Accelerating Data Science Workflows with Kubernetes

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Presenter

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  - University of Missouri
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  - Several years of experience both using and teaching Docker and K8s concepts to researchers and educators around the country as part of NSF-funded GP-ENGINE project (https://gp-engine.umsystem.edu)
  - Lab GitHub: https://github.com/MUAMLL
    - Repo for this Tutorial: https://github.com/MUAMLL/SDSS2025

Learning Objectives

- Introduction to Kubernetes: Container Orchestration
- Kubernetes Architecture: Control Plane vs. Worker Node
- KubeCTL: Interfacing with K8s
- K8s Resource Types
  - PVCs, Pods, Jobs, & Services
- Provisioning Resources
  - YAML Specification Files
- Data Science Workflows in K8s
  - SKLearn
  - Jupyter
  - GPU-enabled Workflows: PyTorch
- Automation with Kubernetes
  - Using 3rd Party Libraries
  - Using the K8s Python Client

Workshop Outline

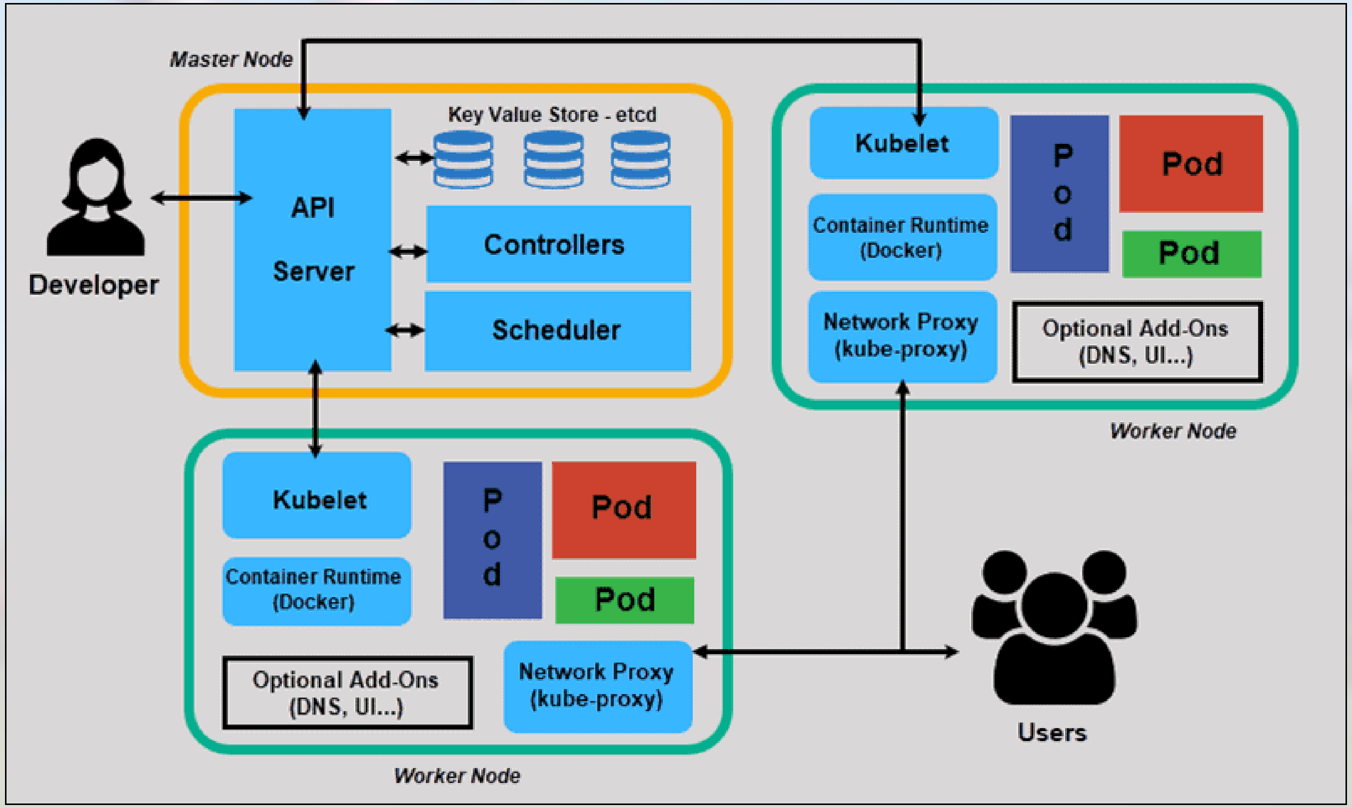
- Introduction to Kubernetes **(Slides)**
  - Container Orchestration
  - Kubernetes Architecture
  - Kubernetes Resource Types
- Interfacing with K8s: KubeCTL and YAML **(Slides)**
  - YAML Definition
  - KubeCTL introduction and syntax
- Introduction to K8s **(Hands-On)**
  - The National Research Platform
  - Creating persistent storage in K8s
  - Spawning a Pod
  - Creating a Job
- Running Data Science Workflows **(Hands-On)**
  - CPU-jobs: Sci-Kit Learn
  - Interactive Pods: Jupyter
  - GPU-jobs: PyTorch
- Automation with Kubernetes **(Slides)**
  - Using 3rd Party Libraries: Jinja2
  - Using the Kubernetes Python Client
- Automating K8s Job Creation **(Hands-On)**
  - Using the Kubernetes Python Client

Introduction to Kubernetes

What is Kubernetes and what is it used for

Kubernetes

- Kubernetes, also known as K8s, is an open-source system for automating deployment, scaling, and management of containerized applications.[1]
- Kubernetes enables both simple and complex container orchestration
- Kubernetes cluster has two main components
  - Master node
  - Worker node

