Kubernetes for GPU Powered Machine Learning Workloads in Academia

The architecture, workload use cases, and open issues

John-Paul Robinson, HPC Architect, Manager, UAB

Camille Rodriguez, Field Engineering Manager, Canonical

THE UNIVERSITY OF ALABAMA AT BIRMINGHAM.

CANONICAL ubuntu

Kubernetes for GPU Powered Machine Learning Workloads in Academia

KubeCon | CloudNativeCon

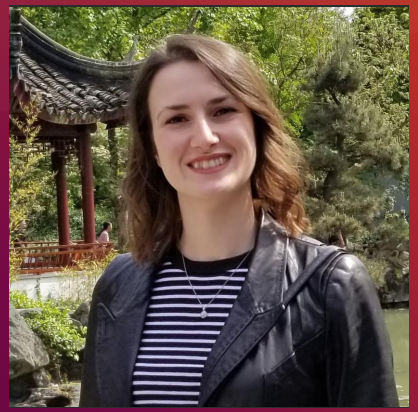
North America 2022

BUILDING FOR THE ROAD AHEAD

DETROIT 2022

October 24-28, 2021

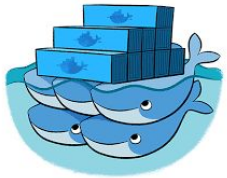
John-Paul Robinson
HPC Architect, Manager
UAB



Camille Rodriguez
Field Engineering Manager
Canonical

Project Overview

- VM based infrastructure already available (Openstack)
- Interest in centralizing work done in containers (laptops, docker swarm, etc.)
- Opportunity to offer a dedicated K8s platform to users
- Collaboration with Canonical to get this done

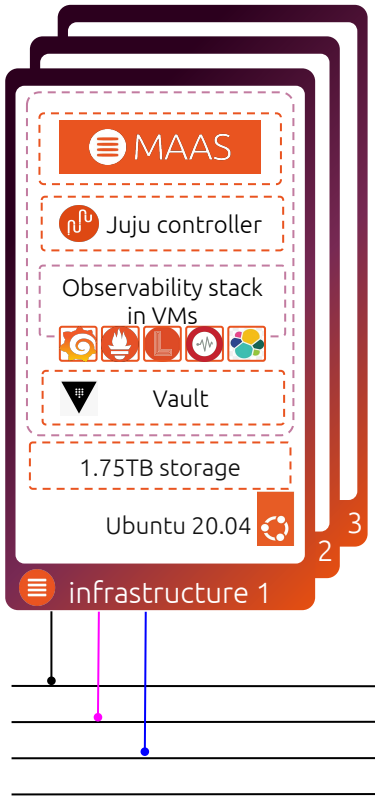


Agenda

- Kubernetes architecture
  - Integrations
- UAB use cases
  - Research workloads
  - ML training
  - CI pipelines
- Research infrastructure
- Future directions

Kubernetes Architecture

Kubernetes Architecture



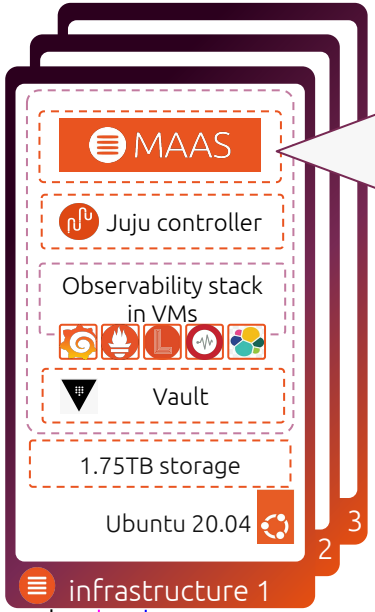
IPMI

Management network

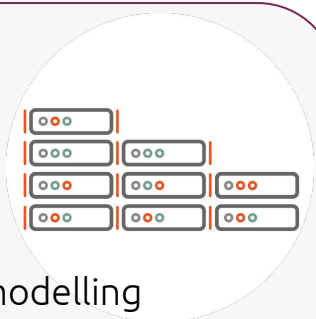
Kubernetes Cluster / API

Storage access

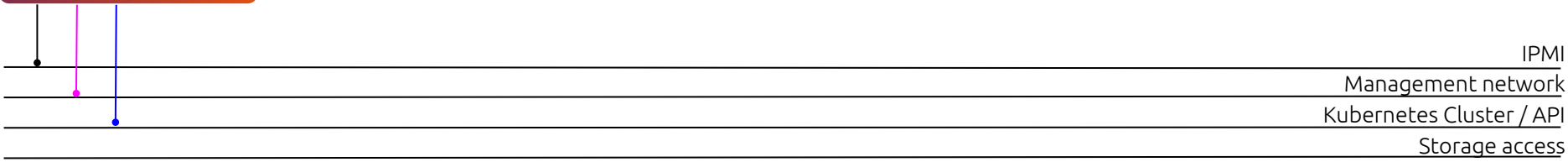
Kubernetes Architecture



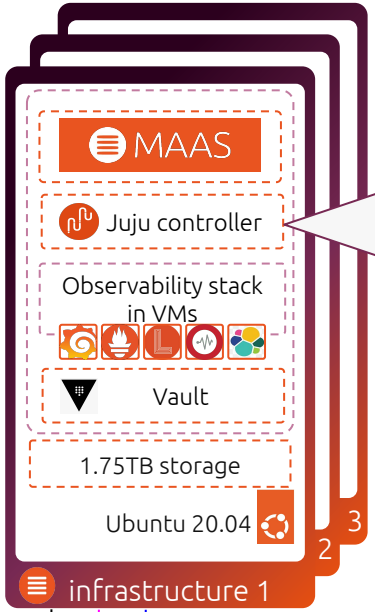
Metal-As-A-Service



- Bare Metal Provisioning
- Asset inventory
- Hardware, storage and network modelling
- Deployment & configuration of physical machines
- KVM & LXD

