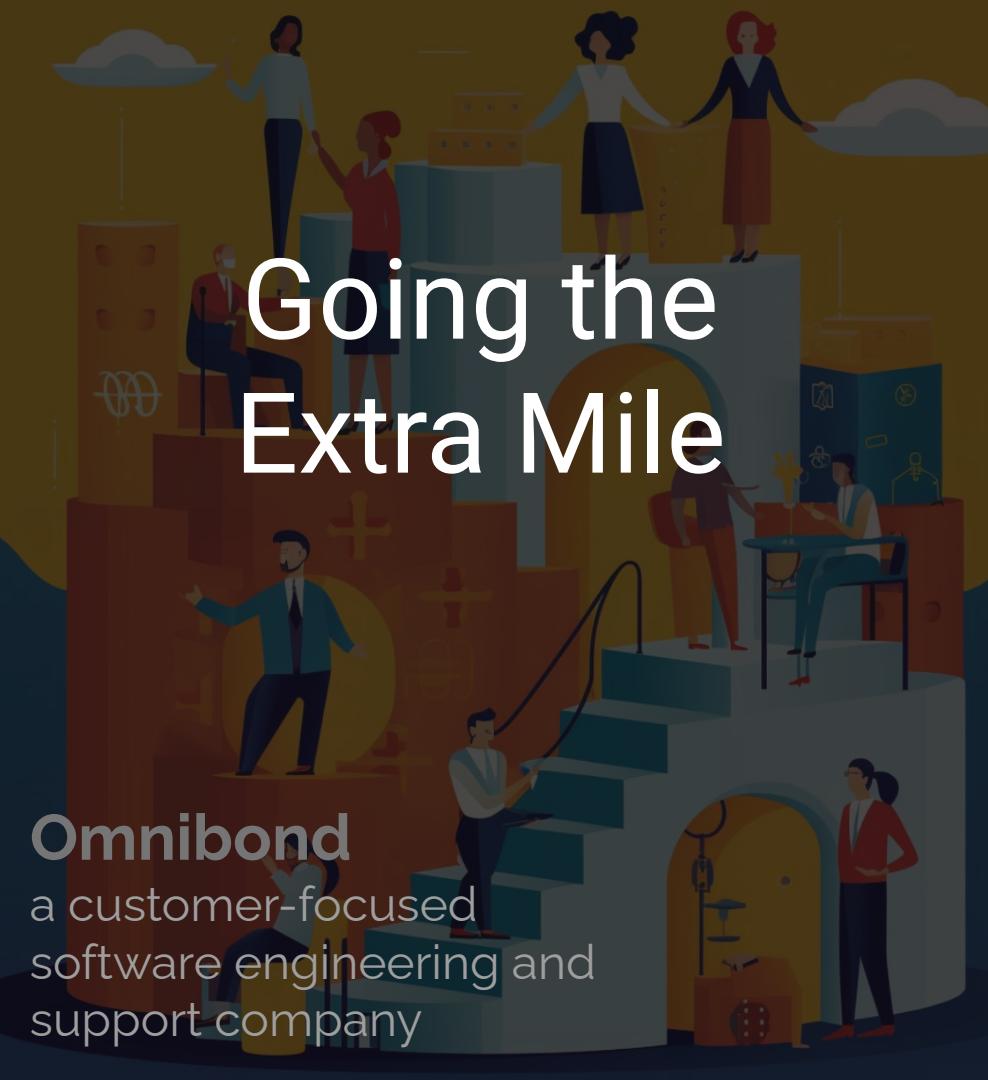
- Over 40 years combined experience in facilitating and supporting academic and corporate research in using the tools and technologies of advanced computing
- Experience at the working and technical, project and executive management levels at Clemson, Purdue and Miami Universities and the National Center 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 Members

- 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



# Software Products

Omnibond  
a customer-focused  
software engineering and  
support company



# Going the Extra Mile

**Omnibond**

a customer-focused  
software engineering and  
support company

I have worked with Omnibond development and support for almost 15 years. They always deliver the highest level of support possible. I have been in Technical Support for 23 years and have worked with different companies across the world. Omnibond is at the top in response time and for going the extra mile to help our customers. I have no reservation in recommending them as a great company.

Reed Harrison

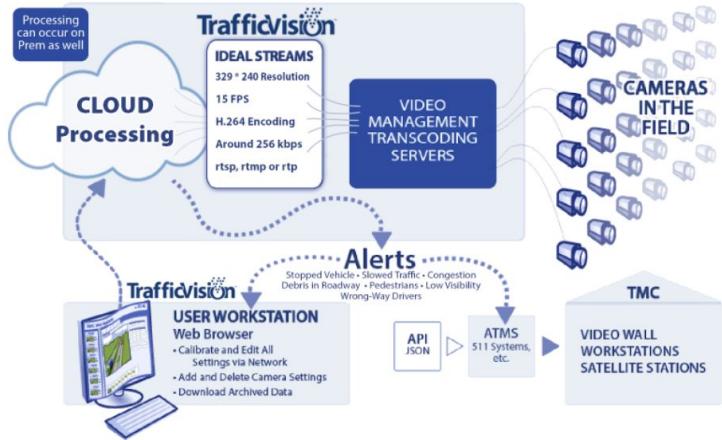
Provo, UT

Support Engineer

Novell/NetIQ/MicroFocus/OpenText

# Real-time HPC & AI **Trafficvision**

Customers



## Features

### Incident Detection

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

### 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

Alerts, Incident Images & Clips

Data CSV export & JSON API



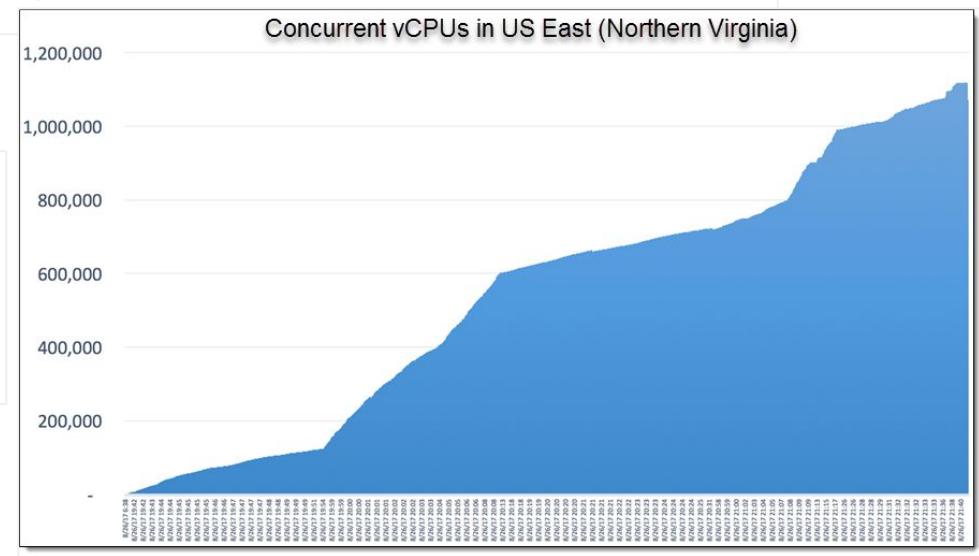
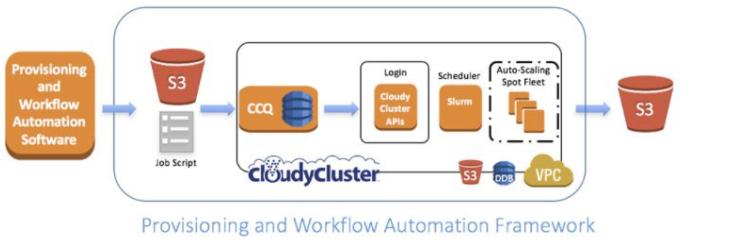
SCDOT

