Reproducible Analysis Workflows on Heterogeneous Resources

Kenyi Hurtado, representing the SCAILFIN team

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Motivation

Major Multi-User Research Facilities involve the comparison of data collected from experiments with “synthetic" data, produced from computationally-intensive simulations.

Comparisons of experimental data and predictions from simulations are abstractions of the specific data analysis techniques developed by the respective communities over several decades. E.g.:

Motivation

Many of these data analysis tasks are often conducted manually or through *ad hoc scripts* that might not be well maintained, making reproducibility and reusability difficult. Many of these tasks do have a well-defined workflow that make automation possible, though.

REANA was created (in collaboration with DASPOS, DIANA and CERN) to address the reproducibility and reusability of the analysis pipeline.

reana

Reproducible research data analysis platform

Motivation

In parallel:

Interest in leveraging Machine Learning (ML) and Artificial Intelligence (AI) techniques, to enhance the analysis of data from these facilities.

In particular, its application with emergent **Likelihood-Free Inference (LFI) techniques** when the predictions for the data are implicitly defined by the simulation, often leading to an intractable likelihood function. This can apply to analysis of data from LHC, LIGO, etc, but such Likelihood-Free algorithms have so far been **implemented mostly on individual machines and in ad hoc scripts because the training workflows are very complicated.**

Introduction

SCAILFIN: Scalable CyberInfrastructure for Artificial Intelligence and Likelihood Free Inference

The SCAILFIN project aims to deploy artificial intelligence and likelihood-free inference techniques and software using scalable cyberinfrastructure (CI) that is developed to be integrated into existing CI elements, such as the **REANA** system, to work on **HPC facilities**.

PI's: Mark Neubauer, Dan Katz Kyle Cranmer, Heiko Mueller Mike Hildreth

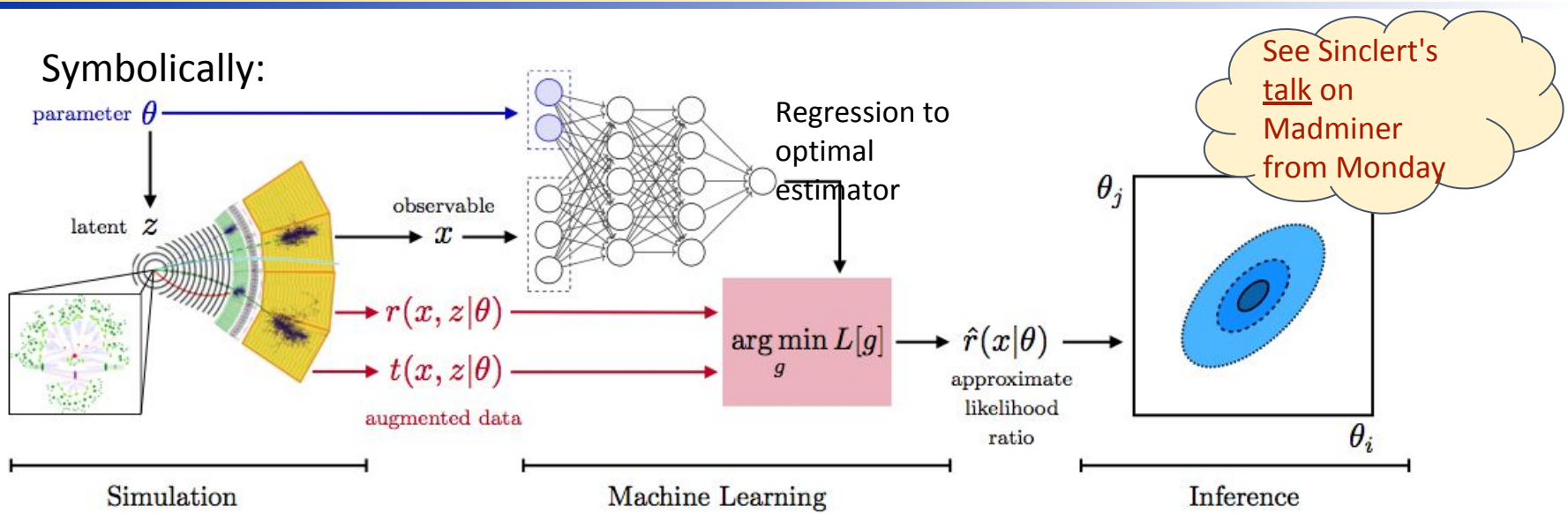
NYU

UNIVERSITY OF NOTRE DAME

Simulation-Based Likelihood Free Inference

arXiv:1805.12244 - PRL
arXiv:1805.00013 - PRD
arXiv:1805.00020 - physics.aps.org/articles/v11/90

Symbolically:



Estimation of optimal estimator lends itself to ML methods:

- Training data derived from simulations
- Can be guided by optimal sampling based on phase space density of generator, sensitivity to physics under study

Today's Topic

SCAILFIN goals

- …
- **Extending the REANA** platform to allow remote **submission** of workflows to **HPC facilities.**
- …

SCAILFIN components

- **REANA** as the Cyber Infrastructure element to deploy AI and Likelihood-Free inference techniques.

- **VC3** (Virtual Clusters for Community Computation) in order to scale REANA to HPC resources.

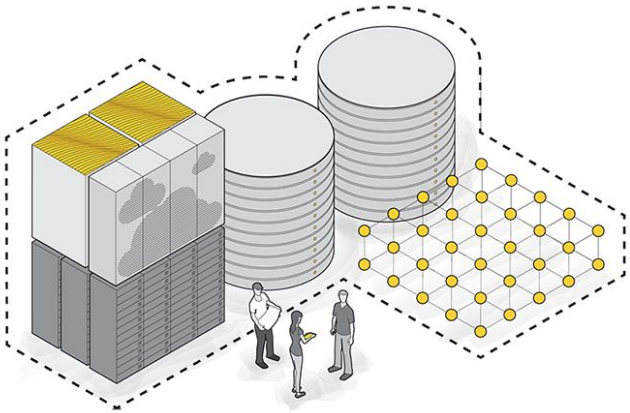
First, a brief overview of these 2 components...

reana: Reproducible Research Data Analysis Platform

Components

- Two major components each consisting of many sub-components
  - reana-client: User facing component.
    - Accepts workflows and and is used as interface to entire REANA system (for user).
  - reana-cluster: Workhorse.
    - Consists of many small pieces which handle workflows, dish out jobs, coordinates results, can be thought of as the job scheduler. Jobs are scheduled via Kubernetes.