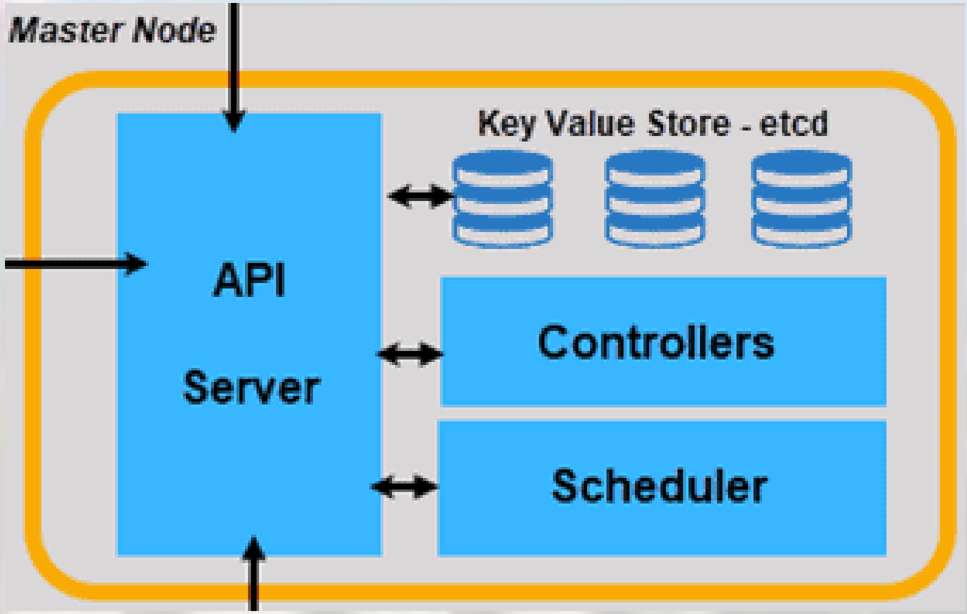


1. https://kubernetes.io/
2. Image: https://phoenixnap.com/kb/understanding-kubernetes-architecture-diagrams
3. Logo: https://commons.wikimedia.org/wiki/File:Kubernetes_logo_without_workmark.svg

Kubernetes

Master node

- Also known as the Control Plane, it is responsible for managing the state of the cluster
- API server: interface between master node and the rest of the cluster
- etcd: distributed key-value store that stores the cluster's persistent information
- Scheduler: responsible for scheduling pods onto the working nodes
- Controller manager: responsible for running controllers that manages the state of the clusters such as replication controller and deployment controller



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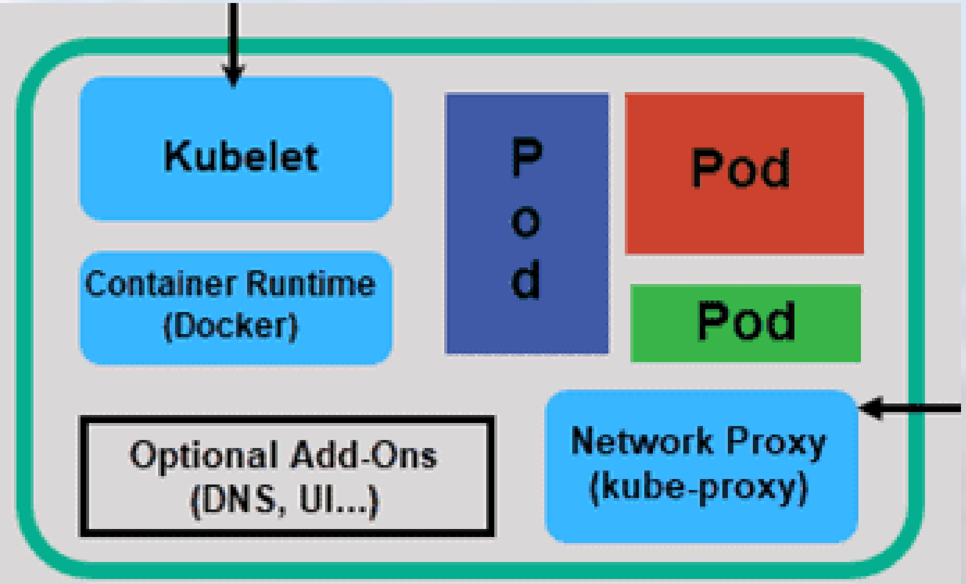
2. Image: https://phoenixnap.com/kb/understanding-kubernetes-architecture-diagrams
3. Logo: https://commons.wikimedia.org/wiki/File:Kubernetes_logo_without_workmark.svg

Kubernetes

Worker node

- The physical machine where the operations takes place, it can run one or multiple pods
- Kubelet: deamon that runs each working node
- Container runtime: is responsible for pulling images from the registry, starting and stopping containers, and managing the container resources
- kube-proxy: responsible for routing traffic to the correct pod and provides load balancing so that the traffic is distributed evenly between the pods



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2. Image: https://phoenixnap.com/kb/understanding-kubernetes-architecture-diagrams
3. Logo: https://commons.wikimedia.org/wiki/File:Kubernetes_logo_without_workmark.svg

Kubernetes concepts

Node, pod, persistent volume, job, deployment, service

Key Kubernetes Concepts

Pod

- Pods are the basic scheduling unit of K8s.
- Pods consist of one or more containers running inside. Each pod has a unique IP address to enable micro services or applications
- Pods can run custom scripts (initcontainer) at runtime to initialize the pod
- Pods generally have limitations on allocated resources and max runtime
- Pods are stateless, meaning all data uploaded or generated by the pod is deleted when the pod terminates