TRIMARC

# Scaling on AWS

AWS News Blog

## 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



### Urgent HPC can Burst Affordably to the Cloud

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



CLEMSON  
UNIVERSITY

Google 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



Trafficvision

# 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

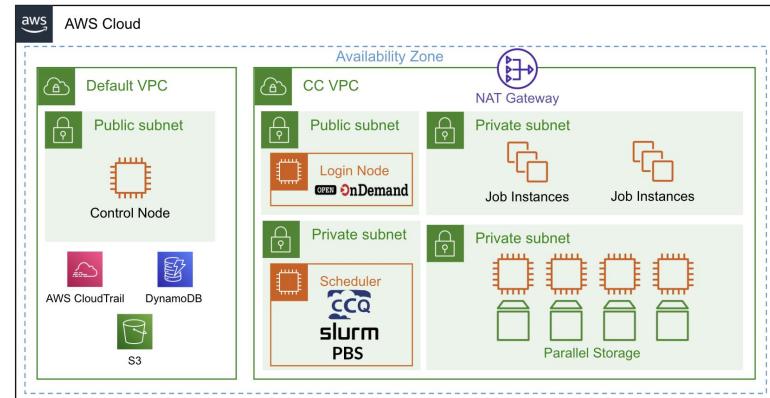
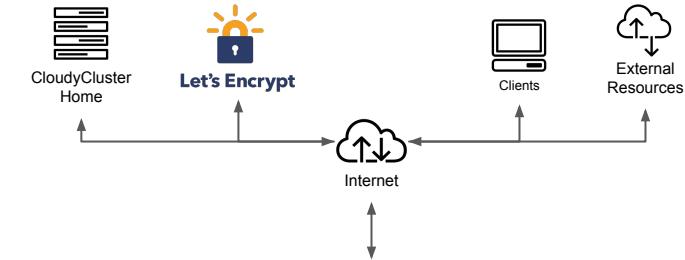
## Includes Familiar Software

**HPC Libraries:** Boost, Cuda Toolkit, Docker, FFTW, FLTK, GCC, Gennetopt, 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:** Mpack, NuPIC, Octave, OpenCV, PICARD, Queue, Scikit-learn, Tensorflow

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



# 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 (Preemptable, 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

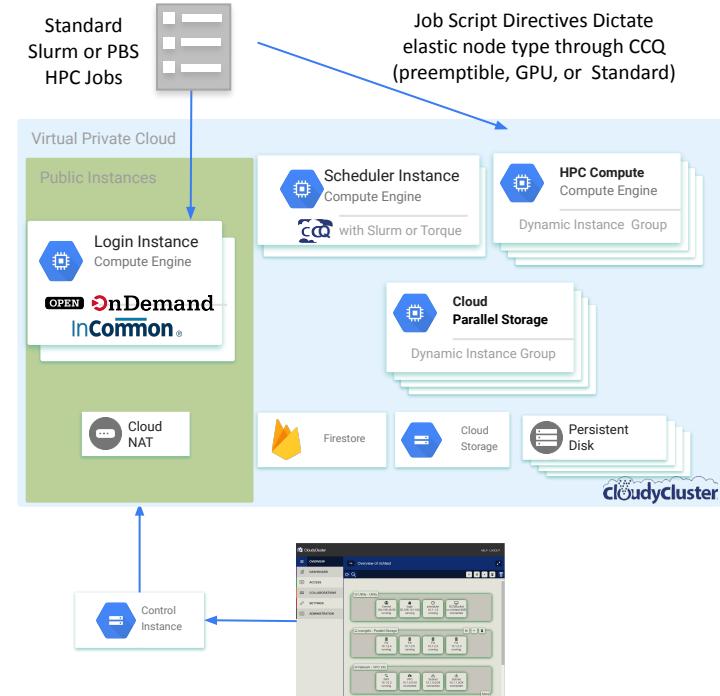
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# HPC User Experience

OPEN  OnDemand

## 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
- The Collaboration Continues



The screenshot shows the CloudyCluster web interface. At the top, there's a navigation bar with links for CloudyCluster, Files, Jobs, Clusters, Interactive Apps, and a user icon. Below the navigation bar, the Open OnDemand & CloudyCluster logo is prominently displayed. The logo features the "OPEN" wordmark in white on a black background, followed by the "OnDemand" logo (a red arrow inside a circle) and the "CloudyCluster" logo (the word "CloudyCluster" in blue with a stylized cloud icon above it). Below the logo, a sub-headline reads: "OnDemand provides an integrated, single access point for all of your HPC resources." A section titled "Message of the Day" follows, which is currently empty. Underneath, a paragraph explains the benefits of using Open OnDemand with CloudyCluster, and a bulleted list details specific features like startup interactive resources, file access, and a job composer tool.



Open OnDemand Deployments

"[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"

# Relion & CRYO-EM

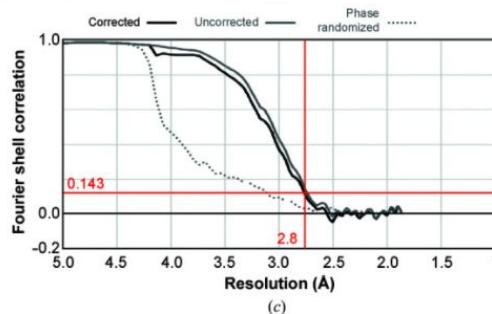
## Working with the Cianfrocco Lab at University of Michigan to test data transfer and scalability to the Cloud for CRYO-EM projects using RELION

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.**

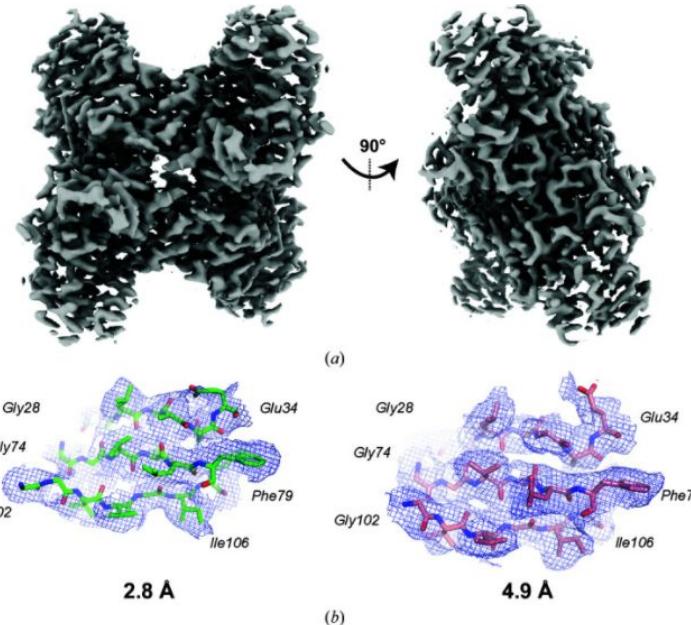
**Cianfrocco is willing to consult with customers in conjunction with Omnibond and CloudyCluster**