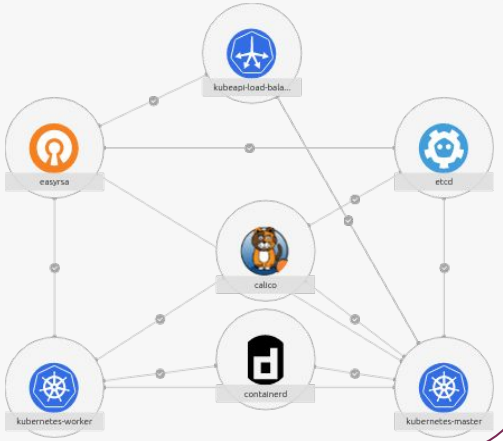


Kubernetes Architecture



Juju Controller

- Operator lifecycle manager
- Deploy OS and applications
- Simple YAML
- Relate applications together in models
- Built-in day 2 operations (updates, scaling, upgrades, etc.)



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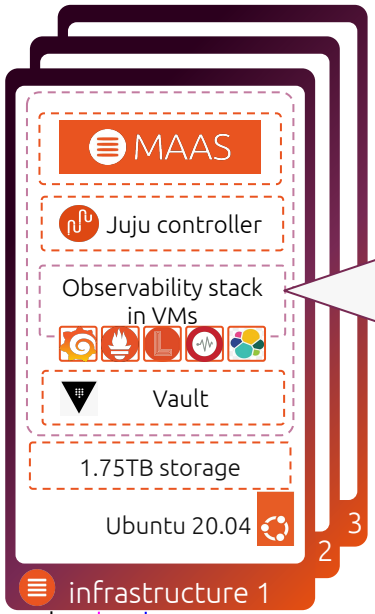
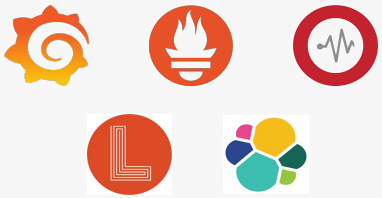
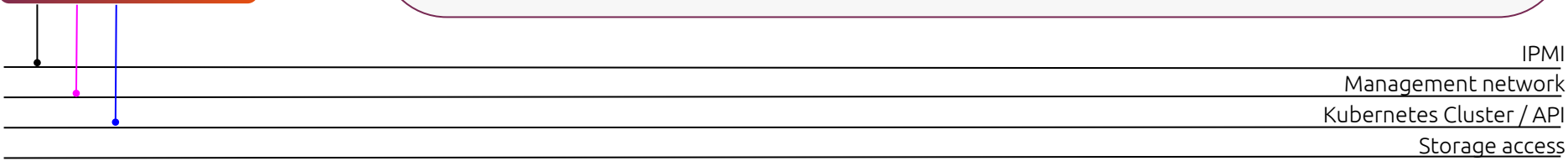


Observability Stack

- Alerting, Monitoring and Logging
- ElasticSearch
- Grafana
- Prometheus
- Landscape server (Ubuntu Management)
- etc.