VC3: Virtual Clusters for Community Computation



VC3: A platform for provisioning cluster frameworks over heterogeneous resources for collaborative science

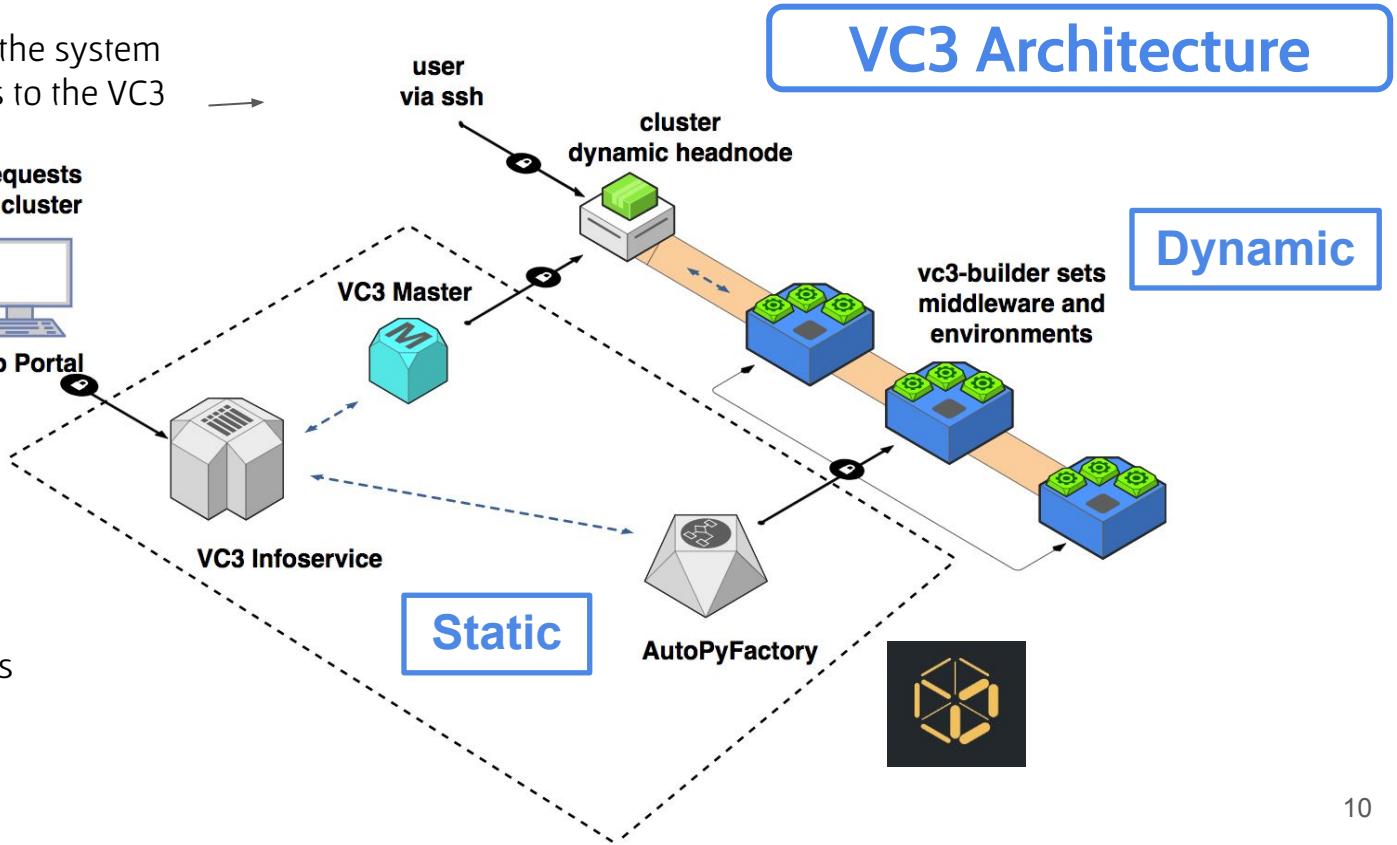
- Overlays "cluster" environment on top of diverse resource allocations
- Similar to cloud services that allow you to stand up clusters, but on "your" resources

https://www.virtualclusters.org

VC3

VC3: Virtual Clusters for Community Computation

User adds an SSH public key to the system that will be used to grant access to the VC3 dynamic headnode



- User defines an allocation
- Selects middleware configuration
- VC3 infrastructure creates VC3 headnode and configures resources
- Workers on compute nodes communicate with VC3 headnode to receive compute workloads

VC3: Virtual Clusters for Community Computation

Features

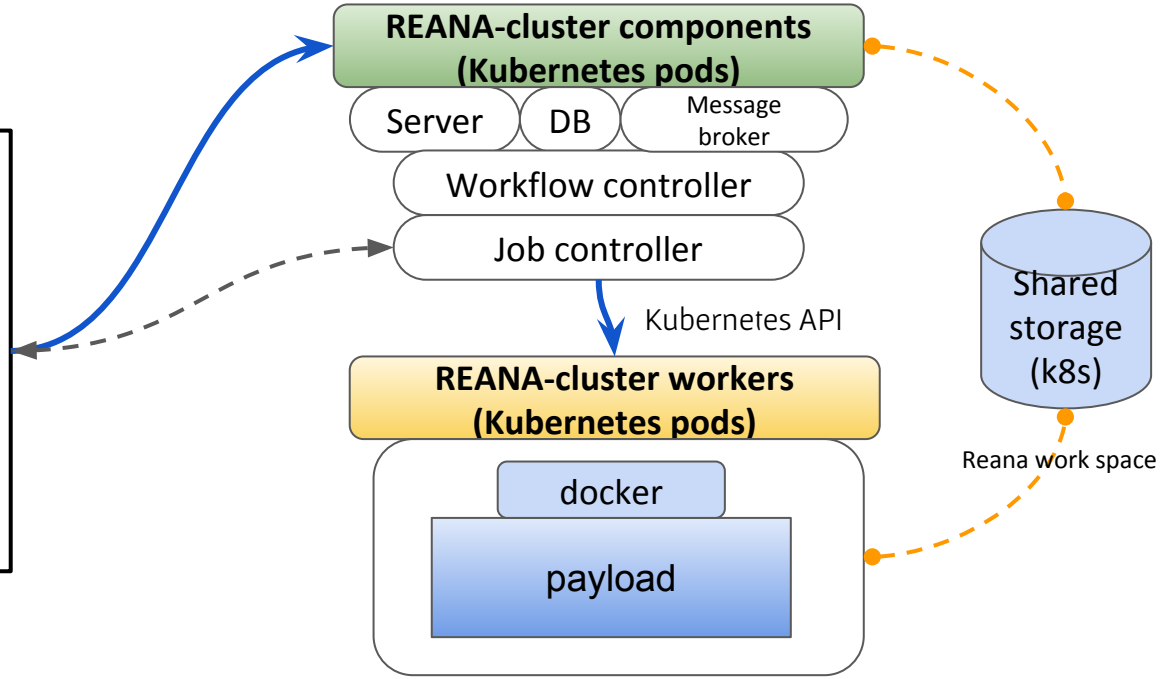
- The user can select its own middleware for submission (E.g.: HTCondor, WorkQueue, Spark, REANA+HTCondor).
- It doesn't matter what the resource target batch system is (as long as it is supported by glite/blah, the translation layer for submission).