Another CRYO-EM project is in progress with the  
ERN  Ecosystem for  
Research  
Networking



## 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>

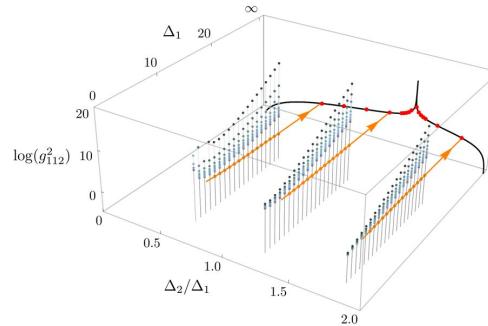


**Figure 5** Final aldolase reconstruction at 2.8 Å resolution. (a) Sharpened aldolase reconstruction at 2.8 Å resolution. (b) Example densities and models for aldolase at 2.8 and 4.9 Å resolution. (c) FSC curve for the final reconstruction.

# SDPB Solver MPI Tuning

## The Problem of Strong Coupling

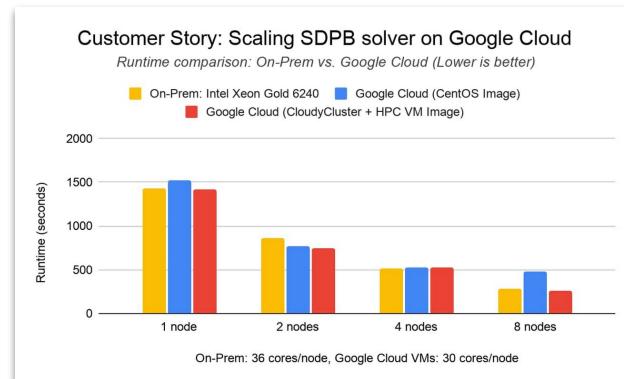
Quantum field theory (QFT) is a universal language for theoretical physics, describing the Standard Model of particle physics, early universe inflation, and condensed matter phenomena such as phase transitions, superconductors, and quantum Hall fluids. A triumph of 20th century physics was to understand 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.

# 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.

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

## 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)
- VDJServer
- UTRC

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

ERIC LAM, University of Hawaii, Manoa, USA

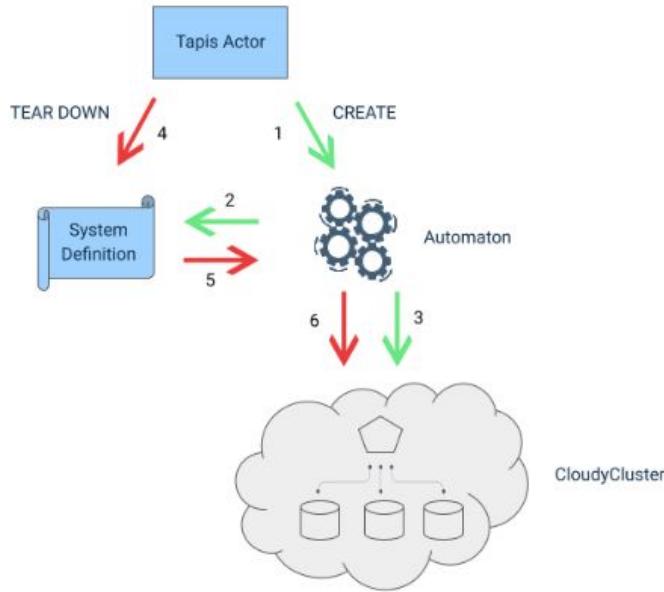
SEAN CLEVELAND, University of Hawaii - Information Technology Services - Cyberinfrastructure, USA

COLE MCKNIGHT, Omnibond Systems, USA

BOYD WILSON, Omnibond Systems, USA

RICHARD CARDONE, Texas Advanced Computing Center, USA

JOE STUBBS, Texas Advanced Computing Center, USA



# The Meta-Scheduler Approach

Scheduler Independent

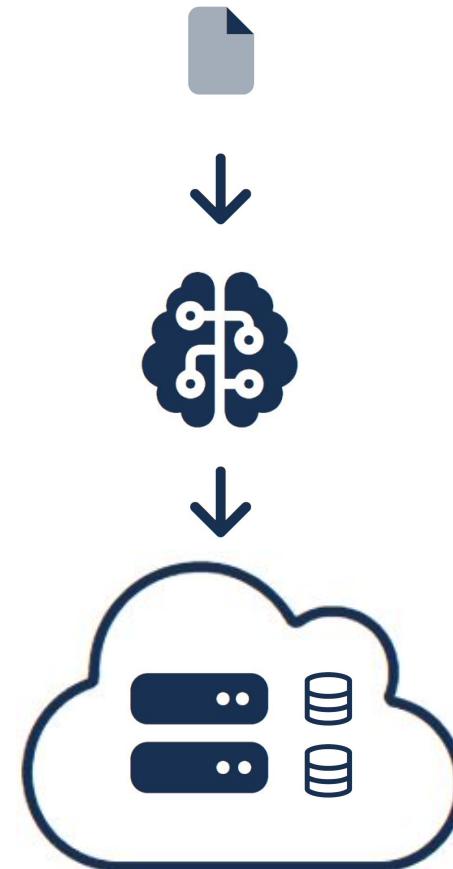
- Torque
- Slurm

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



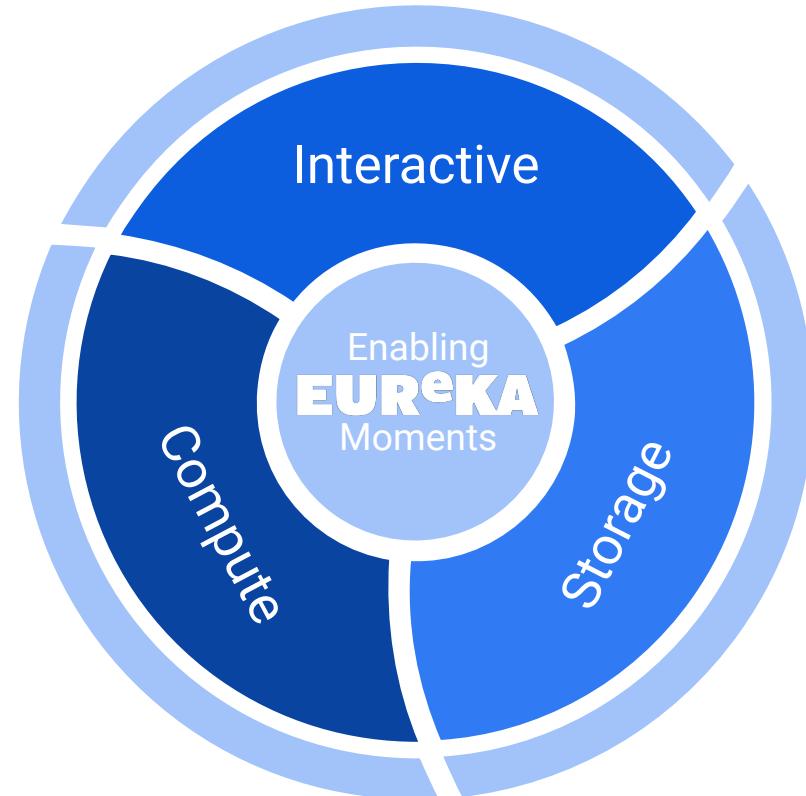
# Project **EUREKA**



see the [show](#)