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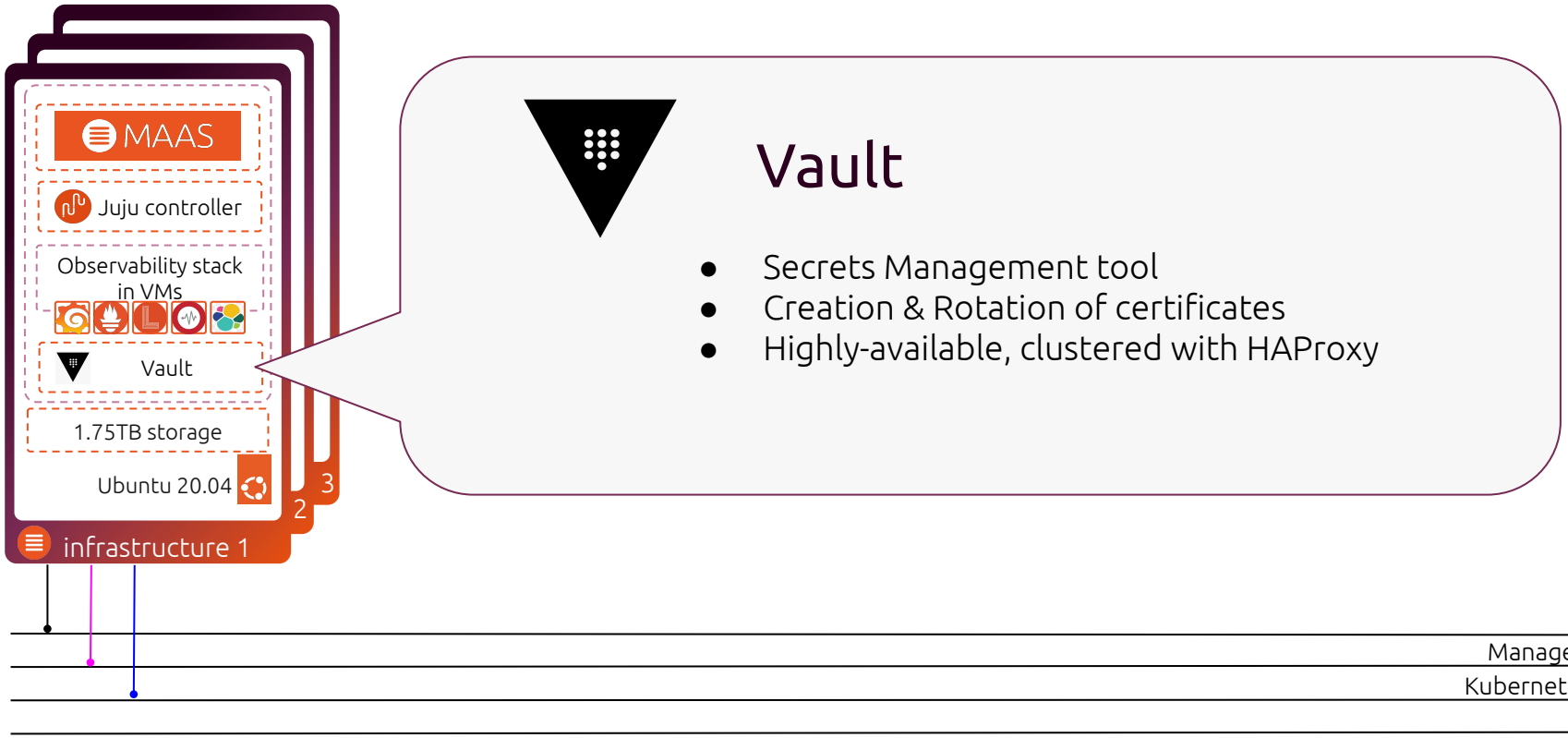

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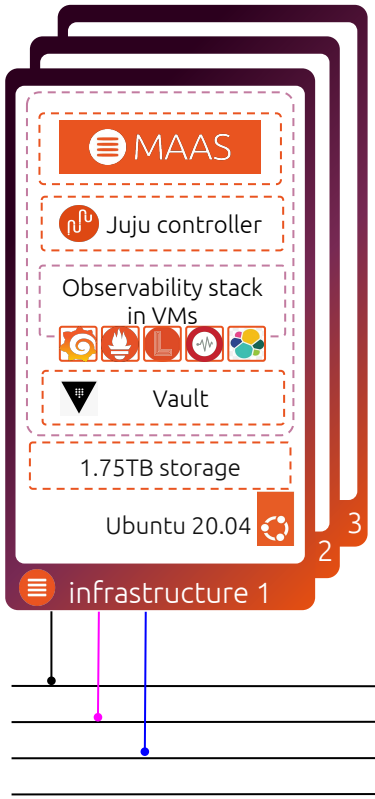

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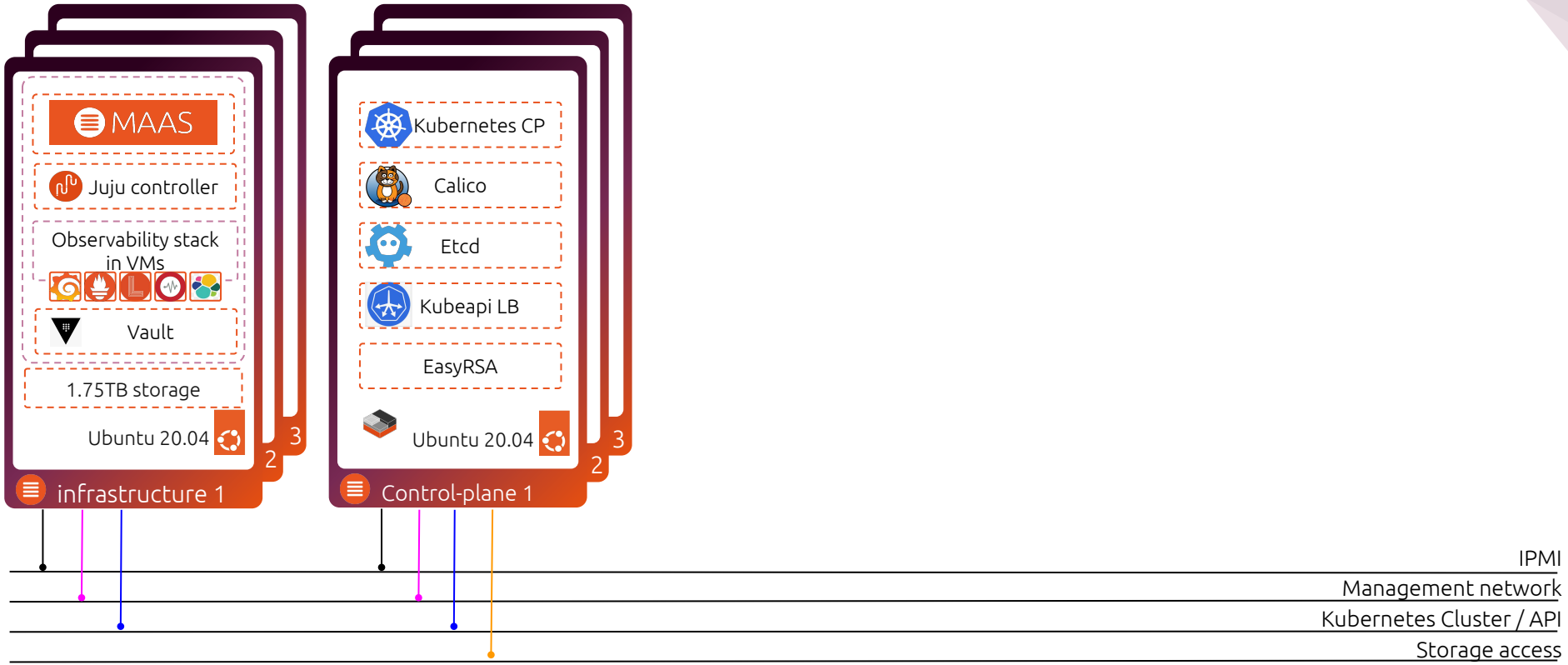