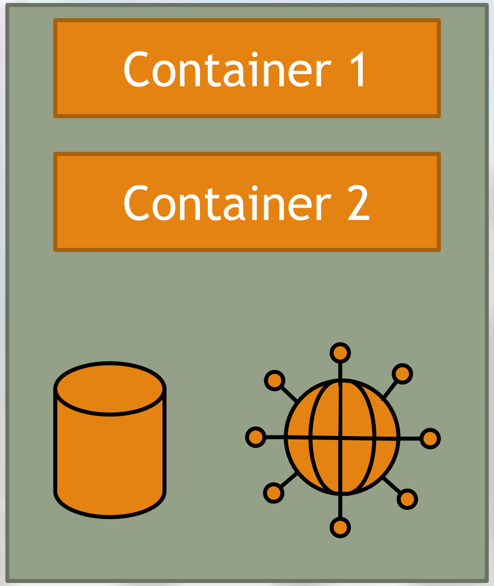
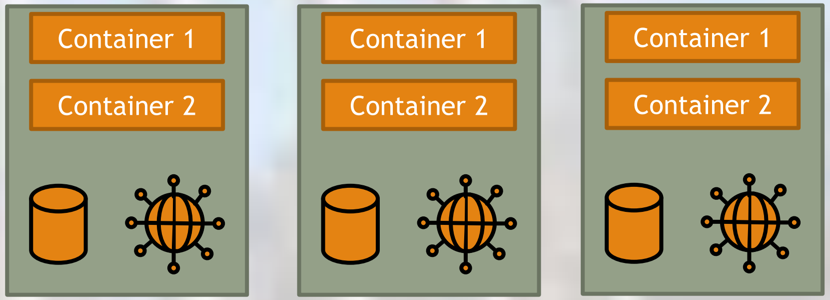


Image: https://aws.plainenglish.io/kubernetes-deep-dive-job-and-cronjob-5ffed1c5fa4e

Key Kubernetes Concepts
ReplicaSet and Deployment

- **ReplicaSet -** its purpose is to maintain a stable set of replica Pods running at any given time. [1]

- **Deployment** - is a higher-level concept that manages ReplicaSets and provides declarative updates to Pods along with a lot of other useful features.[1]



It is recommended to use Deployment instead of ReplicaSets

1. https://kubernetes.io/

Key Kubernetes Concepts

Jobs

- A Job creates one or more Pods and will continue to retry execution of the Pods until a specified number of them successfully terminate.[1]
- A job has virtually access to unlimited resources and can run for extended periods of time
- A job may consist of one pod or multiple pods working in parallel
- Deleting a job will automatically delete its corresponding pod
- A job can create a new pod(s) if any of its pod(s) is deleted or failed for any reason.
- Similar to pods, jobs are stateless

1. https://kubernetes.io/

Key Kubernetes Concepts
Persistent volume

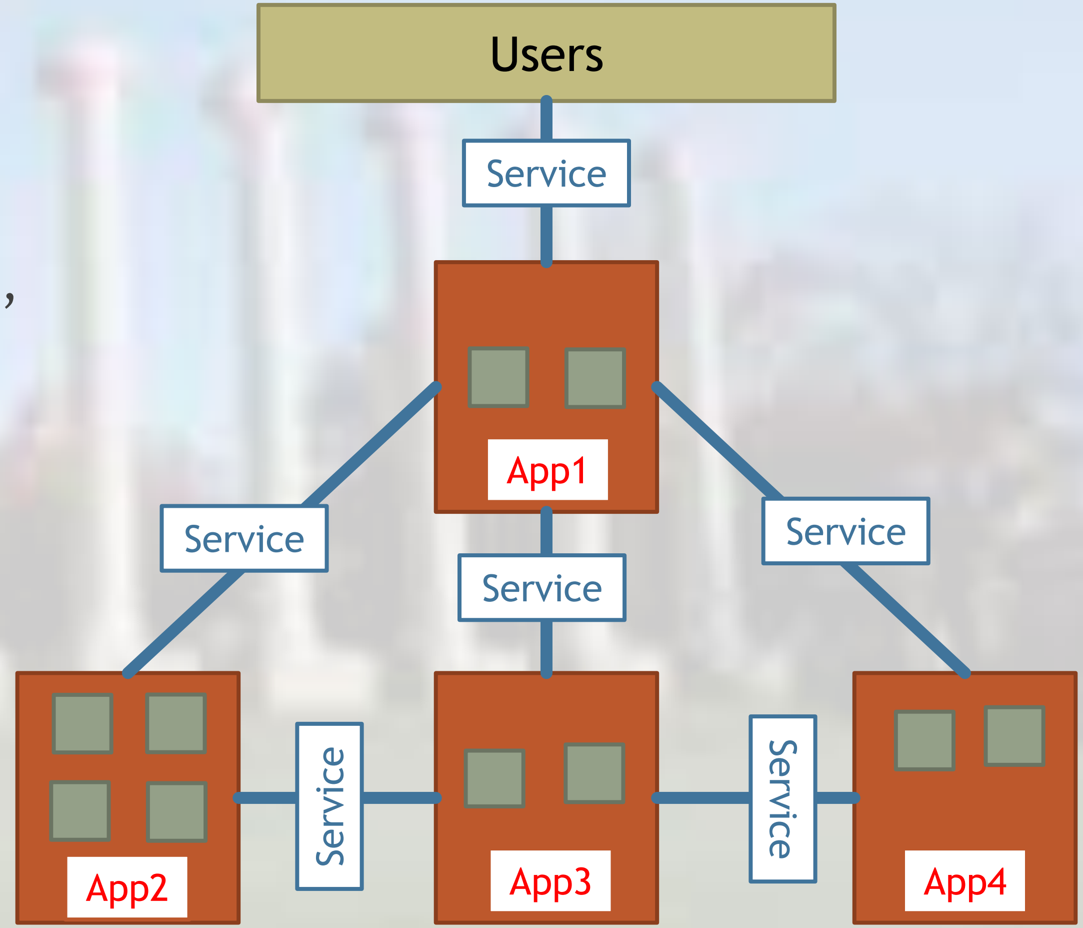
- To maintain the data generated a persistent volume (storage) is needed
- A **persistent volume** is storage on the cluster that has been provisioned by an administrator or dynamically provisioned using storage classes. [1]
- There exists different classes of persistent volumes such as:
  - cephfs
  - Fibre Channel storage
  - NFS storage
- There are different access modes:
  - ReadWriteOnce
  - ReadOnlyMany
  - ReadWriteMany
  - ReadWriteOncePod