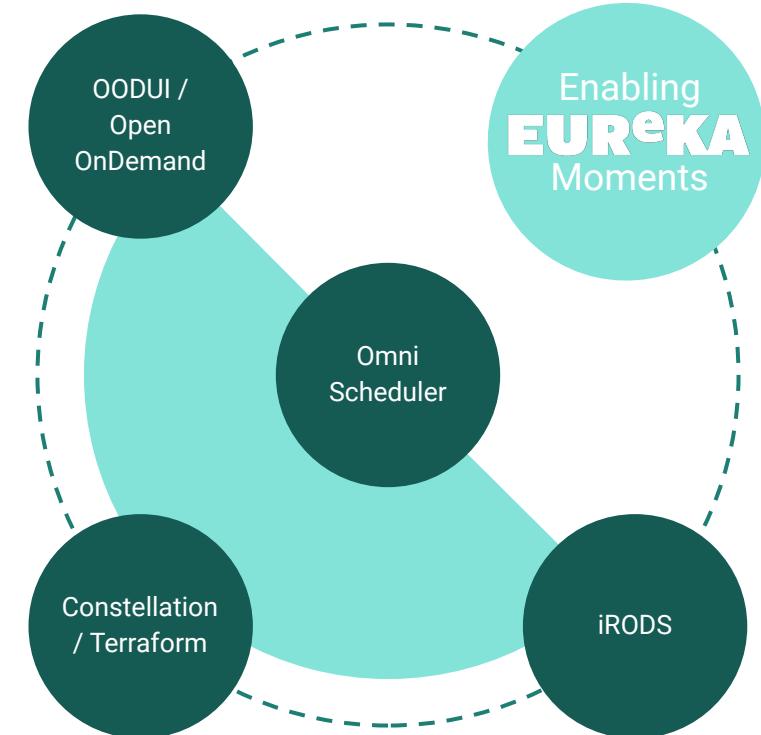
# OOD UI + Eureka Vision

- Interactive
  - Applications & Launchers
  - API Applets & SaaS Apps
  - Project Focused
- Compute
  - Compute Anywhere (HPC, AI, & Beyond)
  - Enable Cloud Specialties
  - Simplify Compute and Storage Interactions
- Storage
  - Integrate Diverse Storage Resources
  - Collaborate First
  - Project Level Data Lifecycle



# Technology

- Cloud Jump UI & Open OnDemand
  - HPC Industry Standard
  - OODUI - Simplify & Empower
- Omni-Scheduler
  - Coordinates UI, Storage, & Compute
- Constellation Driven Terraform
  - Multi-Cloud Enabler
- iRODS
  - Metadata Driven Data Management & Movement
  - Designed for Diverse Storage



# Inside-Out

## Open OnDemand UI

User Experience First  
Design & Usability  
Forward

## Project Leads UI

Leads Projects View  
What's Running  
Utilization Tools

## Admin UI

Global View of Projects &  
Users  
What's Running Globally  
Global Utilization

# Open OnDemand Example Deployments



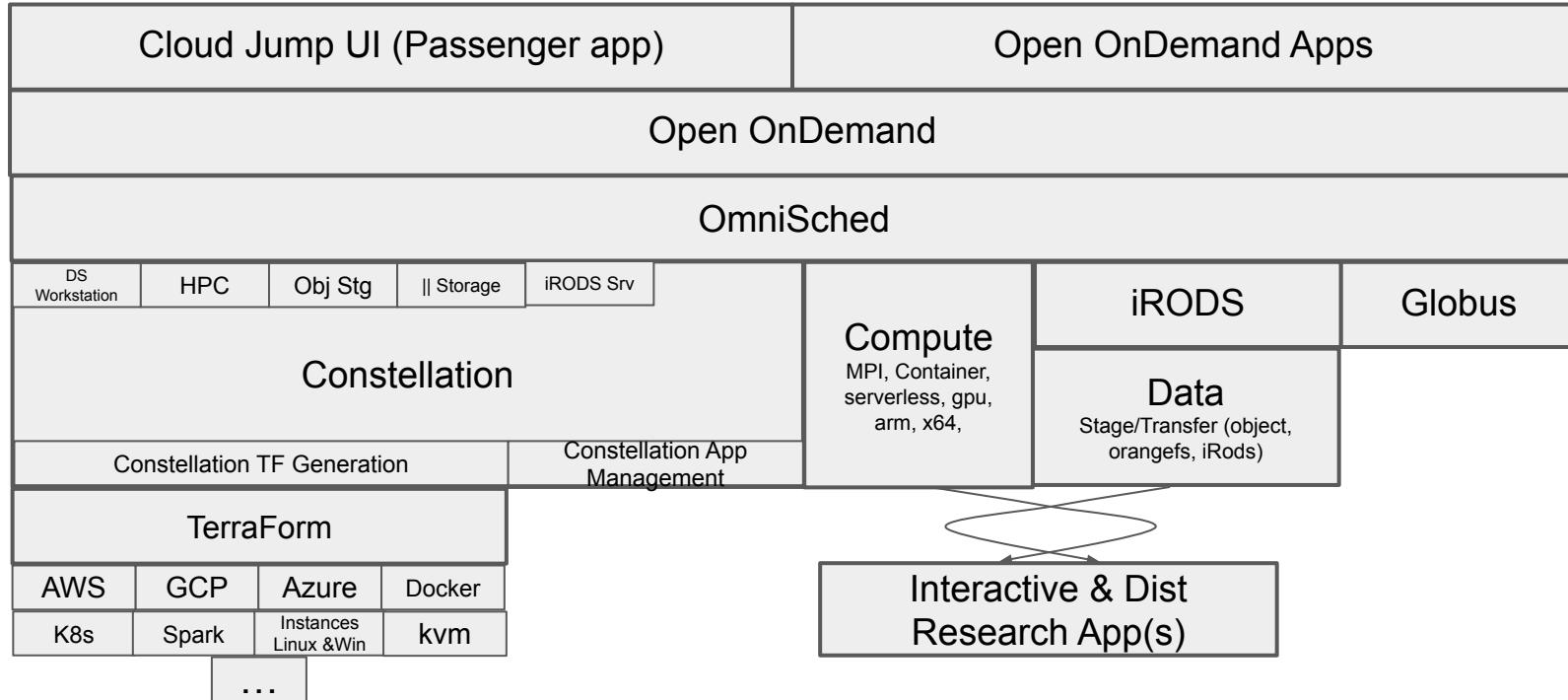
# Don't see an organization?