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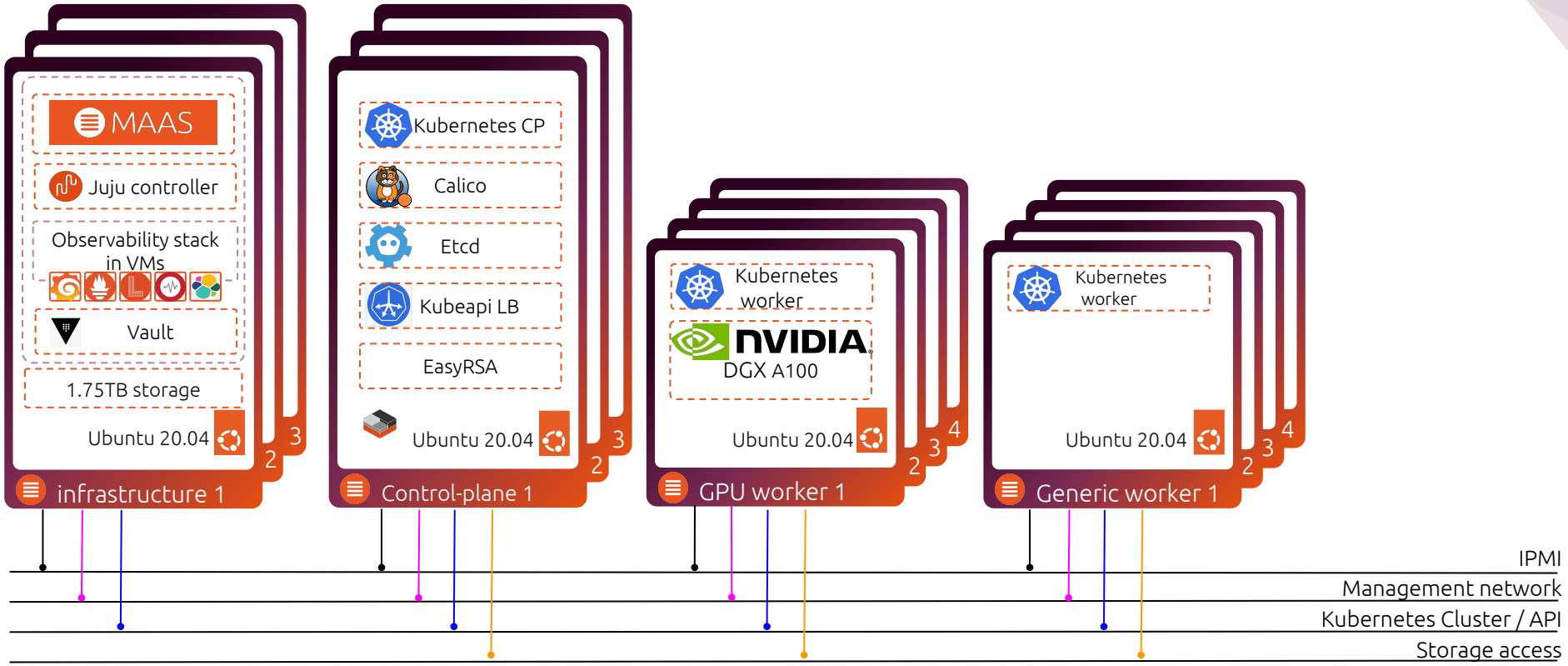

