Enabling Workflows in Livermore Computing

LC User Meeting December 2020

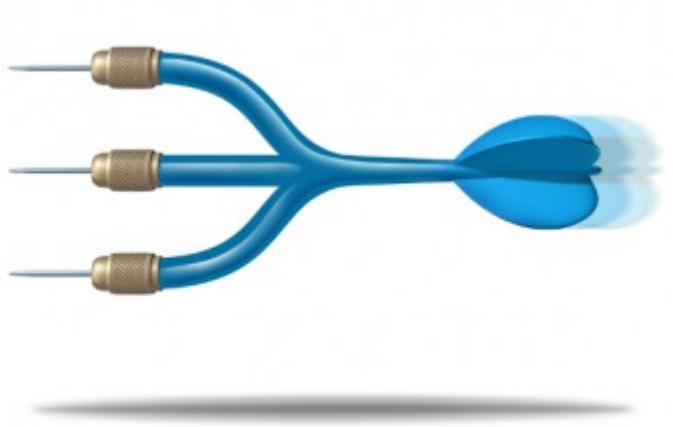
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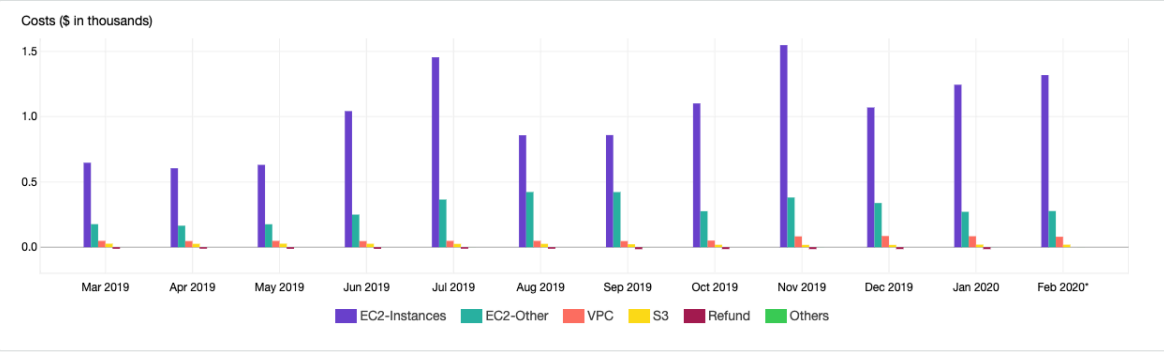
Livermore Computing's Three-Pronged Approach



- Amazon Web Services
- Containers on HPC Systems
- Persistent Data Services Platform

Amazon Web Services

- Leverage AWS for quick and **hopefully** cheap deployments
- Amazon Virtual Private Cloud
- A number of issues/concerns results in not much use.
- A few successful projects using the Amazon Public cloud
  - ZFS on Linux
  - Spack
- LivIT details wrt AWS: https://livcloud.llnl.gov/