The more the merrier!  
Let us know any that  
belong on the list



[openondemand.org/orgs](http://openondemand.org/orgs)

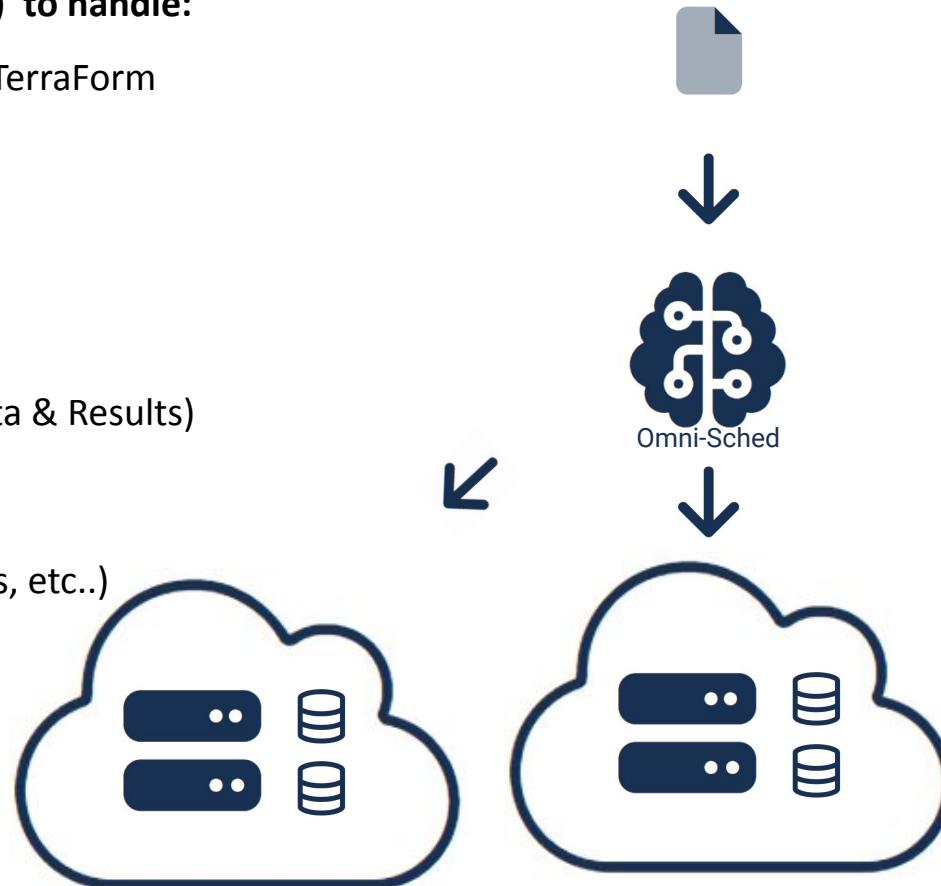
# Eureka - Architecture (Work in Progress) 5/2023



# The Omni-Scheduler Approach

Expand meta-scheduler concept (OmniSched) to handle:

- Cross Cloud - leveraging Constellation / 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
  - Data Science Apps
  - HPC adjacent (publishing, websites, etc..)
  - Enable Apache Spark
  - K8s
  - Etc...
- Scheduling Data Movements
  - iRODS integration