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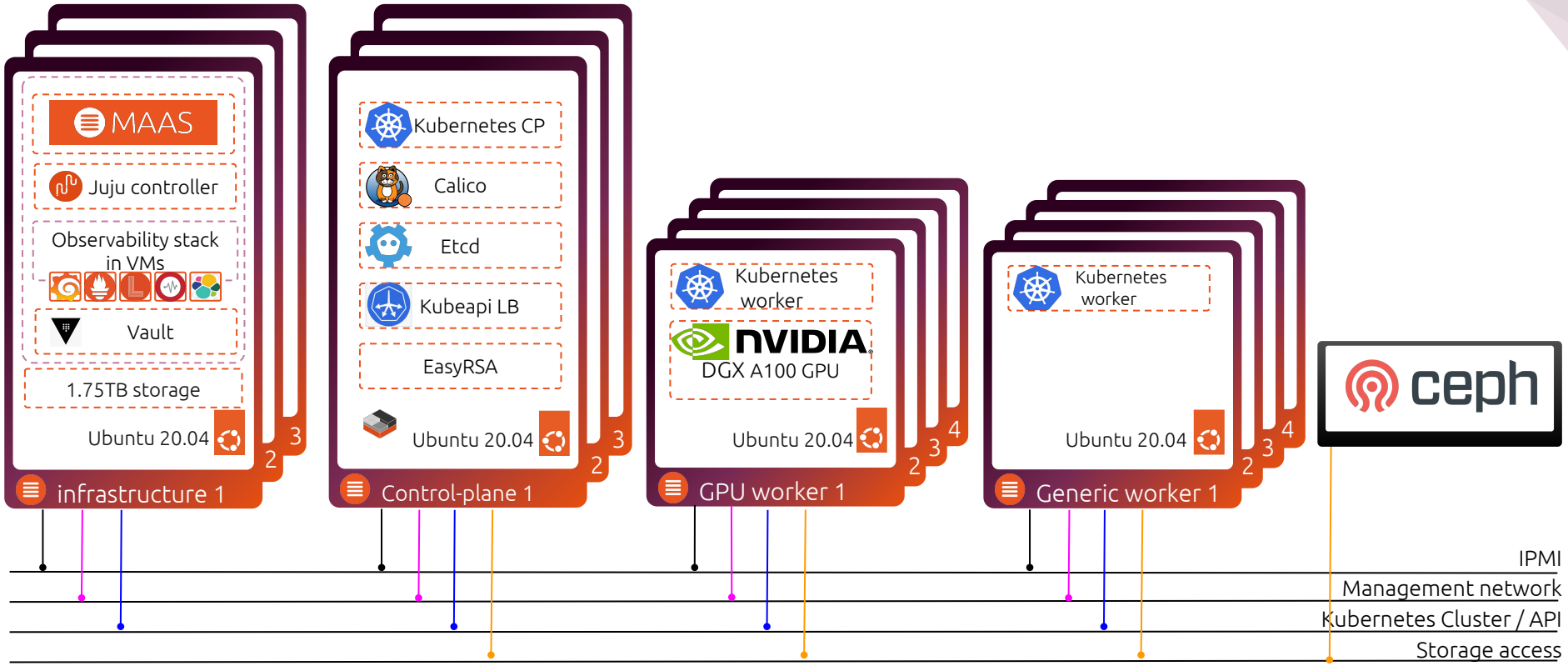

Integrations

NVIDIA GPU Integration

1. Installation of the NVIDIA GPU Operator https://github.com/NVIDIA/gpu-operator

```
$ kubectl get pods -n gpu-operator

NAME                                                  READY   STATUS      RESTARTS   AGE
gpu-feature-discovery-tkxht                           1/1     Running     0          4d15h
gpu-operator-6497cbf9cd-jrgjd                         1/1     Running     0          4d16h
gpu-operator-node-feature-discovery-worker-q5tfd      1/1     Running     0          4d16h
nvidia-container-toolkit-daemonset-wgxg8              1/1     Running     0          4d15h
nvidia-cuda-validator-s728q                           0/1     Completed   0          4d14h
nvidia-dcgm-exporter-vrl72                            1/1     Running     0          4d15h
nvidia-device-plugin-daemonset-hnq7x                  1/1     Running     0          4d15h
nvidia-device-plugin-validator-n6b2r                  0/1     Completed   0          4d14h
nvidia-driver-daemonset-vv4pk                         1/1     Running     0          4d15h
nvidia-mig-manager-c77fx                              1/1     Running     0          4d14h
nvidia-operator-validator-gsb66                       1/1     Running     0          4d15h
```

NVIDIA GPU Integration

Multi-instance GPU (MIG) profiles : allows to split the GPU card into multiple compute.memory slices

- 1 x 7g.40gb
  or
- 2 x 3g.20gb
  or
- 3 x 2g.10gb
  or
- 7 x 1g.5gb

https://docs.nvidia.com/datacenter/tesla/mig-user-guide/index.html

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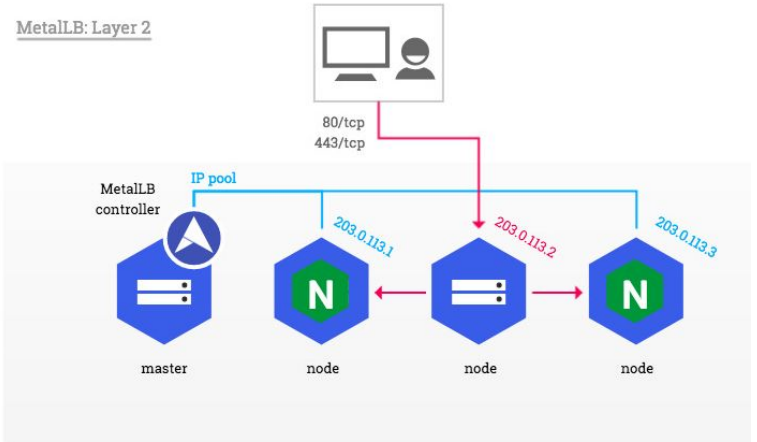
```
$ kubectl label nodes dgx05 nvidia.com/mig.config=all-1g.5gb
$ kubectl get nodes -o yaml | grep nvidia.com/mig-1g.5gb.count:
      nvidia.com/mig-1g.5gb.count: "56"
```

