Building a Scalable Data Science & Machine Learning Cloud using Kubernetes

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Problem(s) with the current platform

- It all started out with a small team of Data Scientists.
- As the team scaled, the (on-prem) server resources were scaled up too.
- But after a point, the server became a bottle neck!
- Dependency hell
- Installation of new versions of software/library took a long time due to IT processes.

- What can be done?

Requirements for the new platform

- Scalability
  - Easily accommodate team growth
- Elasticity
  - Scale up or down the resources based on usage
- Multi Cloud support
- High Availability
- Resource limits
- Authentication/Authorization
- Storage Integration
- Self Service
- Ease of use

Kubernetes for the rescue!

- Scalability
    - Easily accommodate team growth
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Plan

1. Containerize the DS/ML environments/workloads
2. Private Registry
3. SSL Certificates for secure communication
4. Utilize wildcard DNS for Ingresses of the workloads
5. Integrate with LDAP/AD
6. NFS support
7. Build a Highly Available (HA) workload cluster
8. Launch DS/ML workloads

Kubernetes is awesome, but …

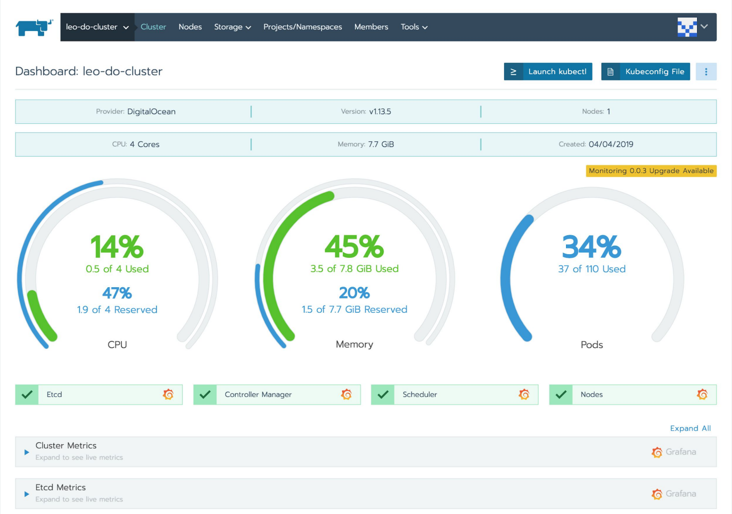
- It's not easy to use!
- Data Scientists don't have time to get a PhD in Kubernetes

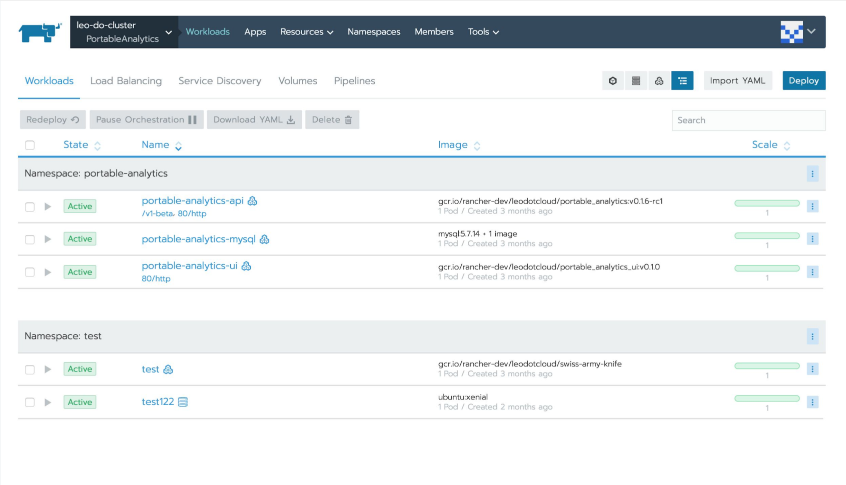
```
> kubectl get nodes
NAME                 STATUS   ROLES                       AGE    VERSION
leo-all-in-one-h1    Ready    controlplane,etcd,worker    105d   v1.13.5
> kubectl get deployments
NAME       READY    UP-TO-DATE    AVAILABLE    AGE
test       1/1      1             1            62d
test111    1/1      1             1            54d
> kubectl get pods
NAME                                 READY    STATUS     RESTARTS    AGE
add-ssh-key-qn82s                    1/1      Running    0           104d
debug-hn-swiss-army-knife-8h5wl      1/1      Running    0           99d
test-5d9bbddf7d-2tfbm                1/1      Running    0           51d
test111-657cc5556b-2v7df             1/1      Running    0           54d
>
```