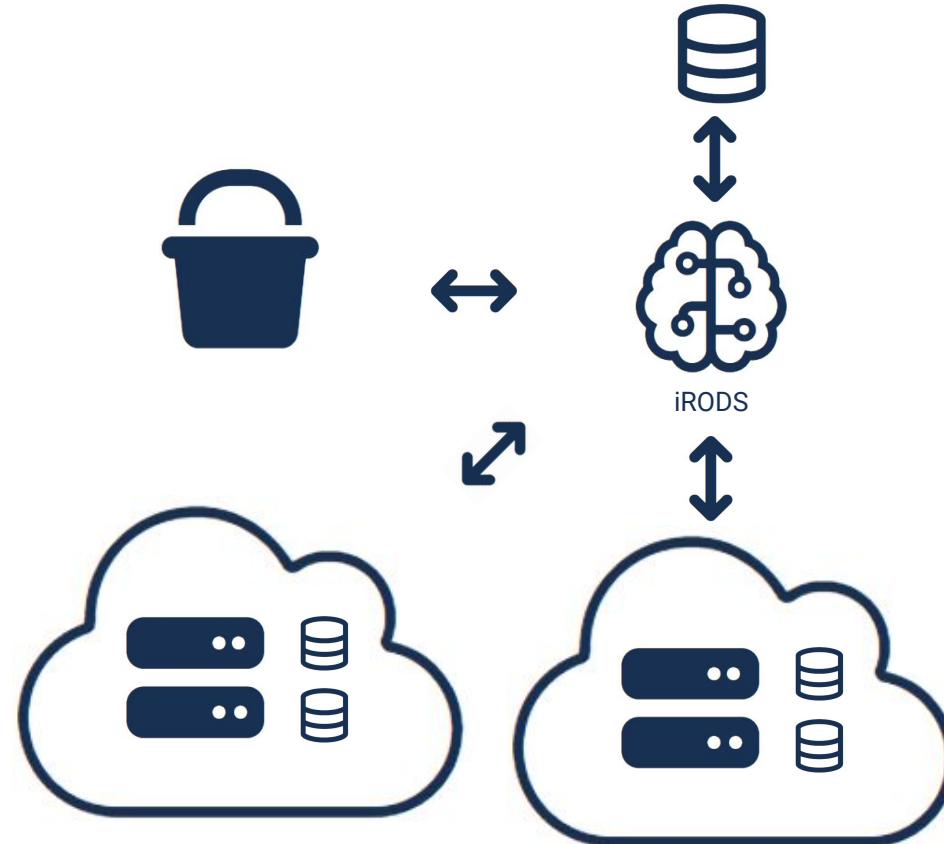
# The Integrated Data Management

In addition to Job based directives

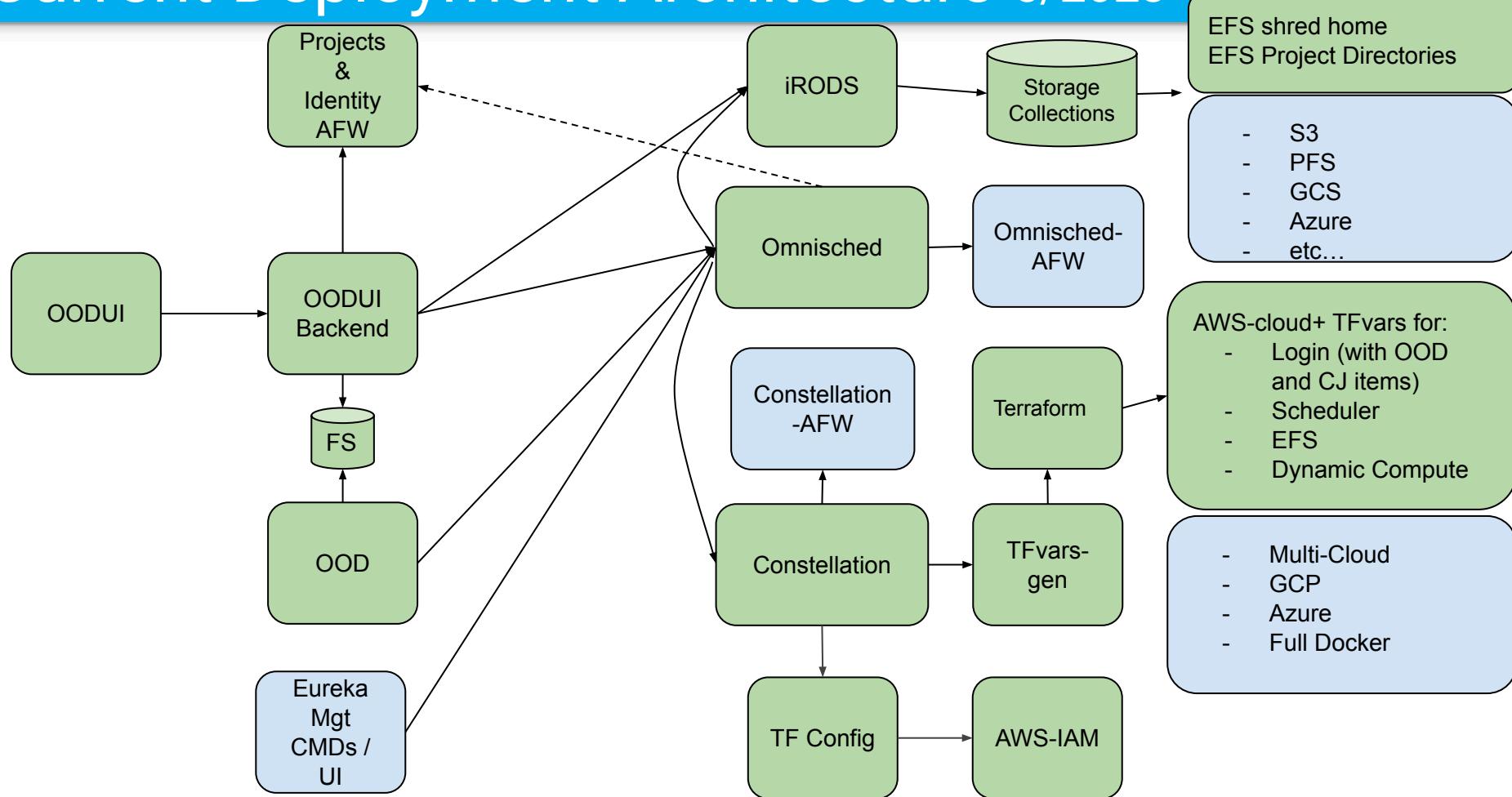
Data Management Capabilities

- Replicate
- Archive
- Ingest
- Tier
- Publish

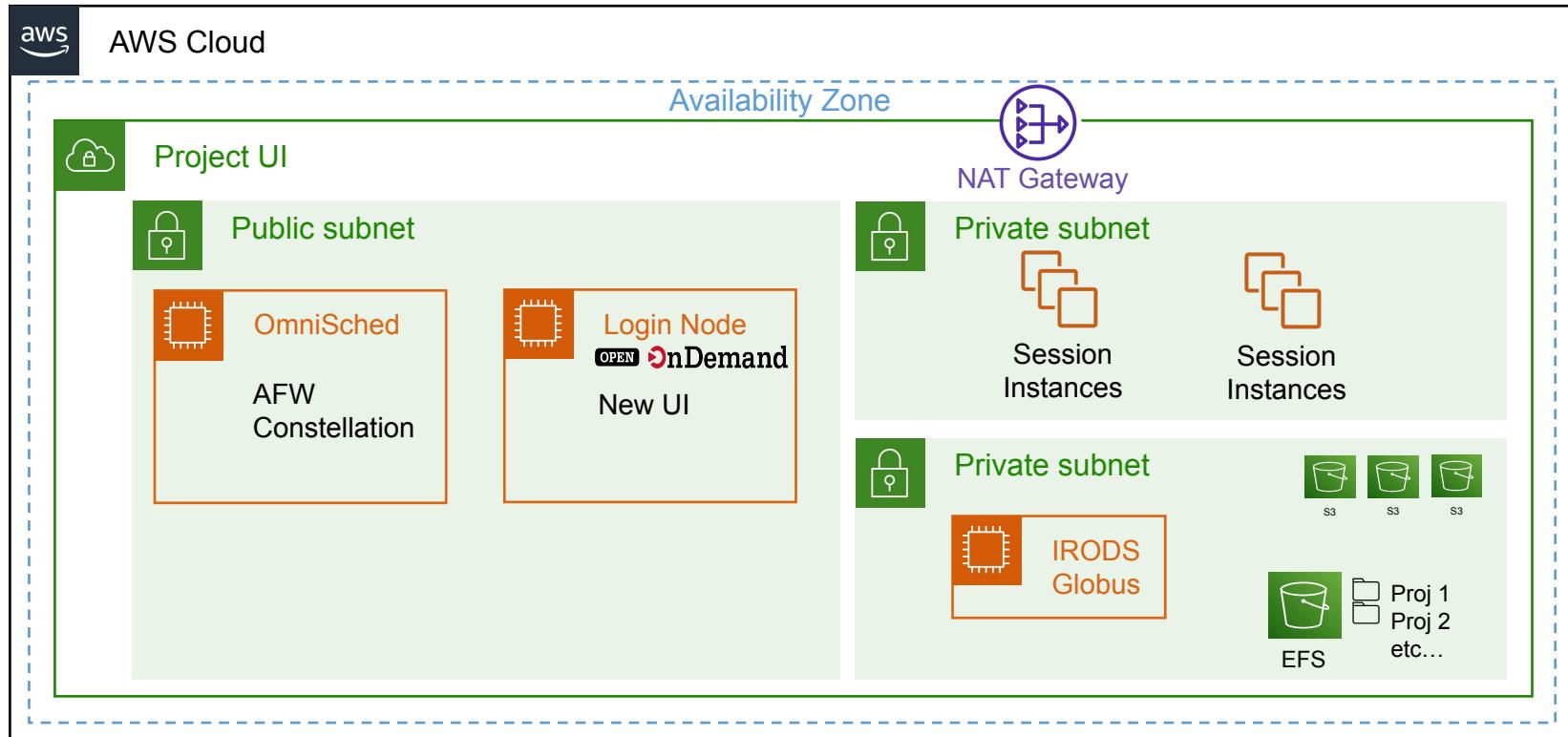
All configured in OOD with iRODS



# Current Deployment Architecture 5/2023

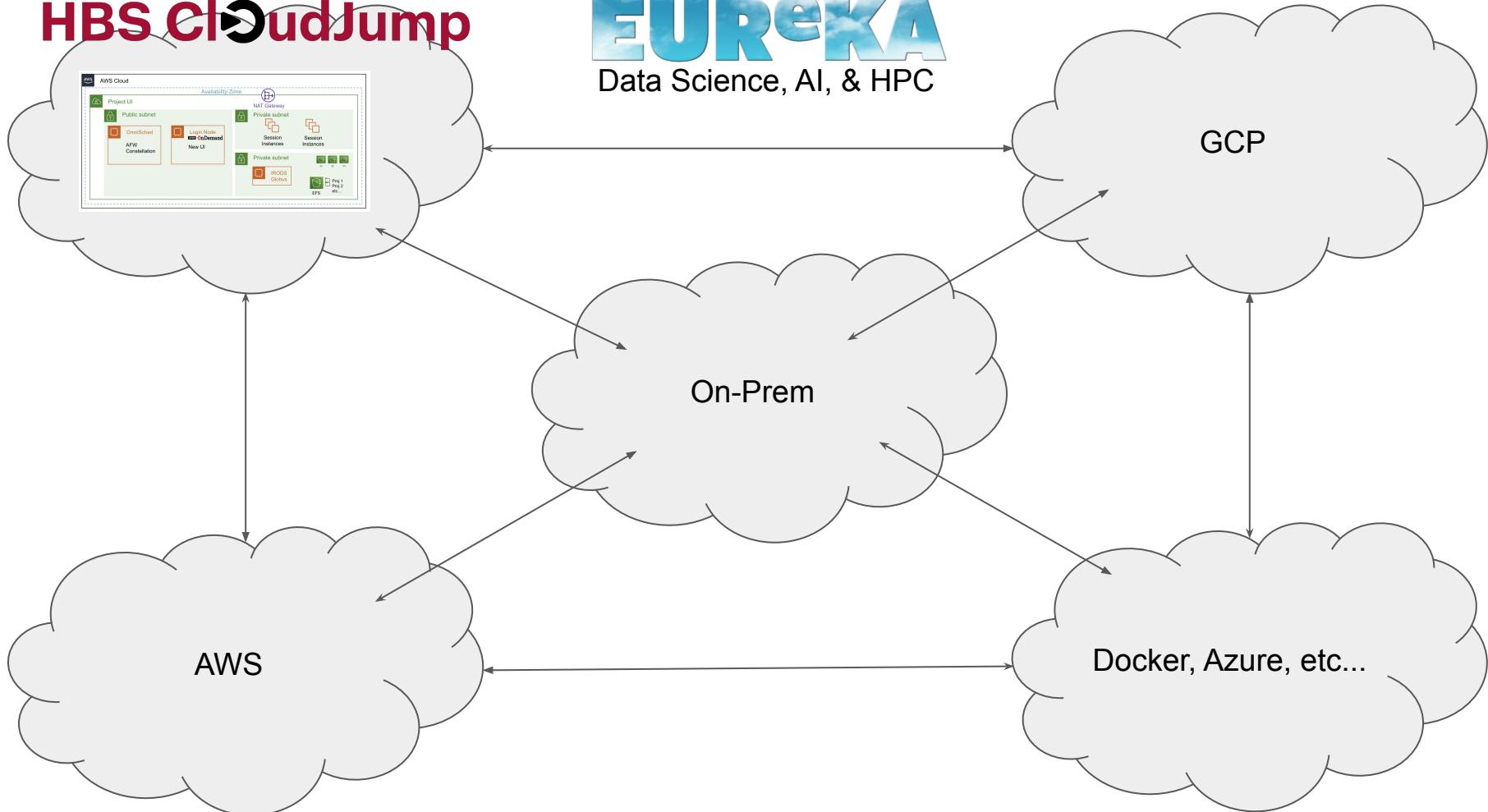


# Deployment Architecture



# HBS CloudJump

Destination  
**EUREKA**  
Data Science, AI, & HPC



# Demo

# EUREKA



see the [show](#)

# Cloud Jump

Data Science Platform

Active Projects New Project

Advanced Discovery Data Science NewProj

Sessions	State	Cores	GPUs	Time
VS Code	Running	2	0	0h 18m
Desktop	Running	0	0	0h 11m
VS Code	Running	0	0	0h 11m
RStudio	Running	0	0	0h 8m