MetalLB

- MetalLB
  - Bare-metal load-balancing in Kubernetes
  - **Layer 2** or BGP mode
  - External IPs assigned by MetalLB
  - NGINX Ingress Controller can perform the TLS termination and the balancing across the nodes



https://kubernetes.github.io/ingress-nginx/deploy/baremetal/#a-pure-software-solution-metallb

SAML Authentication

- Keystone + Keystone-SAML-Mellon charms
- Relate Keystone + Kubernetes-control-plane
- snap client-keystone-auth

- “Self-service” for SSO users
- Access level is defined in SAML
- Leveraging existing tooling to streamline authentication and creation of access files

KEYSTONE

an OpenStack Community Project

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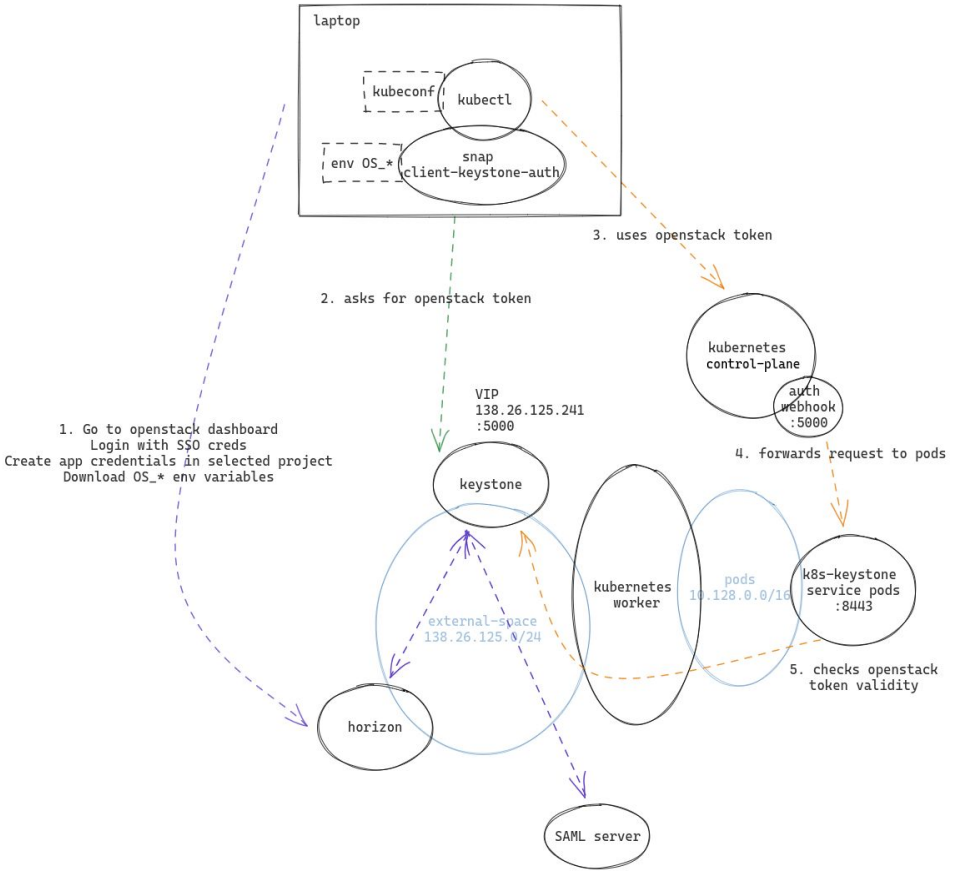

Gitlab Integration

Gitlab registry and Gitlab CI/CD

Each project in Gitlab can host their own container registry and be linked to a Kubernetes namespace.

CI/CD feature lets you connect a project to Kubernetes and use pods as runners. It will install a gitlab agent in your cluster

Research at UAB

University of Alabama at Birmingham

- Public institution
- Located in Birmingham, Alabama (1.2M people)
- One of the largest Academic Medical Centers in the United States.
  - 26,000+ employees
  - $7.15B+ annual economic impact

- UAB Academics + Research
  - ~22,000 enrolled students
  - > 8,000 graduate/researchers
  - +$600M research funding FY21
- UAB IT Research Computing
  - +200 monthly users
  - +15M CPU hours/year
  - Users are 30% of research revenue

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Kubernetes for Research at UAB

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- Why K8s?
  - Micro Services
  - ML/AI Workloads
  - Science Gateways
- K8s as a Research Infrastructure
  - Hardware Allocations
  - Workload Support
- The Future of Research: HPC + K8s