- Explore third party solutions to provide a simpler user experience
- Rancher

Rancher makes it easy, but ...

- A Data Scientist still has to learn about Kubernetes Concepts





- Can it be made much simpler? (Well, let’s build one!)

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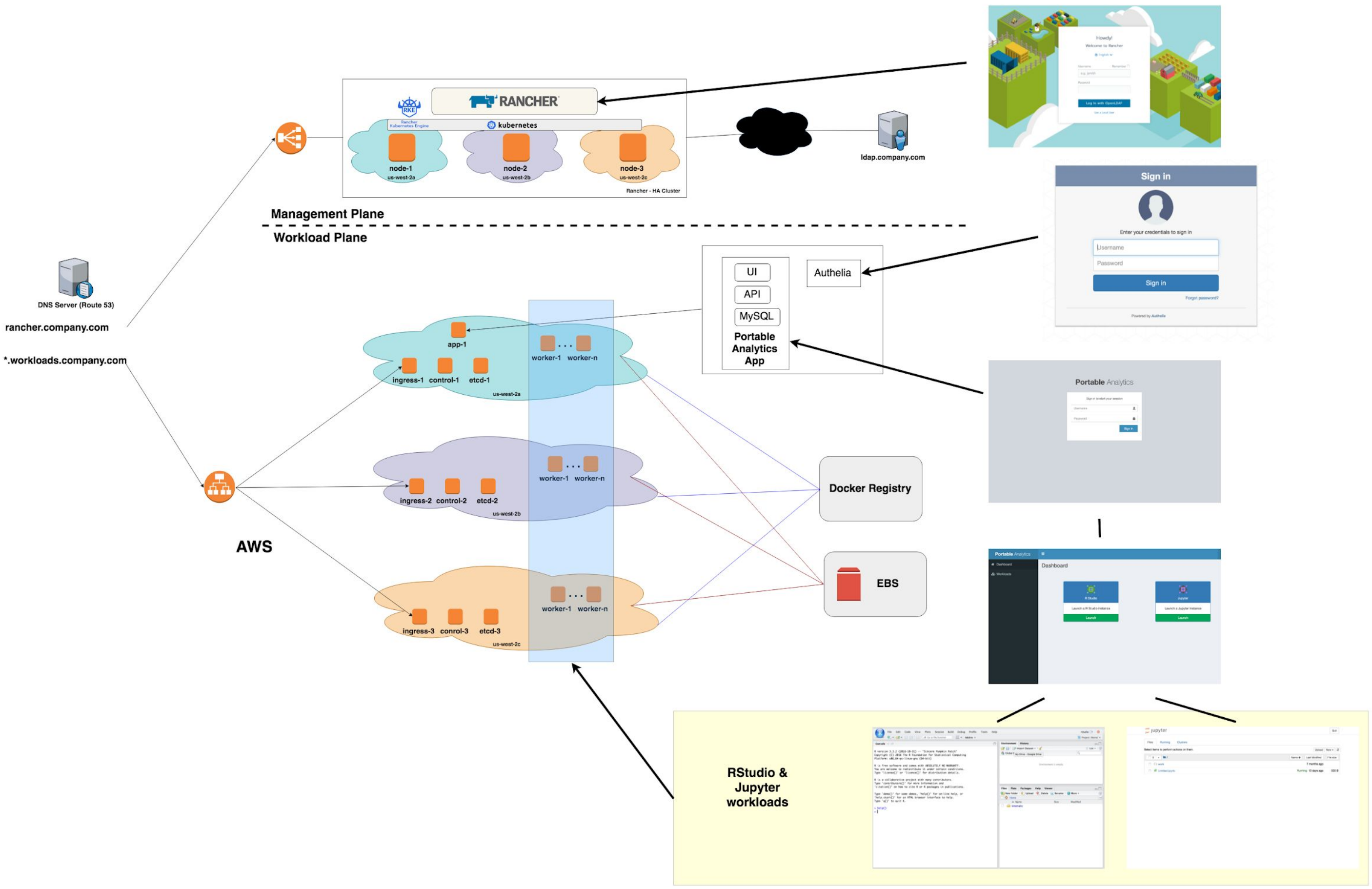
Quick Demo