# Project Eureka - Project Based UI

The screenshot displays the Project Eureka Data Science Platform interface. At the top, a navigation bar includes a menu icon, a logo with three dots, the text "Data Science Platform", and a blue circular icon with the letters "BW".

The main area is titled "Advanced Discovery" and contains a grid of launcher cards. Each card represents a different application or environment:

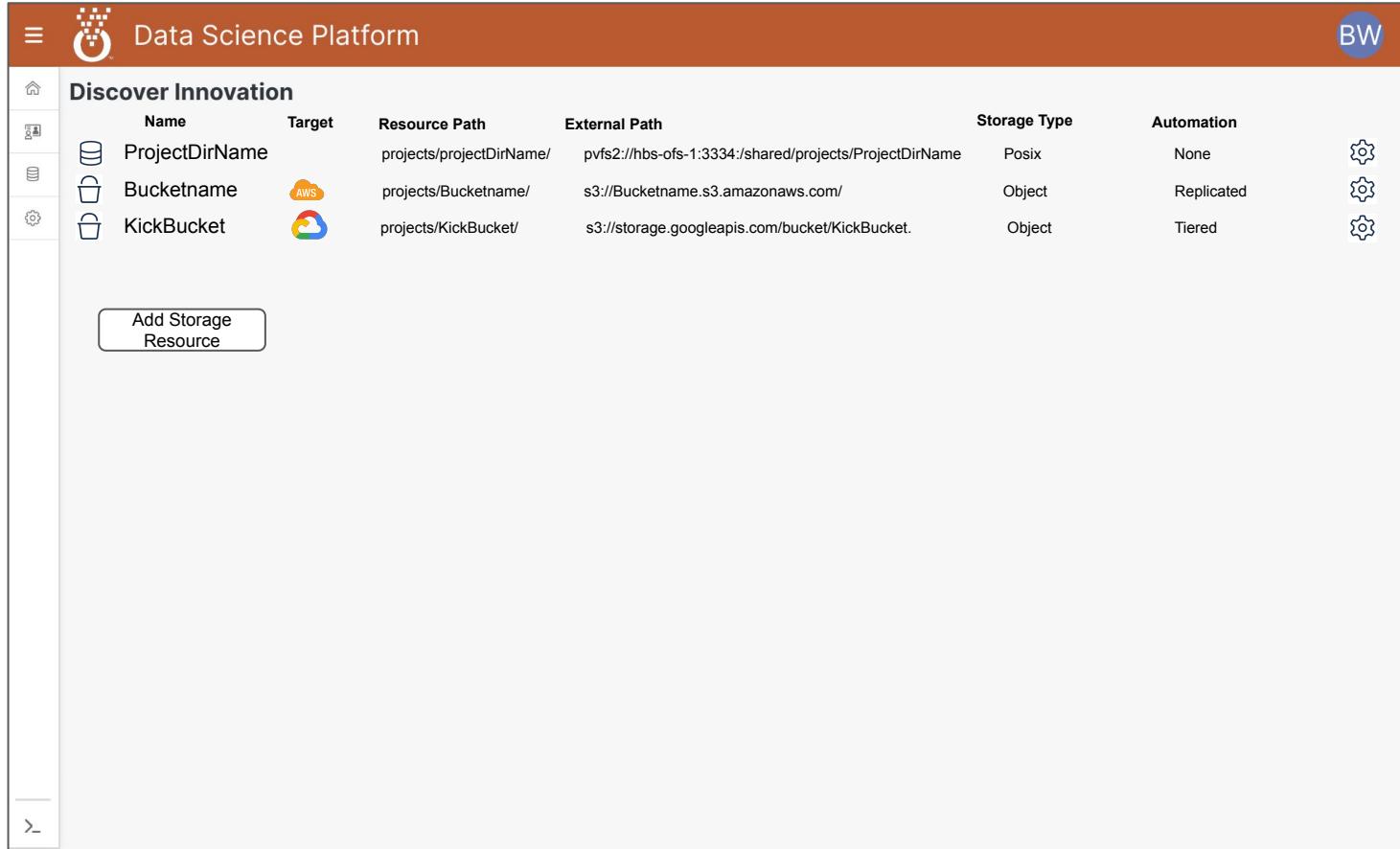
- Desktop**: Cores: 2, RAM: 4, GPU: 0. Status: Available. Buttons: Launch, More.
- VS Code**: Cores: 2, RAM: 4, GPU: 0. Status: Available. Buttons: Launch, More.
- RStudio**: Cores: 2, RAM: 4, GPU: 0. Status: Available. Buttons: Launch, More.
- Jupyter**: Cores: 2, RAM: 4, GPU: 0. Status: Available. Buttons: Launch, More.
- Spyder**: Cores: 2, RAM: 4, GPU: 0. Status: Available. Buttons: Launch, More.
- Stata**: Cores: 2, RAM: 4, GPU: 0. Status: Available. Buttons: Launch, More.
- Spyder2**: Cores: 2, RAM: 4, GPU: 0. Status: Available. Buttons: Launch, More.