K8s Use Cases

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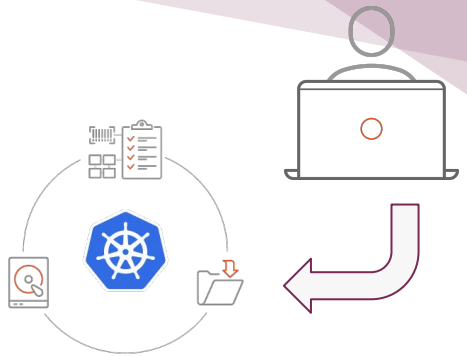
- Microservices for consuming and building RESTful Services
  - Migrate from message-based apps
  - Deploy containerized apps
- Self-service IT Platform for Researchers and Labs
  - User Registration, Auto-provisioning and Group Management
  - Eliminate Ticket-based Workflows
- CI/CD Workflows + GitLab
  - Reduce merge backlog with integration builds
  - Nightly builds for new features
- MLOps: Containers, K8s and Workflows at
  - Kubeflow, MLFlow, NextFlow, PyG with graphgym…
  - Container Registry with GitLab for Code Tracking and Deploy
  - K8s Platform with 32x A100 GPUs



PyG mlflow Kubeflow nextflow kubernetes

High Performance Computing (HPC)

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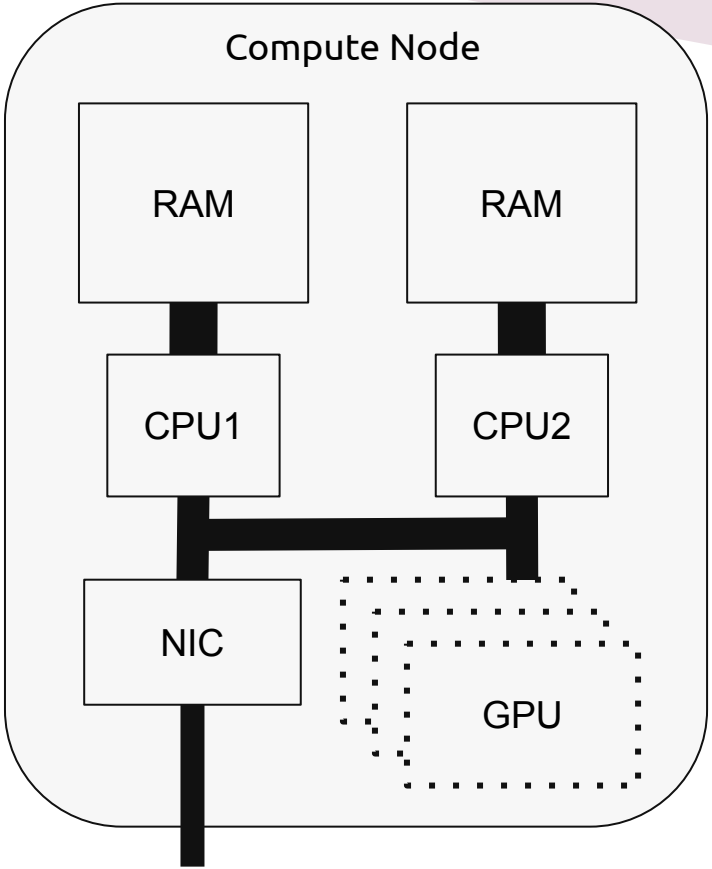
HPC nodes have faster hardware to move lots of data through compute cores

- RAM
  - 384G - 1.5T
- CPUs x 2
  - 24 - 64 core / CPU
- Accelerators (optional)
  - 2,4,8 GPU / node = 1000s cores
- Networking
  - 100Gbps EDR/HDR IB or Ethernet NIC
  - 200Gbps East/West
  - 100Gbps to Internet2 off site



High Performance Compute Clusters

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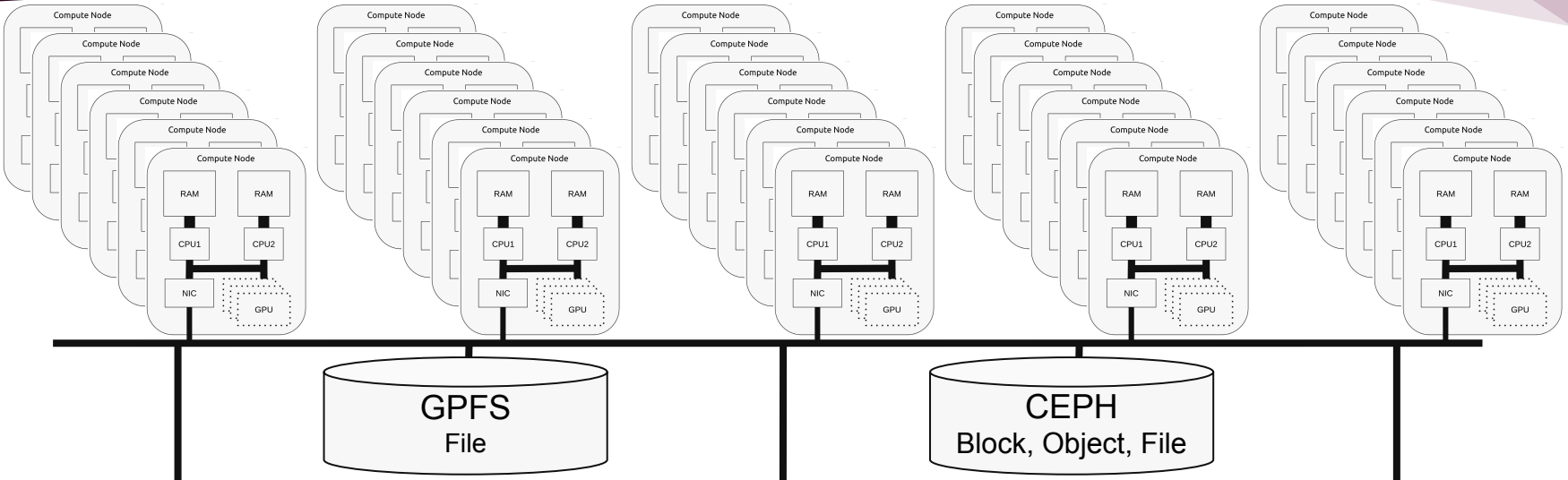