1. https://kubernetes.io/

Key Kubernetes Concepts

Services

- Applications running within distinct pods communicate over the network using the unique IP address assigned to each pod
- Each Pod has a unique IP address assigned at runtime, which changes every time a Pod is restarted, making reliable communication less simple
- Services enable communication between applications running in pods within the cluster and with outside users if necessary
- There are four type of services supported by K8s
  - ClusterIP
  - NodePort
  - LoadBalancer
  - Ingress



Kubernetes usage

Basics of YAML language, kubectl installation and usage

Yet Another Markup Language (YAML)

XML	JSON	YAML

<Servers>
<Server>
<name>Server1</name>
<owner>John</owner>
<created>123456</created>
<status>active</status>
</Server>
</Servers>
	{
	Servers: [
	{
	name: Server1,
	owner: John,
	created: 123456,
	status: active
	}
	]
	}
		Servers:
		- name: Server1
		owner: John
		created: 123456
		status: active

- YAML is a key-value pair file format, similar to JSON and XML
- Kubernetes operations are performed using **YAML** files, known as a Spec file
  - Creating Persistent Storage
  - Creating Pods
  - Creating Jobs
  - Deploying services

Synopsis of YAML language[1]

- Comments in YAML begins with the (#) character and they must be separated from other tokens by whitespaces.
- Indentation of whitespace is used to denote structure.
- Tabs are not included as indentation for YAML files.
- Lists are important
  - List members are denoted by a leading hyphen (-).
  - List members are enclosed in square brackets and separated by commas.
  - YAML always requires colons and commas used as list separators followed by space with scalar values.
- Associative arrays are represented using colon (:) in the format of key value pair. They are enclosed in curly braces {}.

1. https://www.tutorialspoint.com/yaml/yaml_basics.htm

Structure of YAML file

- Each YAML file consists of specific parts, each part is dedicated to hold a type of information that enables us to communicate our needs to the Kubernetes cluster.
- **kind** – tells Kubernetes the type of the resource: pod, job, service, storage
- **metadata** – data about the resource
  - Name is most common attribute to set
- **spec** – the attributes specified in this section depends on the kind
  - We will cover common spec attributes

Pod without mounted volume

We begin by setting the API Version and the type of object we are creating (Pod), as well as the name of the pod

From here we are defining the container to run in this pod

Set the name of the container, the image the container should run, and the command that should run when the container begins

Here, we define the requested and maximum amount of resources our container needs to run, in this case that is 2 CPU cores and 4 GB of RAM

```yaml
apiVersion: v1
kind: Pod
metadata:
 name: python3-pod
spec:
 containers:
  - name: python3-container
   image: python:3.8
   command: ["sleep", "infinity"]
   resources:
    limits:
     memory: 4Gi
     cpu: 2
    requests:
     memory: 4Gi
     cpu: 2
```

Job without mounted volume

We begin by setting the API Version and the type of object we are creating (Job), as well as the name of the job

From here we are defining the pod that is to be started by this job

Set the name of the container, the image the container should run, and the command that should run when the container begins

Here, we define the requested and maximum amount of resources our container needs to run, in this case that is 2 CPU cores and 4 GB of RAM

```
apiVersion: v1
kind: job
metadata:
  name: python3-job
spec:
  template:
      containers:
      - name: python3-pod
        image: python:3.8
        command: ["sleep", "infinity"]
        resources:
          limits:
            memory: 4Gi
            cpu: 2
          requests:
            memory: 4Gi
            cpu: 2
```

Persistent Volume (PVC) Creation

We begin by setting the API Version and the type of object we are creating (PersistentVolumeClaim), as well as the name of the PersistentVolumeClaim

From here we are defining the lass of the persistent volume we are using

Here we define the type of access mode of the persistent volume we are creating

Here, we define the requested size of the persistent volume 50 GB of storage

To increase the size of the persistent volume storage we only need to modify this value
We can only increase but we cannot decrease

```
apiVersion: v1
kind: PersistentVolumeClaim
metadata:
  name: your_name
spec:
  storageClassName: rook-cephfs
  accessModes:
  - ReadWriteMany
  resources:
    requests:
      storage: 50Gi
```

Pod with PVC

We begin by setting the API Version and the type of object we are creating (Pod), as well as the name of the pod

From here we are defining the container to run in this pod

Set the name of the container, the image the container should run, and the command that should run when the container begins

Here, we define the requested and maximum amount of resources our container needs to run, in this case that is 2 CPU cores and 10 GB of RAM

Information of the mounted volume and how it is defined within the pod

```yaml
apiVersion: v1
kind: Pod

metadata:

 name: pod-name-sso

spec:

 containers:

 - name: pod-name-sso

  image: python:3.8

  command: ["sh", "-c", "echo 'Im a new pod' && sleep infinity"]

  resources:

   limits:

    memory: 12Gi

    cpu: 2

   requests:

    memory: 10Gi

    cpu: 2

  volumeMounts:

  - mountPath: /data

   name: anes-pv

 volumes:

  - name: anes-pv

   persistentVolumeClaim:

    claimName: anes-pv
```

Job with mounted volume

We begin by setting the API Version and the type of object we are creating (Job), as well as the name of the job

From here we are defining the pod that is to be started by this job

Set the name of the container, the image the container should run, and the command that should run when the container begins

Here, we define the requested and maximum amount of resources our container needs to run, in this case that is 2 CPU cores and 4 GB of RAM

Information of the mounted volume and it is defined within the job

```
apiVersion: v1

kind: job

metadata:
  name: python3-job

spec:

 template:

    containers:

    - name: python3-pod

      image: python:3.8

      command: ["sleep", "infinity"]

      resources:

        limits:

           memory: 4Gi

           cpu: 2

        requests:

           memory: 4Gi

           cpu: 2

      volumeMounts:

      - name: canada

        mountPath: /Canada

    volumes:

    - name: canada

      persistentVolumeClaim:

        claimName: canada2019-3
```

Interfacing with Kubernetes: KubeCTL installation

- https://kubernetes.io/docs/tasks/tools/
- This link provide options for installing kubectl with:
  - Linux
  - macOS
  - windows

Interfacing with Kubernetes: KubeCTL installation (Linux)

there are three options to installing kubectl on Linux

- Install kubectl binary with curl on Linux
- Install using native package management
- Install using other package management