AWS has not been a great fit

Containers on HPC systems

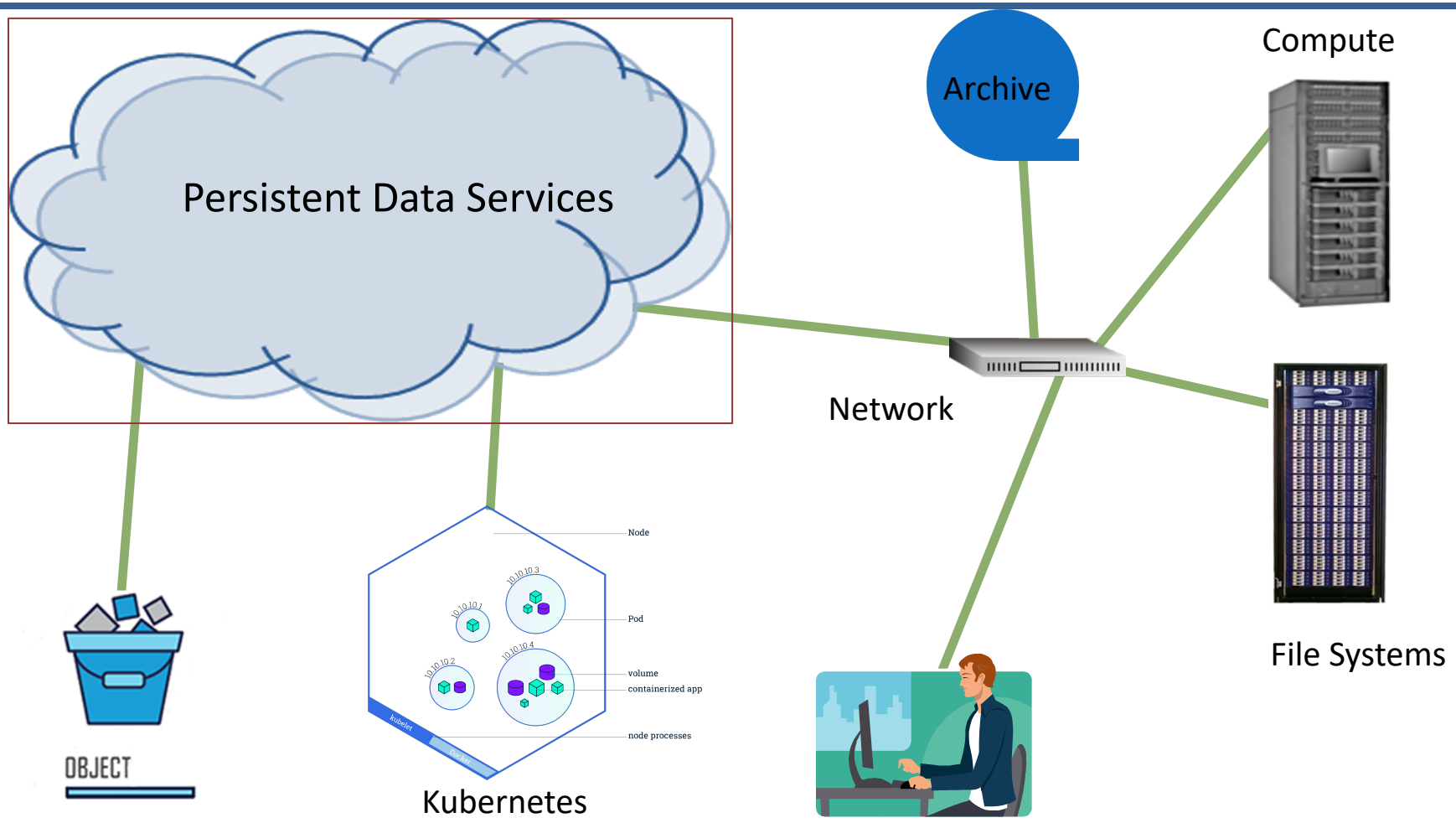


Sierra



Singularity

A Persistent Data Services Platform



LC CZ enclave – RZ system coming soon

A Persistent Data Services Platform Goals

- Deploy a production quality scientific focused cloud platform in our Collaboration Zone.
- Identify both customer and internal to LC applications that can be ported and deployed onto this platform.
- Deploy an Object Storage system that is usable both by the Persistent Data Service Platform and from the HPC systems.

A Persistent Service Platform: Technologies

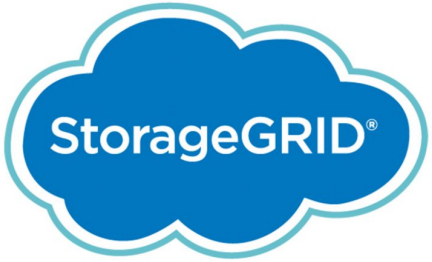
- Kubernetes
  - RedHat OpenShift
- Persistent Storage
  - NetApp Trident – AFF Filers
- Object Storage
  - NetApp – Storage Grid