Slurm HPC Batch

- Open OnDemand
- HPC Desktop
- Matlab
- Jupyter/Rstudio
- MPI, BLAS,
- FSL, FreeSurfer
- BWA, SAMTools
- SnakeMake
- NextFlow

OpenStack Cloud

- Open OnDemand
- Cluster Dev
- Application Dev
- Science Gateways
- Custom ML
- Singularity Builds
- CI/CD
- R-Shiny hosting
- Custom App Envs

K8s Container

- ML/AI Workloads
- CI/CD
- NextGen Science Gateways
- Composable Apps
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- NextFlow
- HPC Archive

High Performance Compute Clusters

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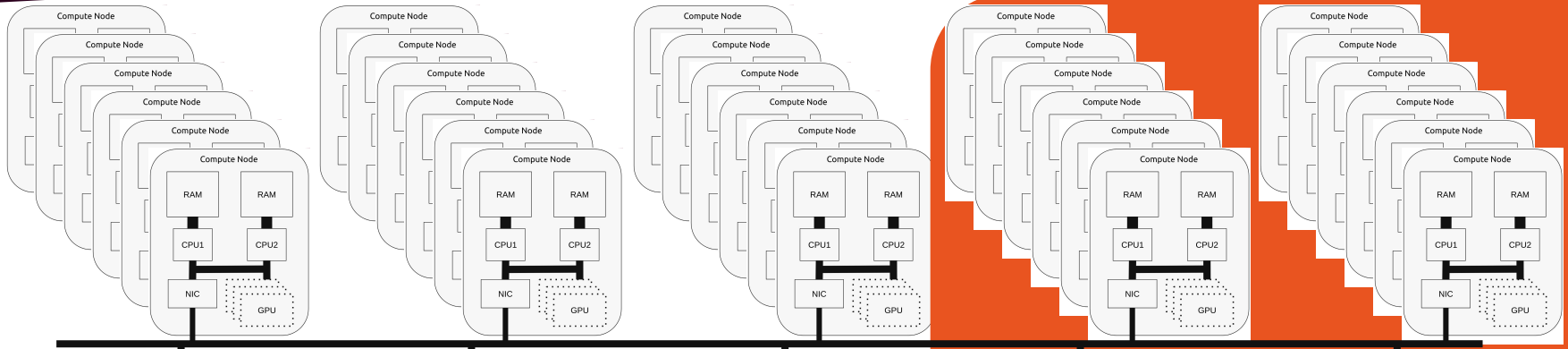

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- NextFlow

NextGen Science Gateways

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HPC Workloads

Instruments & Data Sources

OS | GPFS File System

Environment Modules | GPU

HPC Workloads

CPU | Rest

CPU | GPU

Instrument Mgmt

Web | ML

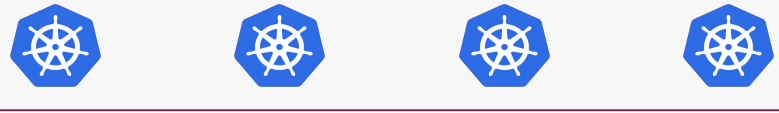
IO | GPU

ML/AI Workload

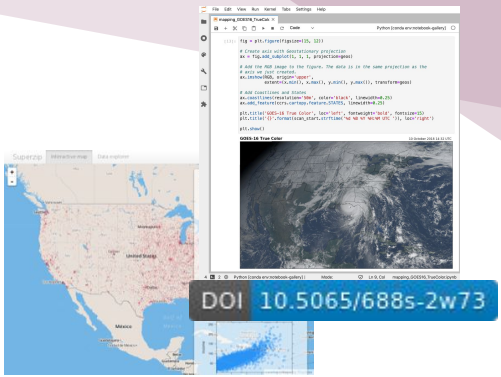
Web | CPU

CPU | GPU

UserPod



Kubernetes Container Engine



RStudio Shiny

Streamlit

jupyter

User Analysis and Composable Apps

Thank you! Questions?

For more info, come see us at booth #P28!

Want to connect ?
jpr@uab.edu
camille.rodriguez@canonical.com