E.g.: Torque (Blue Waters), SLURM (NERSC, PSC–Bridges, Stampede2), HTCondor, LSF, SGE, PBS.

REANA cluster / Workforce Infrastructure
Standard kubernetes deployment

CERN cloud/Openstack

- Openstack with container orchestration engine (coe) working with Kubernetes
- REANA-cluster can be deployed via kubernetes, or can use one deployed accessible for CERN users



Container technologies in HPC facilities

- HPC centers are no strangers to the user's need for containers nowadays.
  - Docker is not an option though (security reasons)
  - User-space container technologies preferred instead. E.g.:
    - Singularity: PSC, Stampede, Comet, etc.
    - Shifter: NERSC, Blue Waters
    - Charlie Cloud: Unprivileged containers using linux user namespaces (linux 4.4+)
    - All options above have mechanisms to run/convert docker images

SCAILFIN Developments to make this work:

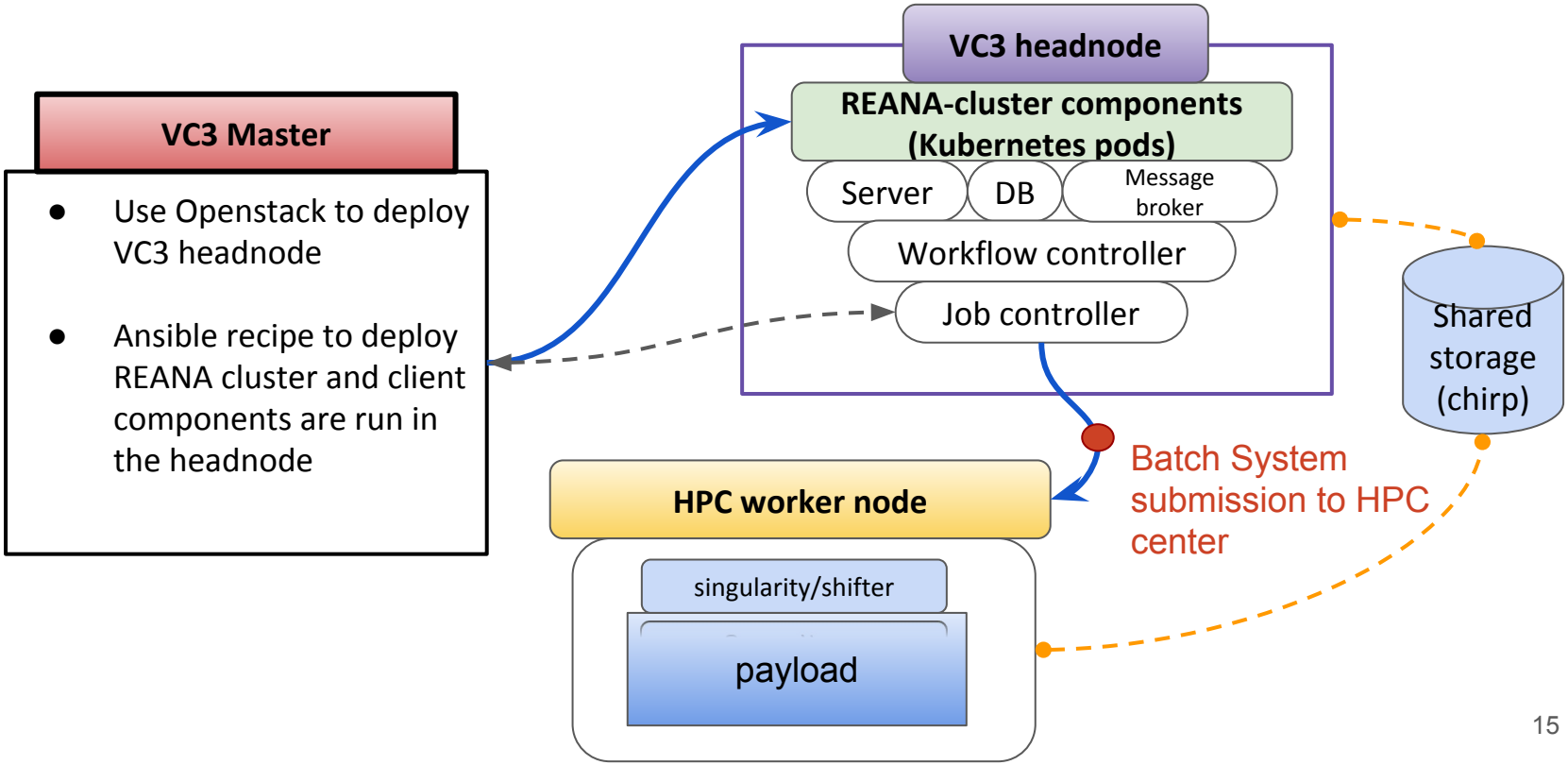
REANA Modifications:

- REANA requires some form of docker supporting container technology
  - Singularity and Shifter support finished.
- REANA expects to submit to a kubernetes cluster
  - Added support for VC3 specialized HTCondor submissions through a modified reana-job-controller and a job_wrapper for every workflow step.
  - The modified reana-job-controller submits each workflow step to a local condor scheduler
- Job Wrapper Auto-detection of container technology for workflow steps. (shifter, singularity)