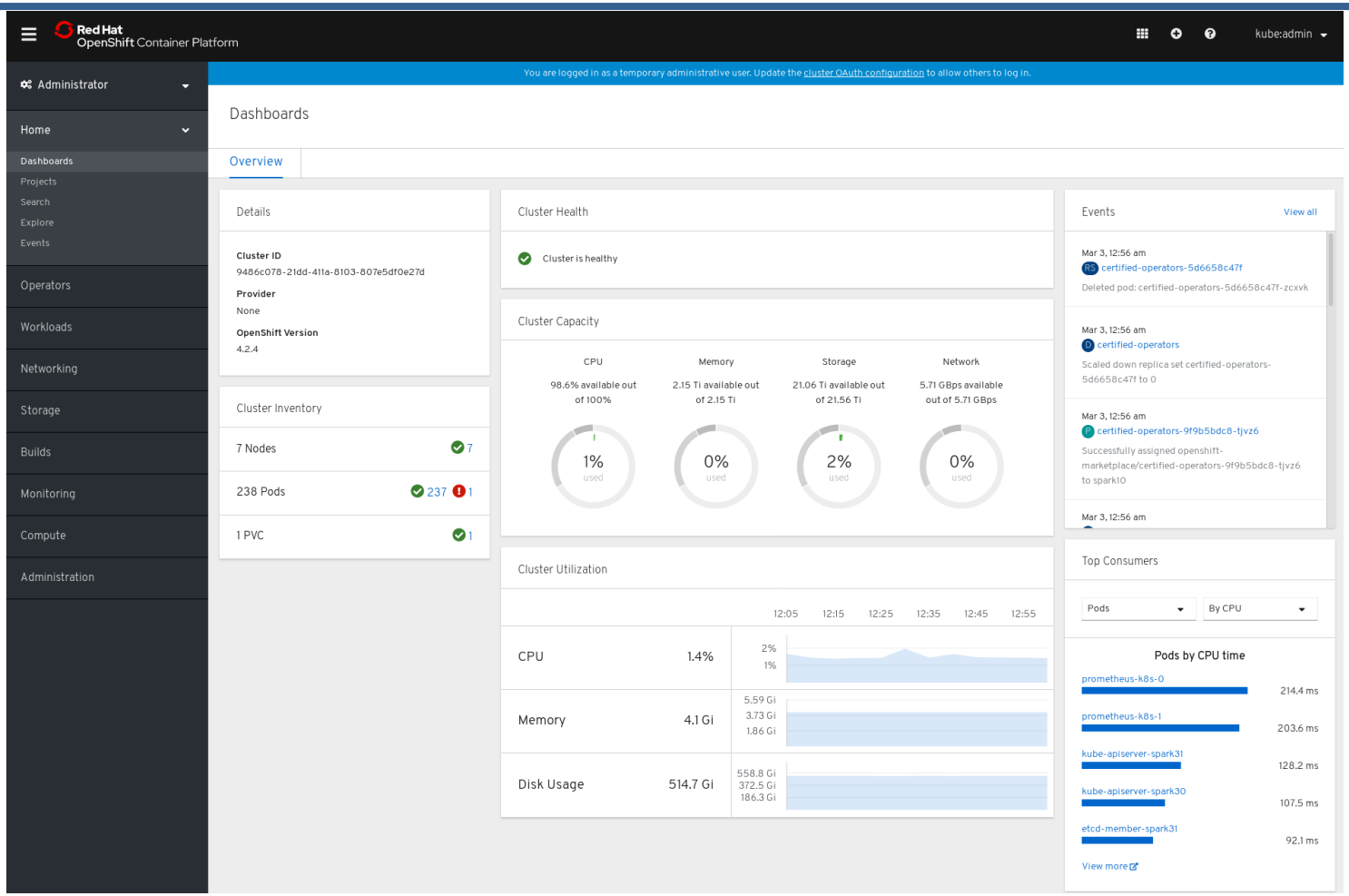


OPENSHIFT





A Persistent Data Services Platform: Openshift



A Persistent Data Services Platform: Simple Deployments

- Anticipated first apps to deploy – database type systems









More to come

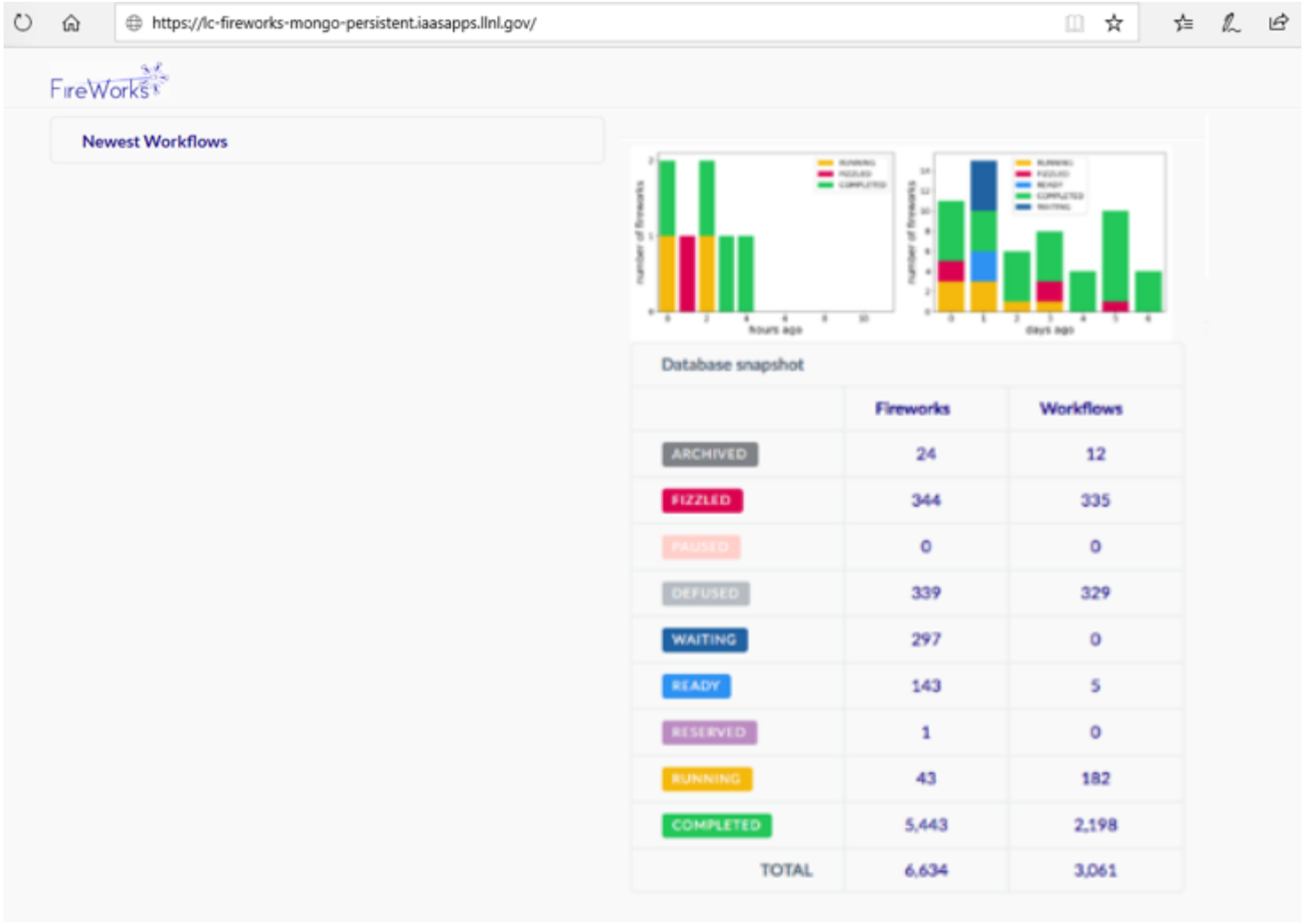
A Persistent Data Services Platform: Workflow Deployments

- Investigating and working with customers on various workflow frameworks.
  - Merlin (LLNL)
  - Sina (LLNL)
  - FireWorks
  - Apache Airflow
  - AiiDA (Automated Interactive Infrastructure and Database for Computational Science)



What workflow tools are you interested in?