Below the discovery grid, there is a section titled "Active Sessions" with a dropdown menu. It shows two active sessions:

- VS Code**: Runtime: 0h 19m, Job Id: 14. Status: Running. Buttons: End, Connect, More.
- Jupyter**: Runtime: 0h 0m, Job Id: 15. Status: Provisioning. Buttons: End, More.

A vertical sidebar on the left features icons for Home, Projects, Data, and Settings, along with a search bar at the bottom.

# Future Storage Collections



The screenshot displays the 'Discover Innovation' section of the Data Science Platform. It lists three storage resources: 'ProjectDirName', 'Bucketname', and 'KickBucket'. Each entry includes its name, target, resource path, external path, storage type, automation status, and a gear icon for configuration.

Name	Target	Resource Path	External Path	Storage Type	Automation	Actions
ProjectDirName		projects/projectDirName/	pvfs2://hbs-ofs-1:3334:/shared/projects/ProjectDirName	Posix	None	
Bucketname		projects/Bucketname/	s3://Bucketname.s3.amazonaws.com/	Object	Replicated	
KickBucket		projects/KickBucket/	s3://storage.googleapis.com/bucket/KickBucket.	Object	Tiered	

**Add Storage Resource**

# Future Collections Access in Storage Manager

The screenshot shows the Data Science Platform Storage Manager interface. The top navigation bar is orange with the title "Data Science Platform". On the far right, there is a blue circular icon with the letters "BW". The main area has a white background and is titled "Discover Innovation". A breadcrumb navigation path is shown: "prj-storage > Folder1 >". On the left, there is a sidebar with icons for Home, Upload, prj-storage, S3 Bucket-1, and GCS Bkt. The "prj-storage" section is expanded, showing two folders: "Folder1" and "Folder2". "Folder1" is selected and expanded, displaying two files: "OmniPasskey.png" and "Screenshot 2023-05-14 at 7.31.42 PM.png". The table columns are "name", "last\_write\_time", "size", "type", and "logical\_path". A callout bubble with a black outline and a light gray background points from the bottom left towards the "GCS Bkt" item in the sidebar. The text inside the bubble is "Additional Storage Collections".

name	last_write_time	size	type	logical_path
OmniPasskey.png	1684165227	3821822	data_object	prj-storage/Folder1/OmniPasskey.png
Screenshot 2023-05-14 at 7.31.42 PM.png	1684165200	205944	data_object	prj-storage/Folder1/Screenshot 2023-05-14 at 7.31.42 PM.png

Additional Storage Collections

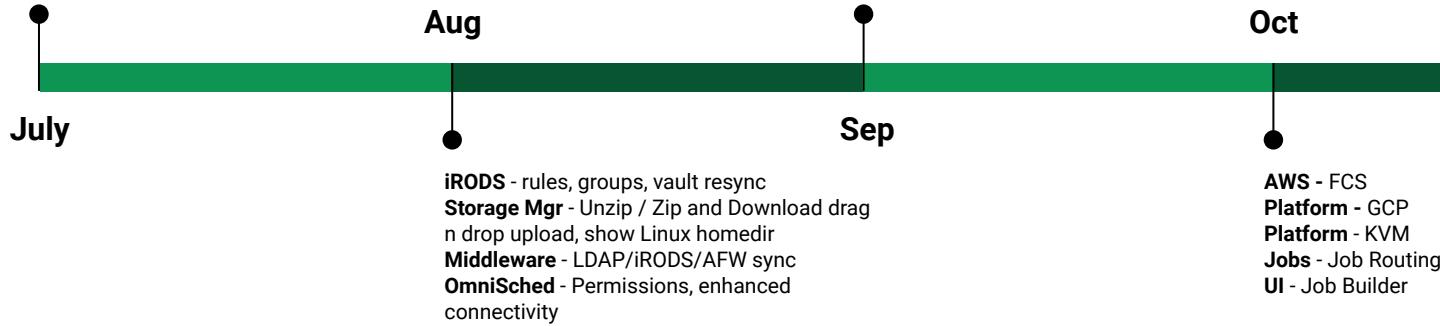
# iRODS: What we're using (so far...)

- iCommands
  - Initialization (default collections, groups, permissions, and metadata)
- REST Client
  - Initialization:
    - Create corresponding iRODS user for each LDAP user
  - Frontend file manager:
    - List files/collections
    - Create collections/files
    - Rename files
    - Upload/download files (stream data)
- NFSRODS
  - Allow apps (e.g., VS Code Server) to directly access iRODS files
- iRODS Rule Language (NREP)
  - Automatically tag collections with custom metadata
- Next
  - OrangeFS MD Syncer (dynamic scratch and linux home sync to iRODS)
    - TBD: How to notify the catalog of file adds, deletes, updates

# Tentative Timeline

**Storage Manager** - Download, Hidden Files,  
Multi-Select, create menu at top  
**Instances** - Start Stop vcpu/ram display in list  
**Project** - directory prefill,  
**Add Launcher** - option in left menu  
**iRODS** - s3 bucket create

**Jobs** - per job scratch, data staging, billing  
tags  
**Launcher** - file search  
**AdminUI** - Initial Admin UI  
**iRODS** - OranegFS Syncer  
**Platform** - local Docker Compute Nodes



# Services

- **Remote Tier 1.5 support**
  - Hand off from HBS to Omnibond to help with:
    - Platform Development
    - Application Integration
    - Applet AI Development
    - Researcher 1 on 1 Support
- **Project Management**
  - Omnibond can optionally provide a portion of a project manager to coordinate the overall project
- **R&D**
  - Cutting Edge Research & Development for future features

# Questions?

**boyd@omnibond.com**

# EUREKA



see the show