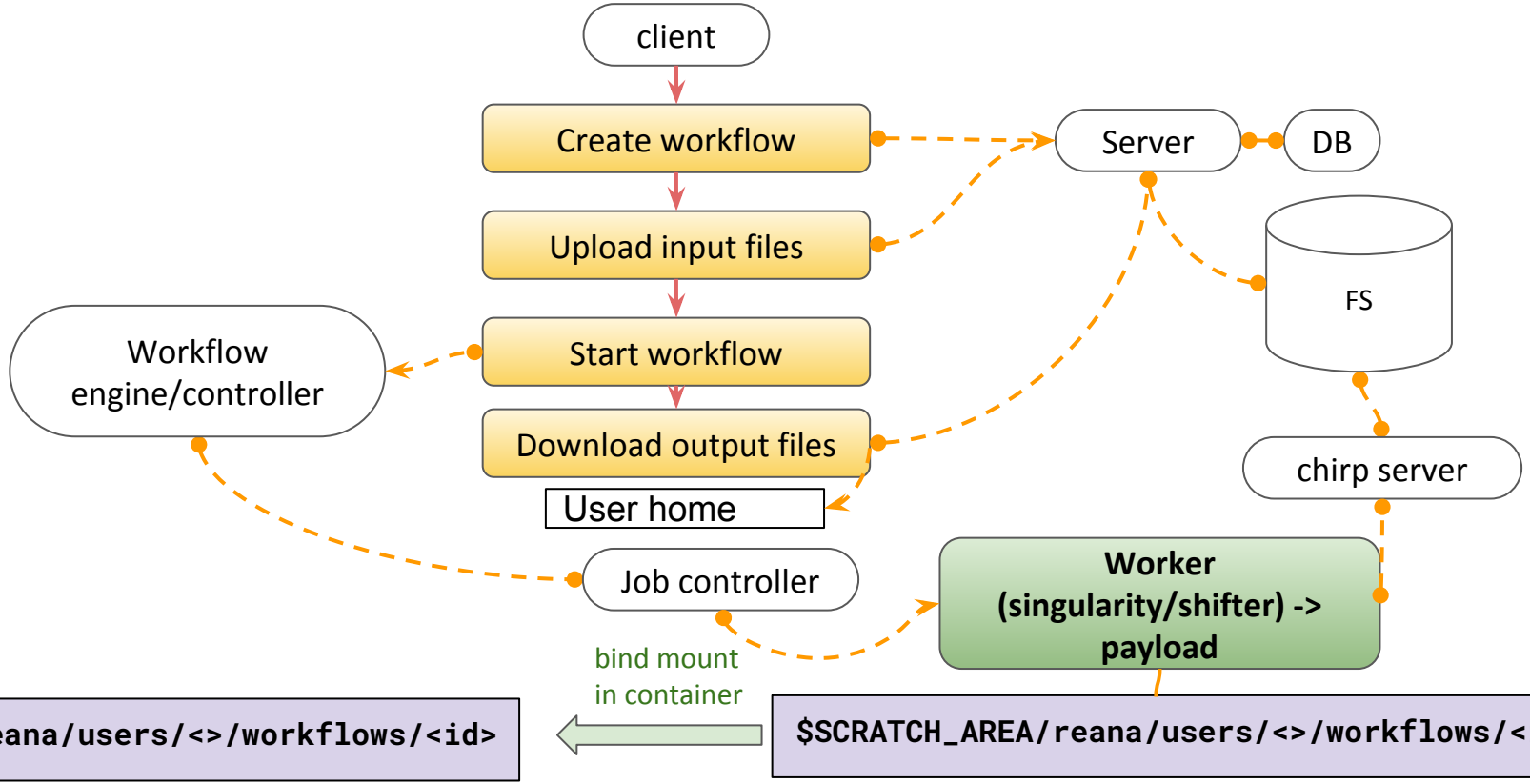
VC3 Modifications:

- Cluster template for REANA+HTCondor
  - Uses the standard HTCondor template as the base to create a condor pool that sends jobs to HPC resources, translating the job to the corresponding batch system submission syntax via bosco.
  - Deploys Kubernetes via minikube
  - Deploys the REANA cluster and client and set up the environment, so the user can interact with them as soon as the VC3 headnode is created.
- Support for GSI-SSH and SSH proxy
  - For Sites like NERSC, BW, etc.

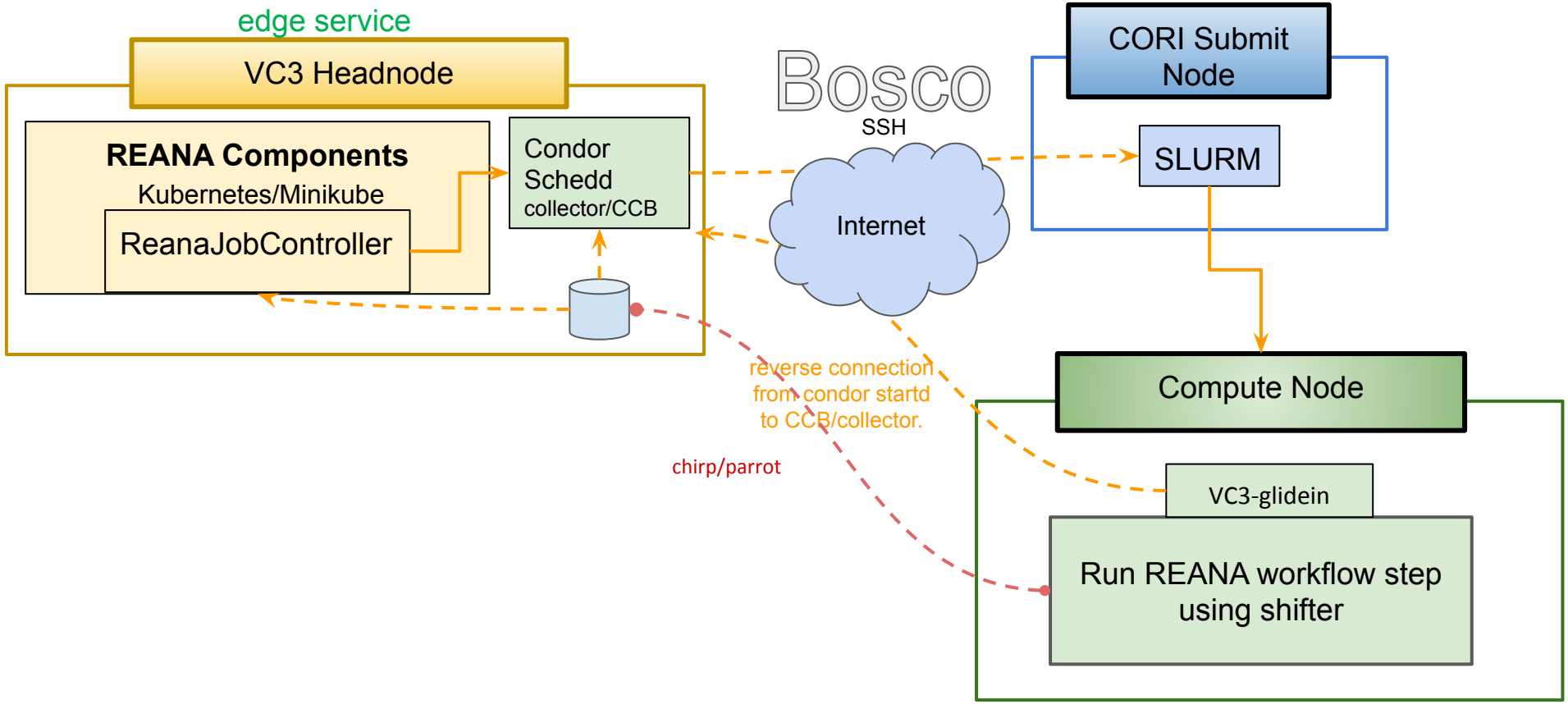
REANA cluster / Workforce Infrastructure SCAILFIN deployment