Interfacing with Kubernetes: KubeCTL installation (Windows)

- There are two options to install Kubectl on windows

- Install kubectl binary with curl on Windows

- Install on Windows using Chocolatey, Scoop, or winget

Interfacing with Kubernetes: KubeCTL installation (MacOS)

- There are many options to install Kubectl on MacOS

- Install kubectl binary with curl on macOS
- Install with Homebrew on macOS
- Install with Macports on macOS

Interfacing with Kubernetes: KubeCTL

- With a published Docker image and prepared YAML Spec file, KubeCTL enables interaction with Kubernetes:

kubectl [command] [TYPE] [NAME] [flags]

where:

- command: Specifies the operation that you want to perform on one or more resources, for example create, get, describe, delete
- TYPE: Specifies the resource type, such as pod or job
- NAME: Specifies the name of the resource, or the path to a Spec file
- flags: Specifies optional flags, such as --server to specify the address and port of the API server

https://kubernetes.io/docs/reference/kubectl/

Interfacing with Kubernetes: KubeCTL cheat sheet

- To create pod

  kubectl create –f pod.yaml

  kubectl apply –f pod.yaml

- To create job

  kubectl create –f job.yaml

  kubectl apply –f job.yaml

Interfacing with Kubernetes: KubeCTL cheat sheet

- To check pod status

  kubectl get pods

  kubectl describe pod pod-name

- To check job status

  kubectl get jobs

  kubectl describe job job-name

- To debug pod

  kubectl logs pod-name

Interfacing with Kubernetes: KubeCTL cheat sheet

- Access Pod interactively

  kubectl exec –it pod-name -- /bin/bash

- Copy data from Nautilus to local machine

  kubectl cp pod-name:path/to/data local/path/

- Copy data to Nautilus from local machine

  kubectl cp local/path/ pod-name:path/to/data

- Exit interactive Pod mode

  Press ctrl+D

Interfacing with Kubernetes: KubeCTL cheat sheet

- To delete pod

  kubectl delete –f pod.yaml

  Kubectl delete pod-name

- To delete job

  kubectl delete –f job.yaml

  Kubectl delete job-name

Interfacing with Kubernetes: KubeCTL cheat sheet

- To create persistent volume

kubectl create –f pvc.yaml

Kubectl apply –f pvc.yaml

- To increase the size of persistent volume

kubectl apply –f pvc.yaml

- To delete persistent volume

kubectl delete –f pvc.yaml

kubectl delete pvc-name

National Research Platform
Nautilus Hyper Cluster

A quick note on Kubernetes Clusters, the NRP, Commercial Clouds, and other K8s Clusters

- All commercial cloud providers support Containers and Kubernetes
- The concepts and examples in this tutorial may require minor modifications to adapt to other environments
- We are using the US National Research Platform solely for demonstration and tutorial purposes
- All Container and Kubernetes concepts are portable to commercial clouds or other research Kubernetes platforms

NSF NRP Nautilus HyperCluster

- The NSF Nautilus HyperCluster is a Kubernetes cluster with vast resources that can be utilized for various research purposes:
  - Prototyping research code
  - S3 cloud storage for data and models
  - Accelerated small-scale research compute
  - Scaling research compute for large scale experimentation
- Resources Available:
  - CPU Cores: 9,769
  - RAM: 167 TB
  - NVIDIA GPUs: 1342

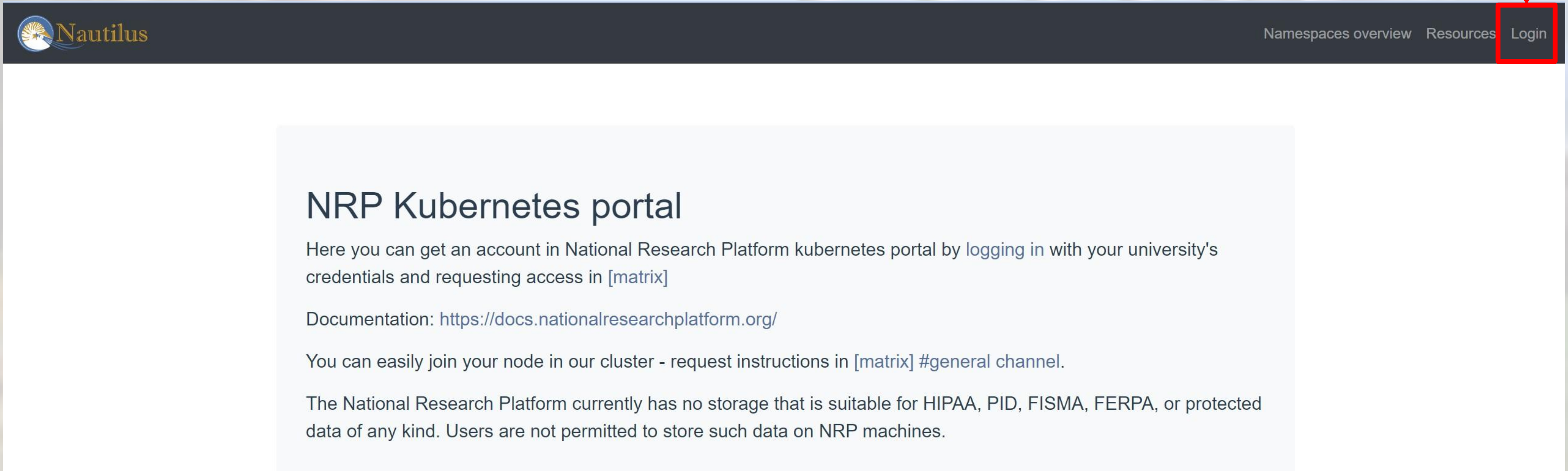
Nautilus Logo: https://portal.nrp-nautilus.io/
Docker Logo: https://developers.redhat.com/blog/2014/05/15/practical-introduction-to-docker-containers
Kubernetes Logo: https://commons.wikimedia.org/wiki/File:Kubernetes_logo_without_workmark.svg

