Interactive HPC using Containers on Nautilus

Introduction to PRP Nautilus, Kubernetes, and Containerized Software

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UC SANTA CRUZ

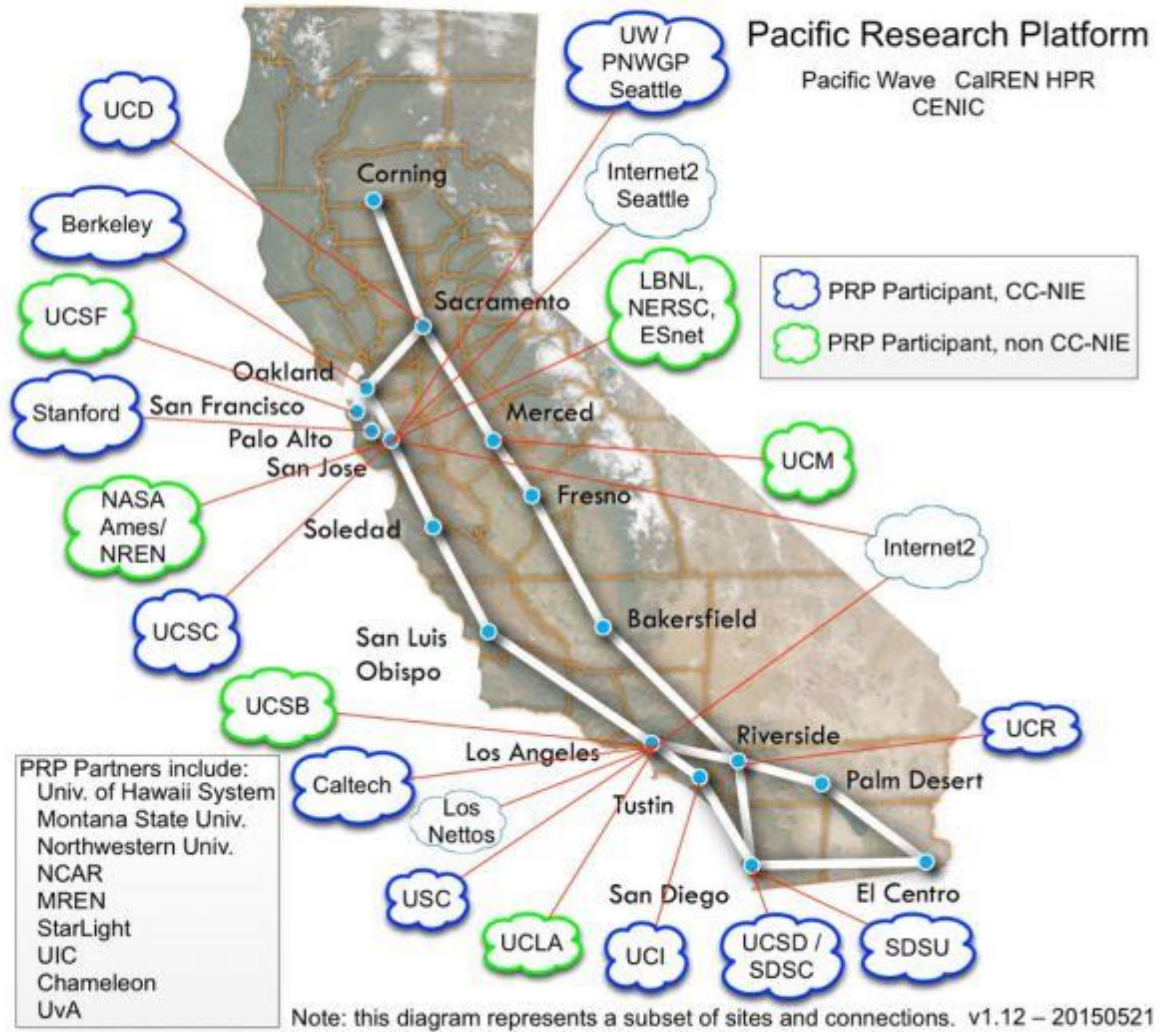
Agenda

1. Introduction
2. Background
    2.1. Pacific Research Platform
    2.2. Nautilus Cluster
3. About Containers and Kubernetes
4. Accessing Nautilus
5. Software Tools
6. Cluster Control
7. Data
8. Other considerations
9. Jupyter
10. Concluding Q&A

What is the Pacific Research Platform?