REANA client / User's perspective
Starting a workflow



SCAILFIN on NERSC



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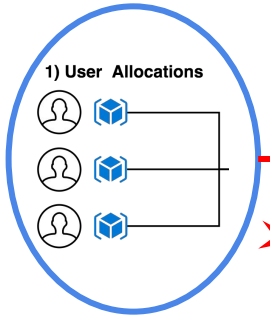
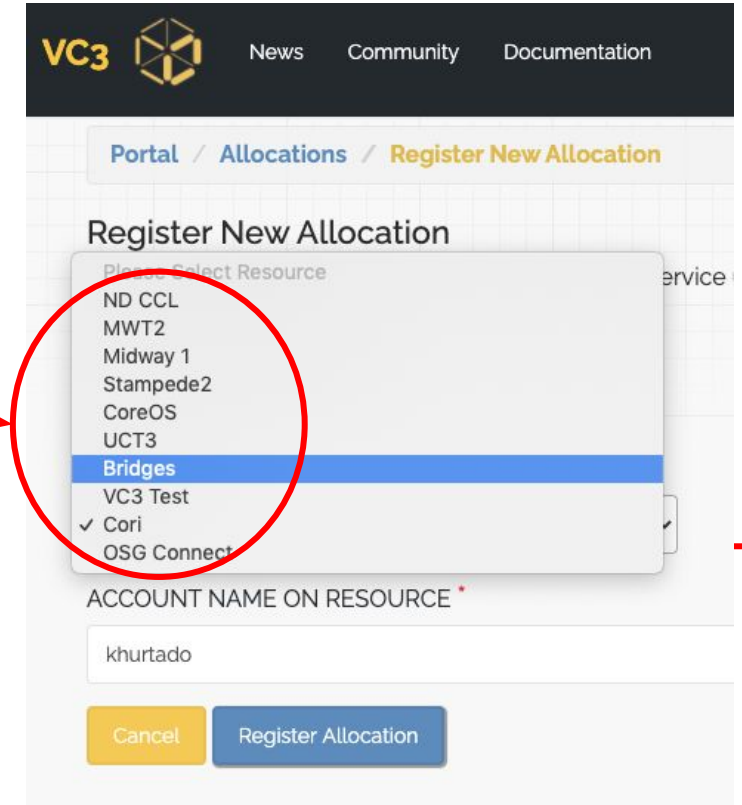
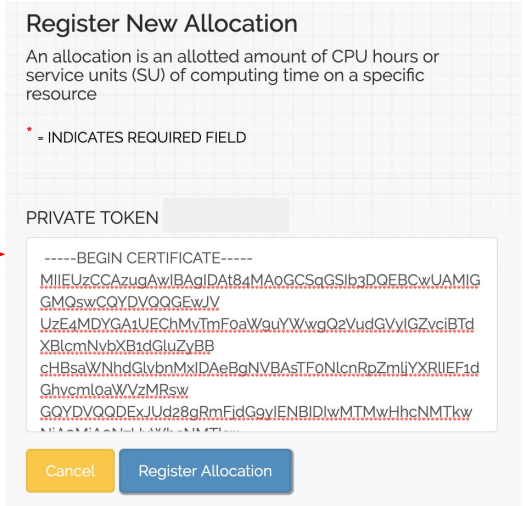
Creating A REANA cluster on VC3

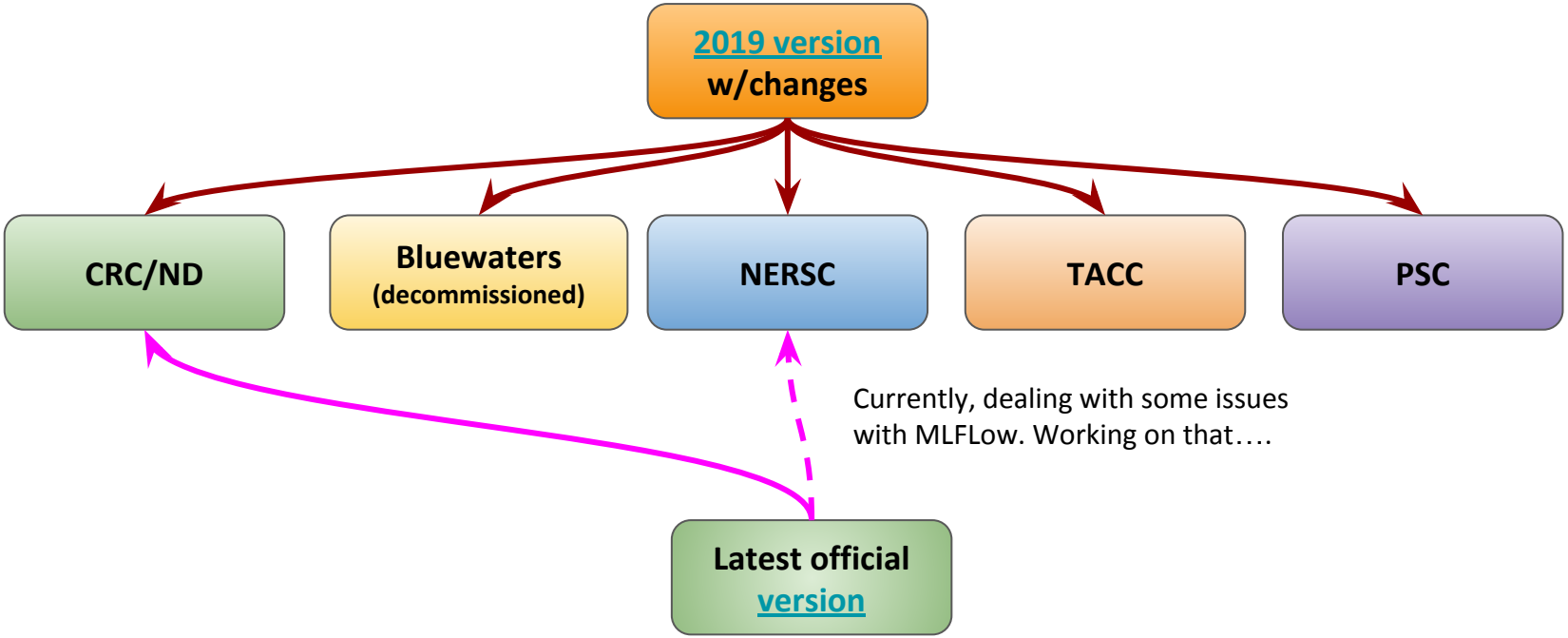





```
$~> ./sshproxy.sh -s weekly -u khurtado -o sshproxy
Enter the password+OTP for khurtado:
hurtadoa@h2ologin1:~> cat sshproxy
```



Running madminer on HPC sites



Conclusions, next steps

- We have successfully managed to run the madminer workflow on HPC sites.
- Current version of VC3+REANA, available on REANA 0.6.0

- Move some of the submission infrastucture from VC3 to REANA, directly
- Currently, working on some MLFlow issues to adapt latest version

Supported by NSF Award OAC-1841448

Links

- SCAILFIN Source code:
  - SCAILFIN's modified RJC
    https://github.com/scailfin/reana-job-controller/tree/job_manager
  - REANA
    - https://github.com/reanahub
  - VC3
    - https://github.com/vc3-project
- Websites
  - https://www.virtualclusters.org
  - http://www.reanahub.io/

Notre Dame Contacts = Main developers

- Kenyi Hurtado
  - khurtado@nd.edu
- Cody Kankel
  - ckankel@nd.edu

Thanks!