Behind the Scenes

Architecture



Registry

- Evaluated multiple options
- Docker Hub was not an option as AWS, GCP, Azure were already being consumed
- Self hosting is quite tedious
- ECR provides a per-AZ endpoint, hard to manage config
- GCR provided a single endpoint with global replication

Cons of GCR:

- The credentials are not simple token values, huge json blob

Main workloads

- RStudio (R programming language)
  - Various versions of R
  - Dependencies (Installation takes a lot of time)
  - Private libraries
  - Open source RStudio container image doesn’t support LDAP integration
- Jupyter (Python programming language)
  - Various versions of Python
  - Conflicting packages
  - Private packages
  - Hard to integrate LDAP support

Disable container auth (and use Ingress authentication)

High Availability

- Use of multiple availability zones (AZ)
- Redundancy (scale=n)
    - Multiple etcd nodes (1, 3, 5 …)
    - Redundant control plane, ingress nodes
    - Workers in different AZs
- Cons of availability zones with EBS:
    - Once a PVC is created in a particular AZ, a dependant workload can't move to a different AZ without loss of data
    - In case of AZ failure, not all users are affected, but it's hard to migrate.
- Future work: Investigate and use EFS

Ingress & DNS

- Easy to bookmark URLs for users
- Wild card DNS
  - Scalable
  - No more change requests after the first one
- Ingress authentication
- SSL Termination
  - Terminate on external LB
  - Reduce overhead on the cluster resources
  - Use Wildcard SSL certificate
- Future work:
  - Input from user for the name of workloads

Authelia

- It’s an open-source full-featured authentication server
- Pros:
  - Per Ingress authentication
  - Easy to setup and use
  - Supports multiple auth backends
- Cons:
  - Doesn’t support a config API endpoint (needs to restart Pod on config change)
- https://github.com/clems4ever/authelia

```
access_control:
  default_policy: deny
  any:
  - domain: '*.alpha.do.mpaluru.com'
    policy: deny
  groups: {}
  users:
    mpaluru:
    - domain: mpaluru-rstudio.alpha.do.mpaluru.com
      policy: allow
    - domain: mpaluru-jupyter.alpha.do.mpaluru.com
      policy: allow
```

Storage

- NFS
  - Easy to guess the shares (use UUID)
  - Could have used dynamic provisioner
- EBS (Initial platform was built using AWS)
  - Pre-create the PVC
  - Mainly for persisting user settings, non critical data

Resource Limits

- One user's workload shouldn't impact another user's
  - Use of Requests/Limits of CPU and Memory
- Different worker planes for various workloads
  - Use of Taints/Tolerations
- Cons:
  - Request/Limits > Node Capacity?
  - Fragmentation
- Future work:
  - Support for GPUs

Summary

- Kubernetes is a great platform for running Data Science/Machine Learning workloads
- Managed Kubernetes Services reduce the overhead of managing master nodes
- Providing a simple UX for end users still places a lot of burden on the cluster operator
- Use a higher level framework instead of working with native k8s manifests
- Support for other DS/ML projects
- Coming soon: https://github.com/k4ds

Questions?

Thank you!