- The PRP is a partnership of more than 50 institutions, led by researchers at UC San Diego and UC Berkeley.
- PRP is an end-to-end high-speed data freeway built on CENIC and Pacific NW GigaPOP fiber optic networks
- Built for data intensive science collaboration
- Led to the rise of data-intensive science collaborations

The PRP 2015-2020



PRP PACIFIC RESEARCH PLATFORM

Larry Smarr
PI
UCSD

Camille Crittenden
Co-PI
UCB

Philip Papadopoulos
Co-PI
UCI

Thomas DeFanti
Co-PI
UCSD

Frank Wuerthwein
Co-PI
UCSD

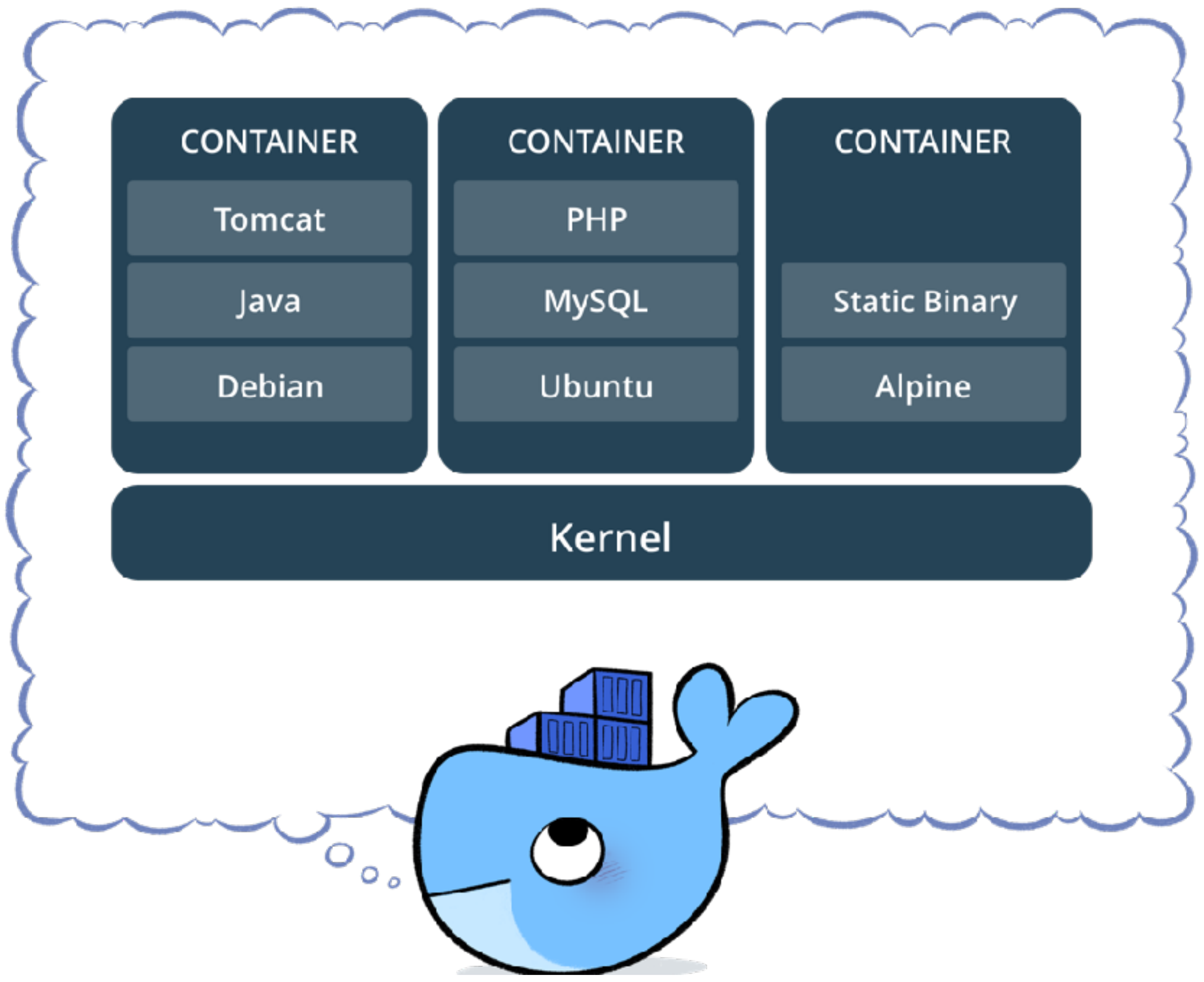
What is Nautilus?