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Backup slides

Notre Dame CCTools

- **Chirp:** Lightweight user-level FS for collaboration across distributed systems such as clusters, clouds, and grids. An ordinary user can share storage space and data without requiring any sort of administrator privileges anywhere. Supports multiple authentication mechanisms.
- **Parrot:** A tool for attaching existing programs to remote I/O systems through the filesystem interface. E.g.:
  - `$ parrot_run vi /chirp/server.nd.edu/mydata`
  - `$ parrot_run cp /path/file /chirp/server.nd.edu/file`

Notre Dame CCTools

- **Chirp:** Integrated with HTCondor. Adding "+WantIOProxy=True" creates a chirp server than can be used between the VC3-headnode and the workers. It also takes care of the authentication.

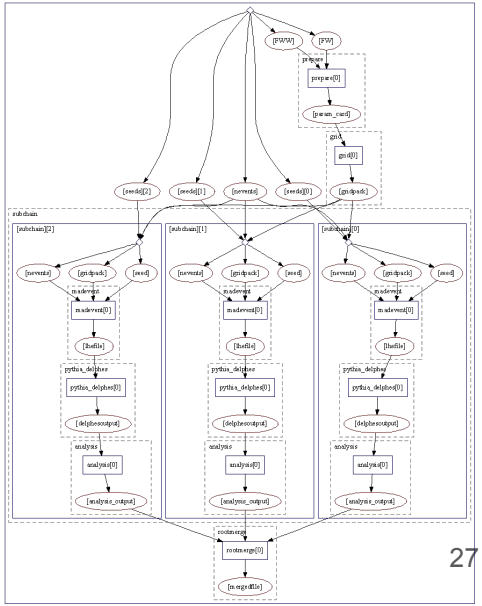
- **Parrot:** Static version available, runs on any x86 architecture. Can be used to interact with the chirp server created by HTCondor.
  - Note HTCondor has its own chirp client, but it doesn't e.g.: recursive copy directories.

reana: Reproducible Research Data Analysis Platform

Features

- Allows creation of tightly defined, container encapsulated workflows
- Built with commodity pieces
- Purpose is to allow complete reproducibility
- Sharing workflows is as easy as sharing a specification
  - (and inputs!)

- Different workflow engines supported. e.g.:
  - CWL (Common Workflow Language) : https://www.commonwl.org/
  - Yadage (YAML based adage): https://yadage.readthedocs.io

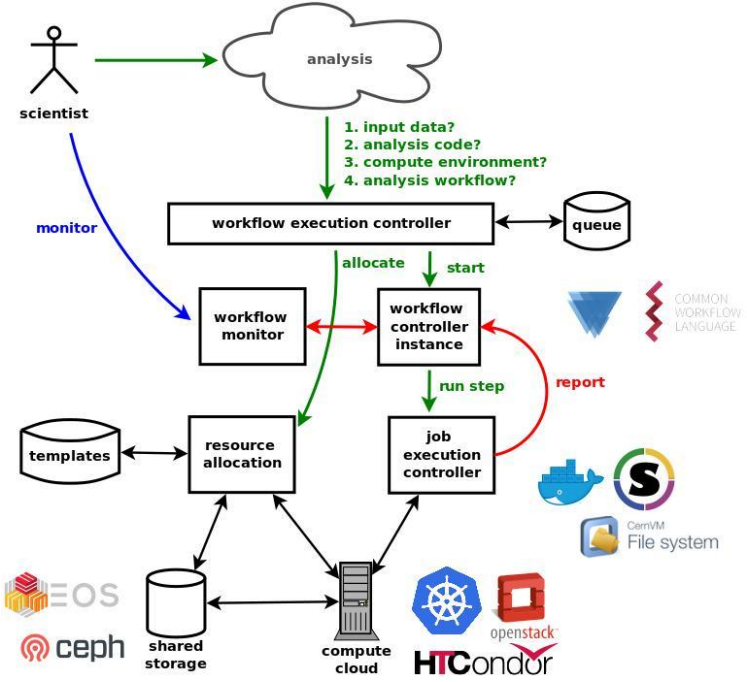


reana: Reproducible Research Data Analysis Platform

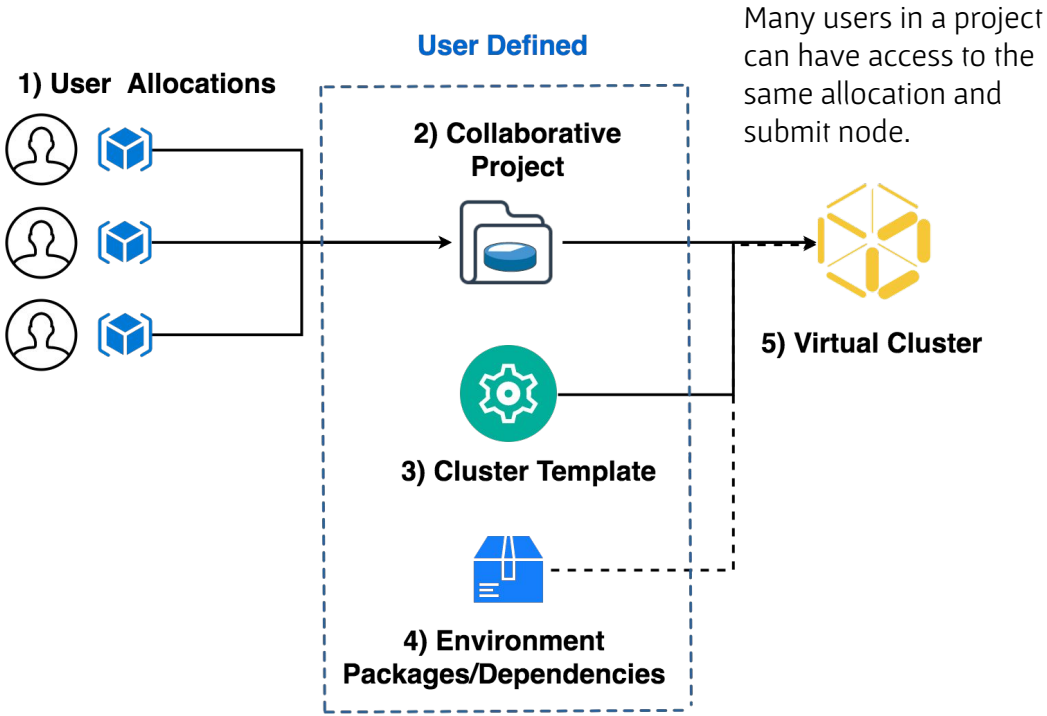
Process

1. Create workflow specification
   (Yadage, CWL, Serial)
2. Upload workflow and inputs to REANA cloud
3. Start workflow
4. Download / pull down results
5. Share workflow specs with others