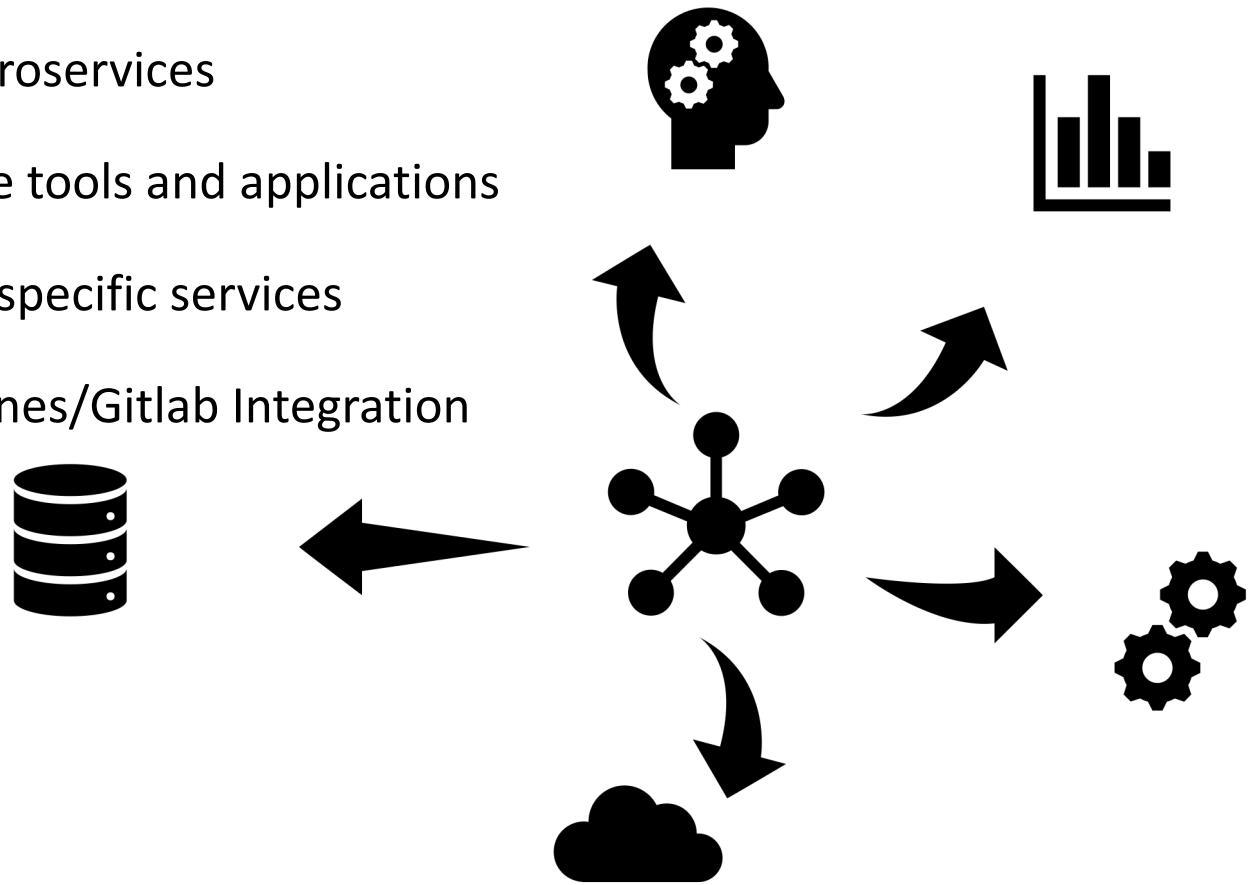
Fireworks Web Interface – Workflow Status



	Fireworks	Workflows
ARCHIVED	24	12
FIZZLED	344	335
PAUSED	0	0
DEFUSED	339	329
WAITING	297	0
READY	143	5
RESERVED	1	0
RUNNING	43	182
COMPLETED	5,443	2,198
TOTAL	6,634	3,061

A Persistent Data Services Platform: Advanced Deployments

- Suite of Microservices
- Data Science tools and applications
- Application specific services
- CI/CD pipelines/Gitlab Integration



Work in progress

Challenges

- Multi-Tenancy Security
- Security compliance
- Knowledge base
- Rapid pace of change







More Information



- https://lc.llnl.gov/cloud/
- lc-hotline@llnl.gov or call (925) 422-4531.



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