- Nautilus1 is a highly distributed, but centrally managed community cyberinfrastructure. It is an on-demand, real-time accessible cluster with >500 GPUs and >7000 CPU cores.
- Approximately 187 nodes provide service from all 10 UC campuses and many partner institutions
- Researchers on more than 30 campuses use Nautilus
- Nautilus advantageously exploits the networking, space, and features of many of the Science DMZs previously built with NSF funding on over 100 US campuses.
- Unlike traditional HPC, Nautilus is interactive

About Containers and Orchestration Schemes…

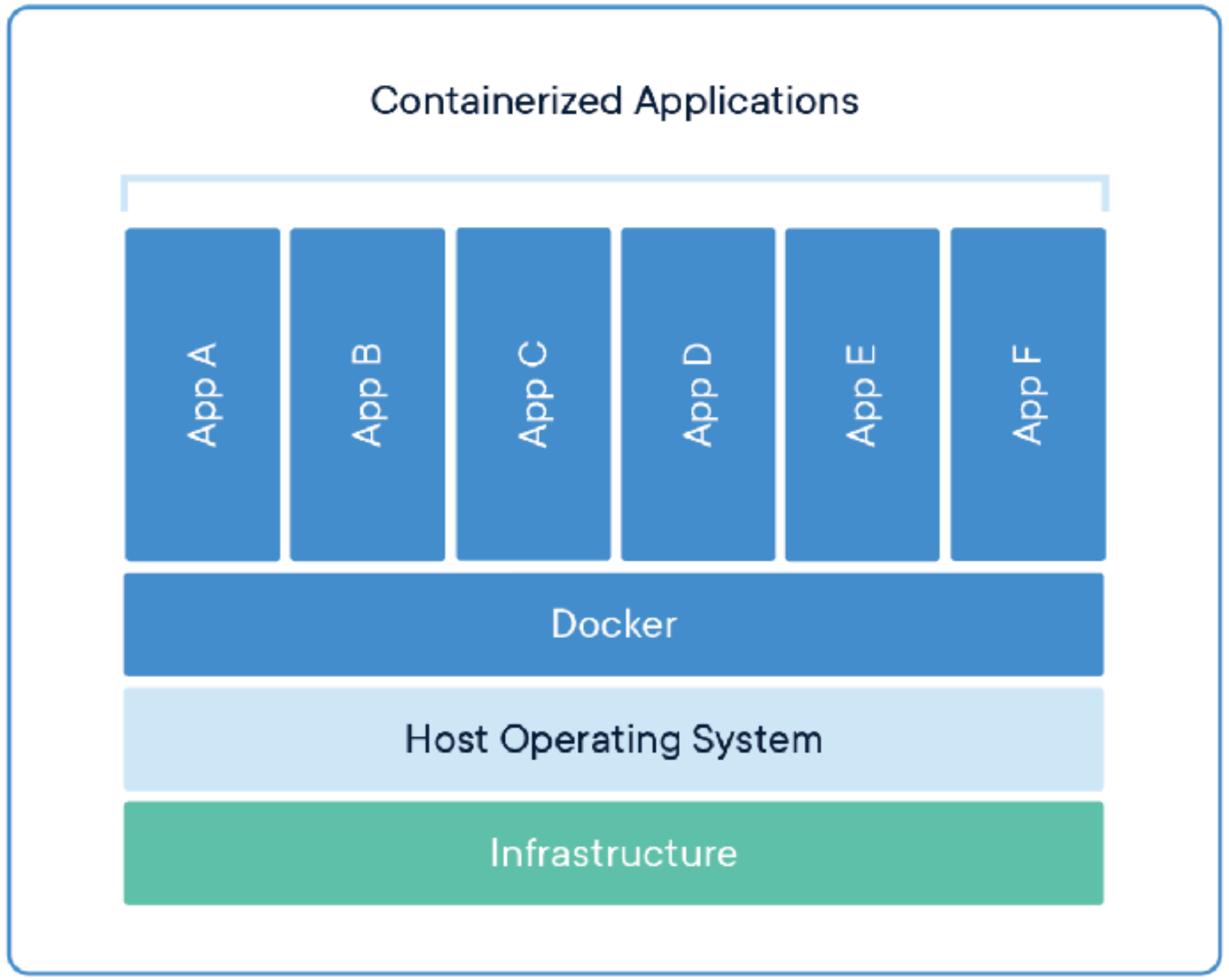
First…what is a container?