Access to Nautilus

- Nautilus Access
  - MU-managed Jupyter Hub
    - https://gp-engine.nrp-nautilus.io/
    - Advantages
      - No manual account creation
      - Ease of use
    - Disadvantges
      - Limited customizability
  - Direct Access with KubeCTL
    - Disadvantages
      - Account and namespace creation
      - KubeCTL installation
    - Advantages
      - High scalability and customizability

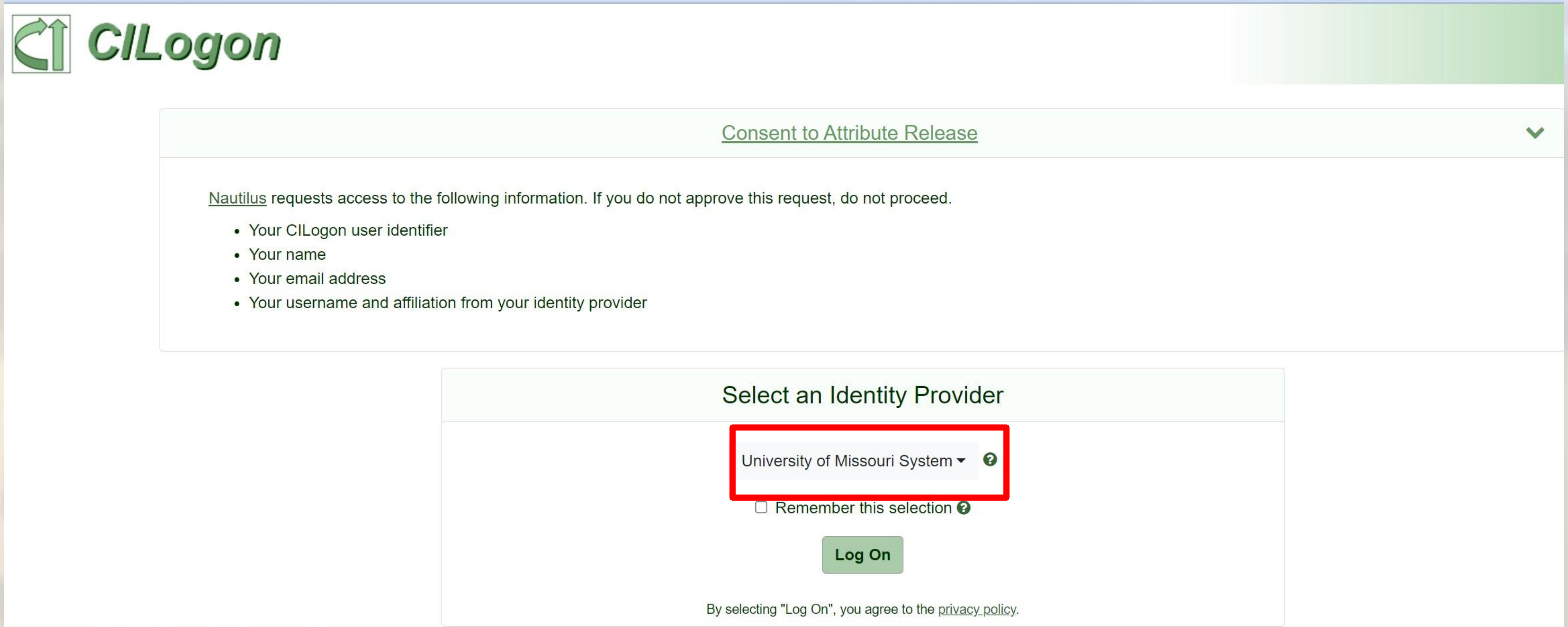
Access to Nautilus

- Follow the steps in getting started
  - https://ucsd-prp.gitlab.io/userdocs/start/get-access/
- Step1: Access Nautilus portal at https://portal.nrp-nautilus.io
- Step 2: Click on login

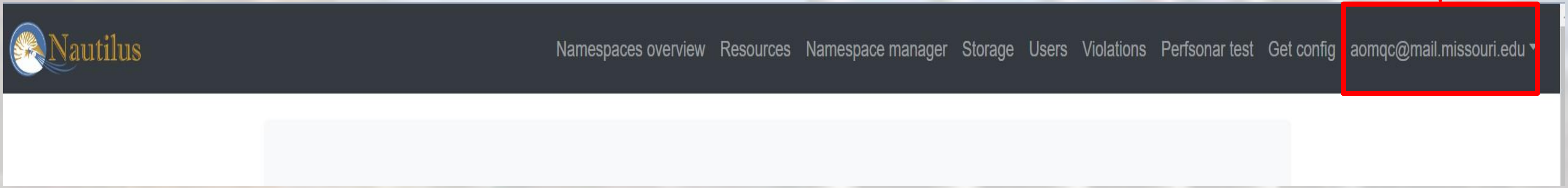


Access to Nautilus

- Follow the steps in getting started
  - https://ucsd-prp.gitlab.io/userdocs/start/get-access/
- **Step 3:** Select identity provider – Either your institution, ORCID, GitHub, or Google



- Follow the steps in getting started
  - https://ucsd-prp.gitlab.io/userdocs/start/get-access/
- Step 4: Contact a Nautilus Namespace Admin
  - Email needs to be visible



- You need to be manually added to a namespace
  - As admins, we can add you to existing namespace or create a namespace for you