Architecture

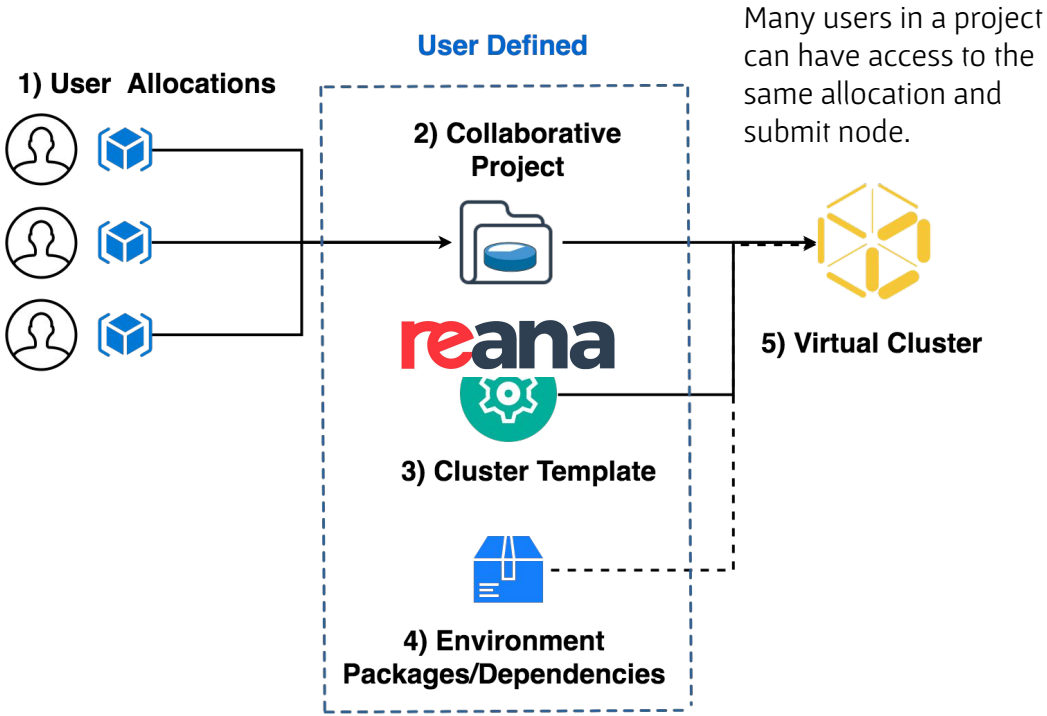


Implementation: A REANA Cluster Template for VC3



Many users in a project can have access to the same allocation and submit node.

Implementation: A REANA Cluster Template for VC3



Many users in a project can have access to the same allocation and submit node.

Using REANA + VC3 on Blue Waters*

Blue Waters cluster:

- Batch system: Torque
- Container technology: Shifter
- Authentication mechanisms:
  - Multi-factor authentication (Password + RSA token)
  - GSI-SSH tokens

Virtual cluster created on top of Blue Waters:

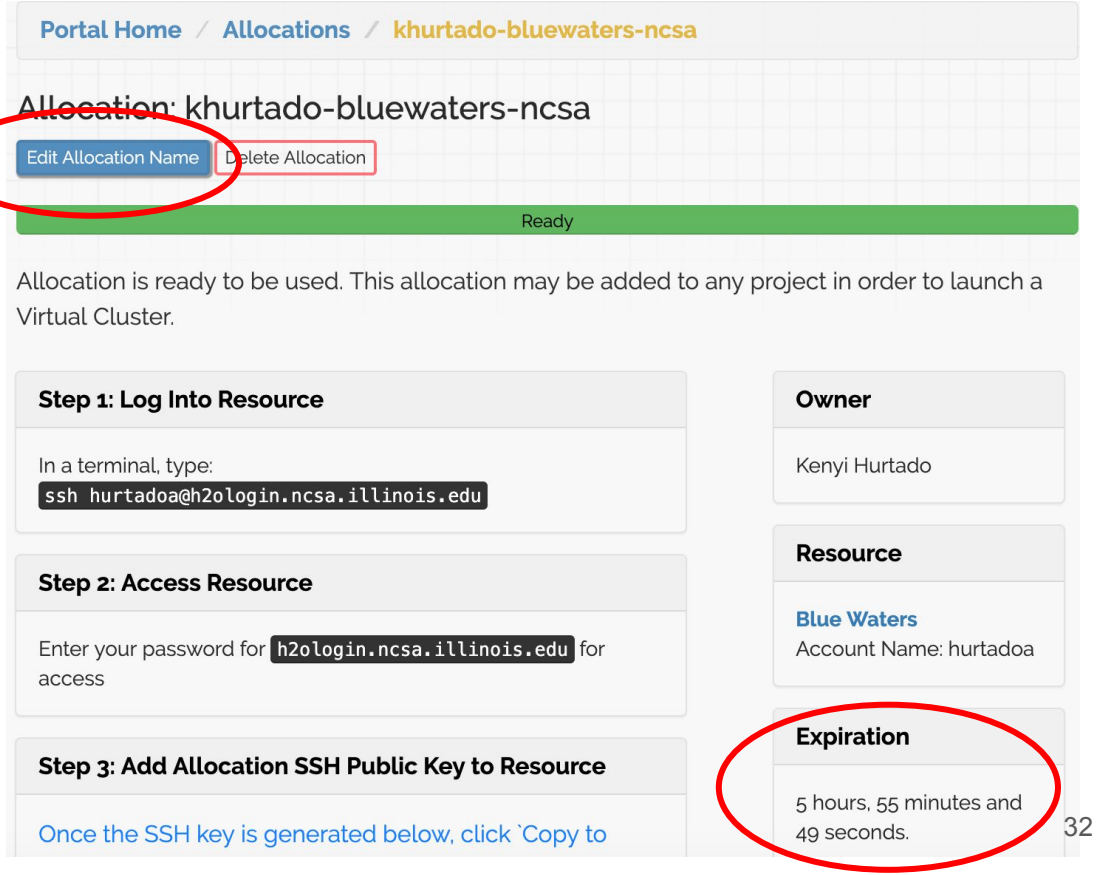
- VC3 Submit node with kubernetes (via minikube) and a REANA cluster deployed on the fly.
- HTCondor as the middleware
- VC3 authenticates with Blue Waters via GSI-SSH

*Note: Infrastructure worked out of the box on other resources such as the ND HPC Cluster and XSEDE/Pittsburgh