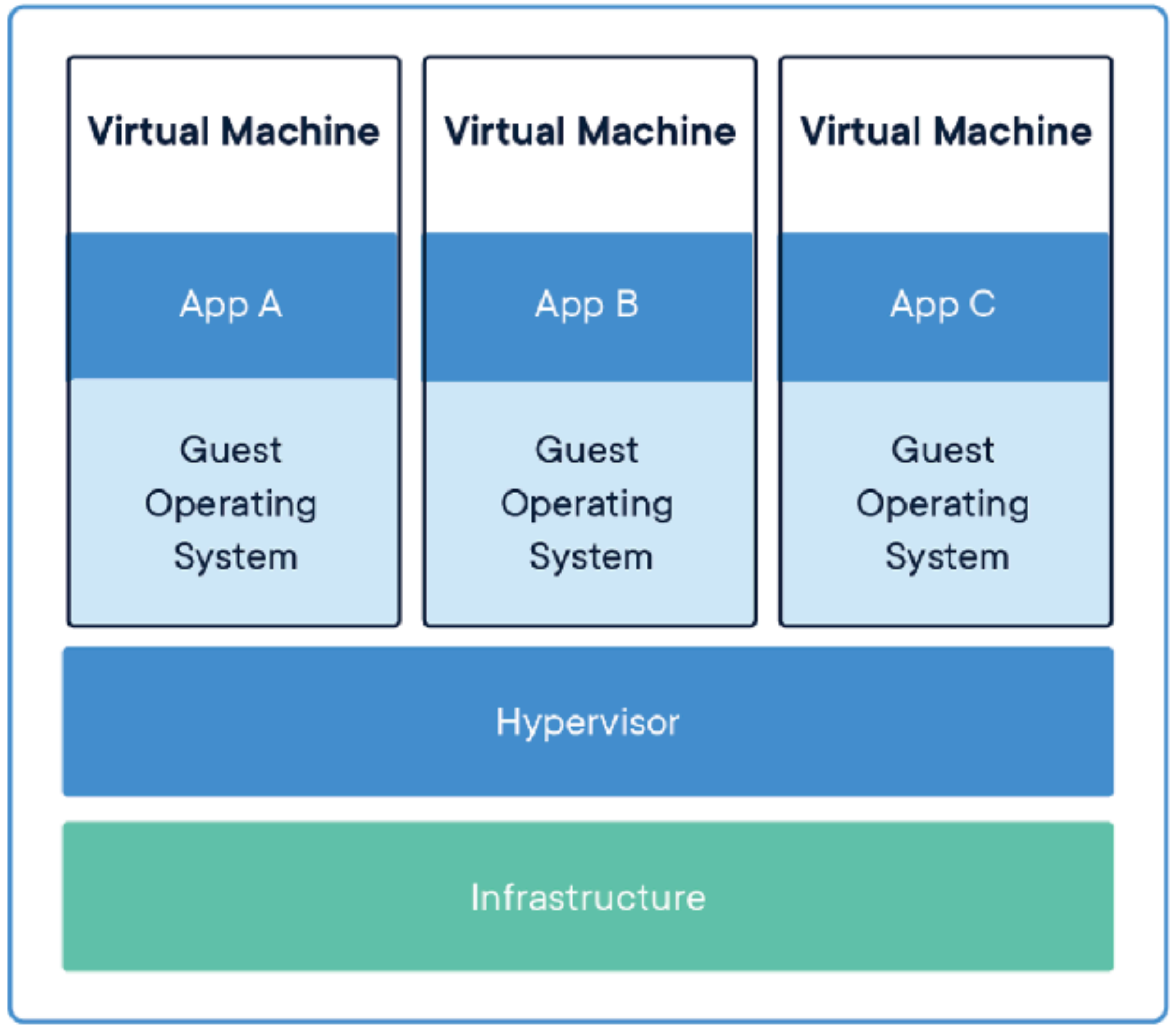
Containerization is the packaging of software code with just the operating system (OS) libraries and dependencies required to run the code to create a single lightweight executable.