Automating Jobs in K8s using Bash and Python

Automating GPU Jobs in K8s using Bash and Python

- Nautilus is set up for parallel computing allowing for the running of multiple jobs at the same time
- Automation of jobs handling (submission, deletion) is key for the smooth operation
- There are multiple ways to automate the job handle processes
- We present here two ways:
  - jinja + bash
  - Nautilus Job Launcher library

jinja & bash

- We need a Python and/or Jupyter environment with these libraries:
  - yaml: to read/write yaml files
  - jinja2: to create and update templates that can be used to generate yaml files
  - os: to generate directories
- Text editor such as Notepad++ to write bash files

jinja & bash

- from jinja2 import Template
- Define template
  - It needs to be a multi line string
  - The variables to be updated are denoted by double braces {{.}}
  - The name of variable between the braces is used as reference
- j2_template1 = Template(template1)

```
template1 ='''apiVersion: batch/v1
kind: Job
metadata:
  name: anes-job-train-exp{{ exp_num }}-{{ network }}-{{ data_type }}-pretrain
spec:
  template:
    spec:
      containers:
      - name: anes-pod-train-exp{{ exp_num }}-{{ network }}-{{ data_type }}-pretr
        image: gitlab-registry.nrp-nautilus.io/jhurt/cgisegment:e98e742e
        command: ["/bin/sh","-c"]
        args:
        - python3 main.py --task train --output_dir /canada2019-3/{{sourcedir}}/e
        volumeMounts:
        - name: canada2019-3
          mountPath: /canada2019-3
        resources:
            limits:
              memory: 12Gi
              cpu: "4"
              nvidia.com/gpu: 2
            requests:
              memory: 12Gi
              cpu: "4"
              nvidia.com/gpu: 2
      volumes:
      - name: canada2019-3
        persistentVolumeClaim:
            claimName: canada2019-3
      restartPolicy: OnFailure
  backoffLimit:

'''
```

jinja & bash

- We use a loop to auto generate the files
- We need to define variables in a dictionary where:
  - Keys: variable names as defined in the template
  - Values: values of the variables for this iteration
- Apply values to the template using:

  output_file = j2_template1.render(data)
- Save the yaml file to the appropriate location

```
for exp in list(range(8)):
    exp_num = exp + 1

    if os.path.exists('{}/exp{}'.format(source_dir,exp_num)):
        shutil.rmtree('{}/exp{}'.format(source_dir,exp_num))
    os.mkdir('{}/exp{}'.format(source_dir,exp_num))

    for folder in folders_list:

        parts     = folder.split('_')
        network   = parts[0]
        data_type = parts[1]


        data = {'sourcedir':source_dir,
                'exp_num':exp_num,
                'network':network,
                'data_type':data_type,
                'outputdir':dict1[folder][0],
                'configfile':dict1[folder][1]}

        output_file = j2_template1.render(data)

        fileout = open('{}/exp{}/job_exp{}_{}_{}.yaml'.format(source_dir,exp_num
        fileout.write(output_file)
        fileout.close()
```

jinja & bash

- Now that all yaml files have been generated we need bash files to
  - Submit jobs
  - Delete jobs after they finish
- We will write a bash file for each operation
  - Bash for job submission
  - Bash for deletion of completed jobs
- Execute bash file in the terminal

```
@ECHO OFF

Rem This batch file executes kubectl commands to create training jobs

::echo %kubectl%
SET exp_list=2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

(for %%a in  (%exp_list%) do (
    echo %%a

    kubectl create -f experiments\exp%%a/job_exp%%a_deeplab_img.yaml
    kubectl create -f experiments\exp%%a/job_exp%%a_deeplab_tci.yaml
    kubectl create -f experiments\exp%%a/job_exp%%a_deeplab_img_pretrained.yaml
    kubectl create -f experiments\exp%%a/job_exp%%a_deeplab_tci_pretrained.yaml

    kubectl create -f experiments\exp%%a/job_exp%%a_unet_img.yaml
    kubectl create -f experiments\exp%%a/job_exp%%a_unet_tci.yaml
    kubectl create -f experiments\exp%%a/job_exp%%a_unet_img_pretrained.yaml
    kubectl create -f experiments\exp%%a/job_exp%%a_unet_tci_pretrained.yaml
))

echo "batch complete"
```

```
@ECHO OFF

Rem This batch file executes kubectl commands to delete training jobs

::echo %kubectl%
SET exp_list=1 2 3 4 5 6 7 8

(for %%a in  (%exp_list%) do (
    echo %%a

    kubectl delete -f experiments_2\exp%%a/job_exp%%a_deeplabv3_img.yaml
    kubectl delete -f experiments_2\exp%%a/job_exp%%a_deeplabv3_tci.yaml
    kubectl delete -f experiments_2\exp%%a/job_exp%%a_deeplabv3plus_img.yaml
    kubectl delete -f experiments_2\exp%%a/job_exp%%a_deeplabv3plus_tci.yaml

    kubectl delete -f experiments_2\exp%%a/job_exp%%a_unet_img.yaml
    kubectl delete -f experiments_2\exp%%a/job_exp%%a_unet_tci.yaml
    kubectl delete -f experiments_2\exp%%a/job_exp%%a_unetplus_img.yaml
    kubectl delete -f experiments_2\exp%%a/job_exp%%a_unetplus_tci.yaml
))

echo "batch complete"
```

jinja & bash

- We can use bash in addition to Powershell and Jinja2 to automate K8s job launch
- Creation of template Kube Spec YAML with environment variables (preceded by $)
- Bash scripting combined with environment variables to set the Dataset and/or Model to train and automatically launch the job

```
spec:
  template:
    spec:
      containers:
        - name: myContainer
          image: $CONTAINAER_IMAGE
          workingDir: $WORKDIR
```

Template YAML

```
Dirs="mydir1 mydir2 mydir3 mydir4"
Container=“ubuntu:20.04”

for Dirpath in $Dirs; do
   CONTAINER_IMAGE=$Container WORKDIR=$Dirpath envsubst < template.yml | kubectl apply -f -
done
```

Bash Script

Nautilus Job Launcher

- This Nautilus Job Launcher is an open-source Python library that enables automation of launching jobs on the NRP Nautlius HyperCluster.
  - https://github.com/MU-HPDI/Nautilus-Job-Launcher

- Installation:
  - Use the latest .whl pushed to GitLab's PyPI repository:

```
pip3 install --extra-index-url https://gitlab.nrp-nautilus.io/api/v4/projects/2953/packages/pypi/simple nautiluslauncher
```

  - You can clone this repository and use pip to install it:

```
pip3 install nautilus-job-launcher
```

Automating GPU Jobs on Nautilus

Nautilus Job Launcher

- The Nautilus Launcher can be used as
  - an application at the command line that will kick off jobs from a YAML config file
  - it can be utilized as a library integrated into other Python applications.