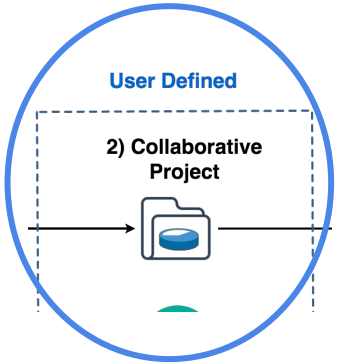
Allocation authentication mechanisms

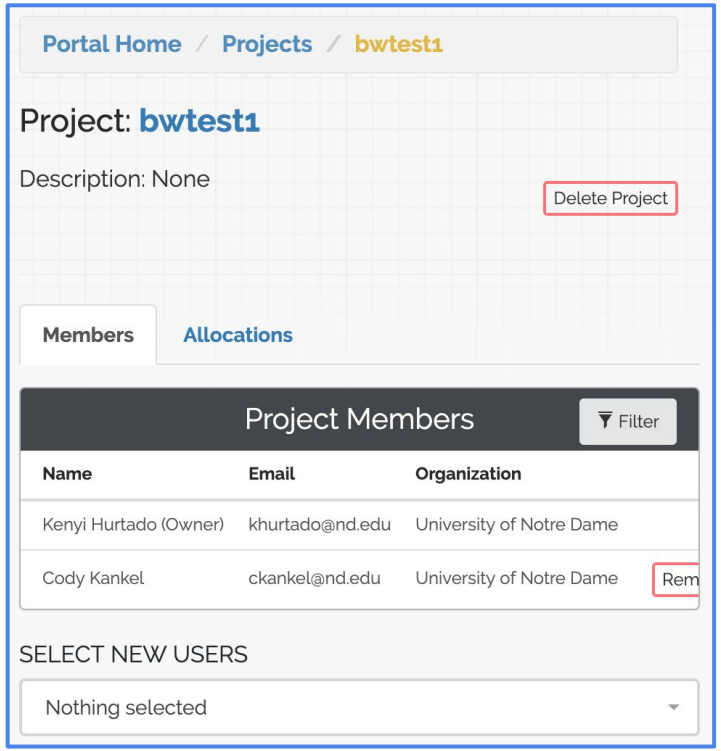
The auth mechanisms available in VC3 are:

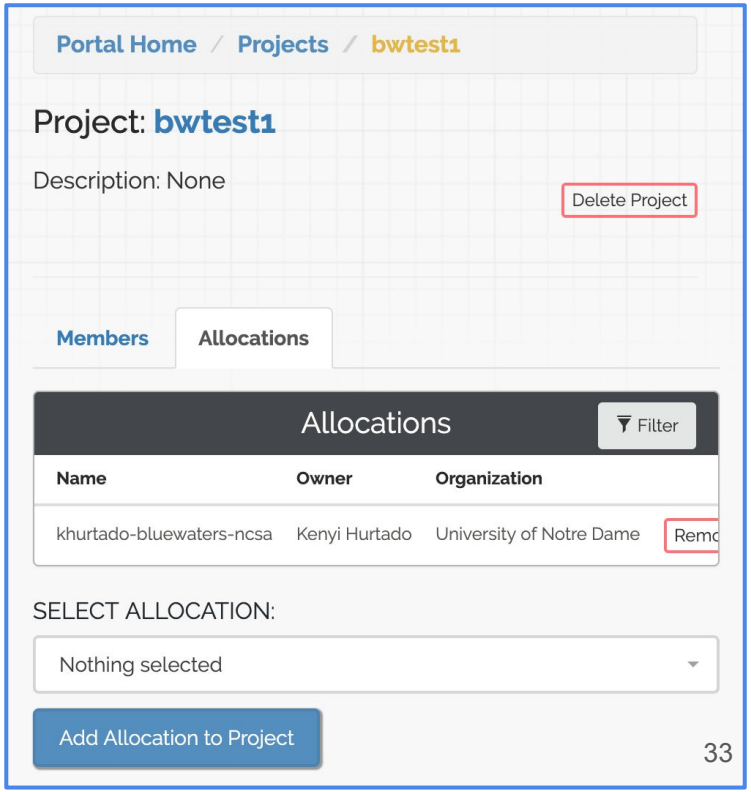
- SSH keys
- GSI tokens
  - Available on XSEDE HPC Systems
  - Requires renewal. The website shows when the proxy expires and the "Edit Allocation Name" button allows users to change
  - Some HPC centers have procedures to increase the default 12 hours expiration time to e.g.: 10 days (NERSC case, and previously done at BW)
- SSH proxy
  - NERSC



Creating A REANA cluster on Blue Waters







Creating A REANA cluster on Blue Waters

Launch New Virtual Cluster

Project: bwtest1

* = INDICATES REQUIRED FIELD

VIRTUAL CLUSTER NAME (A-Z, 0-9, _ AND -)*

reanabwv1

CLUSTER TEMPLATE FRAMEWORK *

REANA+HTCondor

NUMBER OF COMPUTE WORKERS: *

2

ENVIRONMENT

Select Environment

ALLOCATIONS*

khurtado-bluewaters-ncsa

EXPIRATION

If not specified, expiration defaults to 6 hours from launch, when your virtual cluster will automatically be terminated.

HOURS:

98

Cancel | Launch Virtual Cluster

Creating A REANA cluster on Blue Waters

My Virtual Clusters

Filter

Name	Project	Head Node	Workers	State	Cluster Template
khurtado-ndvc1	scailfin-dev	128.135.158.232	3 Requested 3 Running 0 Queued 0 Error	Running All requested compute workers are running.	reana+htcondor
khurtado-reanabwv1	bwtest1	128.135.158.188	2 Requested 2 Running 2 Queued 0 Error	Running Requesting 0 less compute worker(s).	reana+htcondor

End result is a REANA cluster deployed on the VC3 headnode

Components are deployed via Kubernetes (minikube)

```
(reana) [khurtado@khurtado-reanabwv1 ~]$ reana-cluster status
COMPONENT             STATUS
job-controller        Running
server                Running
db                    Running
workflow-controller   Running
message-broker        Running
REANA cluster is ready.
(reana) [khurtado@khurtado-reanabwv1 ~]$ kubectl get pods
NAME                                                      READY   STATUS      RESTARTS   AGE
batch-serial-7e79ee48-036f-4049-87ee-a3dc66d8a1da-tl7zd   0/1     Completed   0          5h54m
db-69744557df-wg4mt                                       1/1     Running     0          5h55m
job-controller-5c7f4c8b4f-sgnj6                           1/1     Running     0          5h55m
message-broker-b7d66cf55-m9p4n                            1/1     Running     0          5h55m
server-58dc985c77-n2qpn                                   2/2     Running     0          5h55m
workflow-controller-668f69d4bc-x62w7                      2/2     Running     0          5h55m
```

VC3: Virtual Clusters for Community Computation

Constraints

- At present, workers need outgoing network connection for a virtual cluster to work.
  - So, resources like ALCF/Theta are out of the scope with this approach.
  - But e.g.: XSEDE resources like NERSC, Blue Waters, Stampede or PSC-Bridges do meet the outgoing network requirement for example.