From https://www.scalyr.com/blog/containers-benefits-and-making-a-business-case

Software Containers versus Virtual Machines





Containers are an abstraction at the app layer that packages code and dependencies together. Multiple containers can run on the same machine and share the OS kernel with other containers, each running as isolated processes in user space.

Virtual machines (VMs) are an abstraction of physical hardware turning one server into many servers. The hypervisor allows multiple VMs to run on a single machine. Each VM includes a full copy of an operating system, the application, necessary binaries and libraries - taking up tens of GBs.

From https://www.docker.com/resources/what-container

Kubernetes Cluster vs. Traditional HPC

- Both K8s and HPC schedulers are workload managers
- HPC focuses on high throughput jobs with distributed memory
- Jobs are scheduled and resources can be allocated based on sophisticated accounting schemes
- K8s allows for interaction with running jobs (pods)
- K8s scheduler matches pods to appropriate nodes, more sophisticated scheduling is possible, but atypical

What is Kubernetes (K8s)

K8s is an open-source container orchestration system for automating software deployment, scaling, and management.

Key K8s Concepts

- **Control Plane** manages the workload, handles internode communications, keeps knowledge of the cluster state, provides scheduling services, manages resources, and exposes the K8s API so that both internal and external interfaces can be used.
- **Nodes** - a node is a physical machine were containers are deployed. Each node must run a container runtime (in Nautilus, it is 'Containerd').
- **Namespaces** provides a way for K8s to partition cluster resources across multiple or many users in an exclusive way.
- **Pods** - pods are the basic scheduling unit of K8s. Pods consist of one or more containers running inside. Each pod gets a unique IP address (important!) so that micro services or applications can access the pod without contention. Pod IP addresses are ephemeral.
- **Services** are a set of pods working together.

Pods in Nautilus

Pods are the smallest, most basic deployable objects in Kubernetes. A Pod represents a single instance of a running process in your cluster.

Pods contain one or more containers, such as Docker containers.