- You must have your Kubernetes config file in ~/.kube/config to use this library!

Automating GPU Jobs on Nautilus

Nautilus Job Launcher

- Command line: The job launcher is invoked as a library and uses a configuration file (YAML):

```
python3 -m nautiluslauncher -c cfg.yaml
```

- You can choose to perform a dryrun by passing a --dryrun flag:

```
python3 -m nautiluslauncher -c cfg.py --dryrun
```

- cfg.yaml: this file contains the required configuration for the Job launcher library to work

Nautilus Job Launcher

- Configuration requires three keys:
- Namesapce (required):
  - the namespace on the Nautilus cluster you'd like to use
- Jobs (required):
  - list of dictionaries that define all of the parameters for each job
- Defaults (optional):
  - It is a starting place for all jobs in your config.
  - All jobs will use the defaults as the beginning configuration and then whatever is placed in each job will be added to **or override** what is present in the defaults key

```
defaults:
    container: python:3.8
    workingDir: /mydir

jobs:
-
    container: python:3.7
-
    workingDir: /mydir2
-
    container: python:3.7
    workingDir: /mydir2
```

Key	Description	Default	Type
job_name	The name of the job	required	str
image	The container image to use	required	str
command	The command to run when the job starts	required	str/list[str]
workingDir	Working directory when the job starts	None	str
env	The environment variables	None	dict[str, str]
volumes	The volumes to mount	None	dict[str, str]
ports	The container ports to expose	None	list[int]
gpu_types	The types of GPUs required	None	list[str]
min_cpu	Minimum # of CPU Cores	2	int
max_cpu	Max # of CPU cores	4	int
min_ram	Min GB of RAM	4	int
max_ram	Max GB of RAM	8	int
gpu	# of GPUs	0	int
shm	When true, add shared memory mount	false	bool

Automating GPU Jobs on Nautilus

Nautilus Job Launcher

- Library usage:
- The Job launcher can be integrated with user's application/library
- This can be done in different ways:
  - import Job launcher into the user's scripts.
  - utilize a dictionary to configure your jobs and integrate that into your application
  - from a YAML file

Automating GPU Jobs on Nautilus

Nautilus Job Launcher

import Job Launcher into the user's scripts.

```
from nautiluslauncher import Job, NautilusAutomationClient

client = NautilusAutomationClient("mynamespace")
images = ["python:3.6", "python:3.7", "python:3.8"]
for i, img in enumerate(images):
    j = Job(job_name=f"test_python_{i}", image=i, command=["python", "-c", "print('hello world')"])
    client.create_job(j)
```

Automating GPU Jobs on Nautilus

Nautilus Job Launcher

Utilize a dictionary to configure your jobs

```
from nautiluslauncher import NautilusJobLauncher

my_jobs = {
    "namespace": "mynamespace",
    "jobs": [
        {"image": "python:3.6", command: ["python", "-c", "print('hello world')"], "job_name": "myjob1"}
        {"image": "python:3.7", command: ["python", "-c", "print('hello world')"], "job_name": "myjob2"}
        {"image": "python:3.8", command: ["python", "-c", "print('hello world')"], "job_name": "myjob3"}
    ]
}

launcher = NautilusJobLauncher(my_jobs)
launcher.run()
```

Automating GPU Jobs on Nautilus

Nautilus Job Launcher

from a YAML file

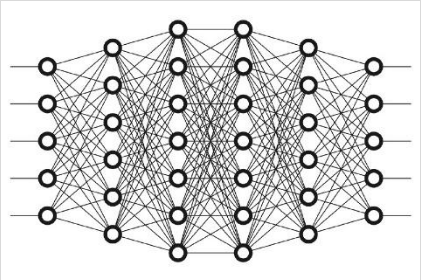
```
from nautiluslauncher import NautilusJobLauncher

my_file = "myCfg.yaml"

launcher = NautilusJobLauncher.from_config(my_file)
launcher.run()
```

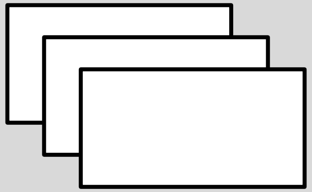
Deep Learning on Nautilus: Transformer Research

Nautilus

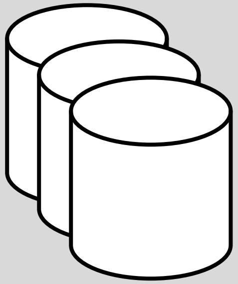


9 Deep Neural Architectures

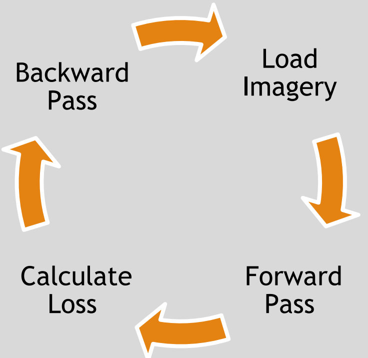
27 Trained Models



124.74 TB Imagery Processed



3 Open Source HR-RSI Datasets



- 8,100 Epochs
- 30M iterations
- 1.7B parameters

Wall Clock Time: 76 days, 10 hours

https://www.freecodecamp.org/news/want-to-know-how-deep-learning-works-heres-a-quick-guide-for-everyone-1aedeca88076/
https://commons.wikimedia.org/wiki/File:PyTorch_logo_icon.svg
https://www.clipartmax.com/download/m2K9A0m2b1m2i8i8_4-o-clock-clip-art-clock-face-clip-art/

MUAMLL/SDSS2025

- NRP Portal

  https://portal.nrp-nautilus.io

- JupyterHub Instance:

  https://gp-engine.nrp-nautilus.io/

- Tutorial Repository for this Tutorial:

  https://github.com/MUAMLL/SDSS2025

- Git Clone Command:

  git clone https://github.com/MUAMLL/SDSS2025.git