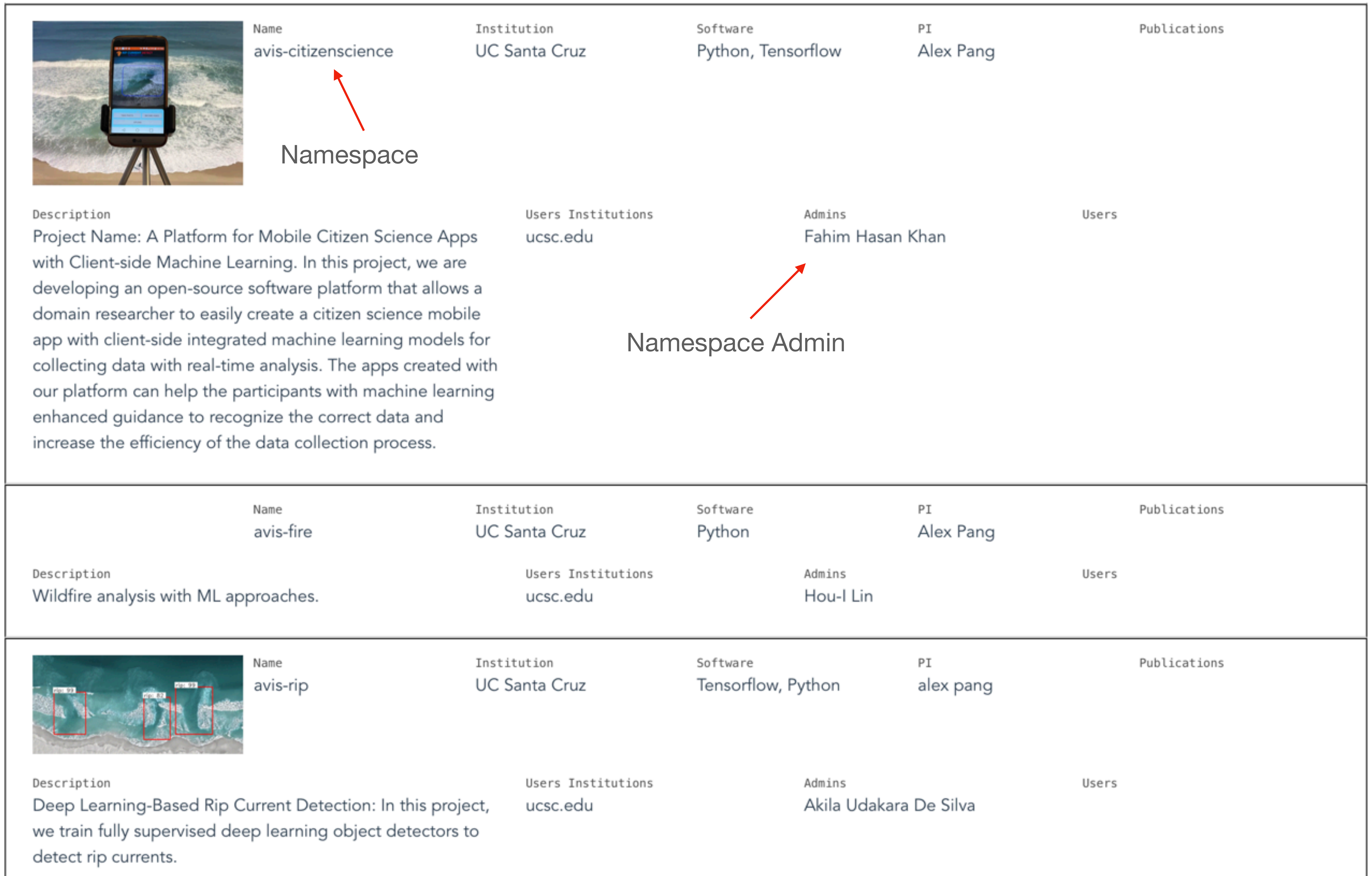
Pods also contain shared networking and storage resources for their containers:

- Network: Pods are automatically assigned unique IP addresses. Pod containers share the same network namespace, including IP address and network ports. Containers in a Pod communicate with each other inside the Pod on localhost
- Storage: Pods can specify a set of shared storage volumes that can be shared among the containers

Pods running on a cluster are automatically able to communicate with other pods

Managing Users with Namespaces

Groups of users working together



Name	Institution	Software	PI	Publications
avis-citizenscience	UC Santa Cruz	Python, Tensorflow	Alex Pang	

Namespace

Description	Users Institutions	Admins	Users
Project Name: A Platform for Mobile Citizen Science Apps with Client-side Machine Learning. In this project, we are developing an open-source software platform that allows a domain researcher to easily create a citizen science mobile app with client-side integrated machine learning models for collecting data with real-time analysis. The apps created with our platform can help the participants with machine learning enhanced guidance to recognize the correct data and increase the efficiency of the data collection process.	ucsc.edu	Fahim Hasan Khan	

Namespace Admin

Name	Institution	Software	PI	Publications
avis-fire	UC Santa Cruz	Python	Alex Pang	

Description	Users Institutions	Admins	Users
Wildfire analysis with ML approaches.	ucsc.edu	Hou-I Lin	

Name	Institution	Software	PI	Publications
avis-rip	UC Santa Cruz	Tensorflow, Python	alex pang	

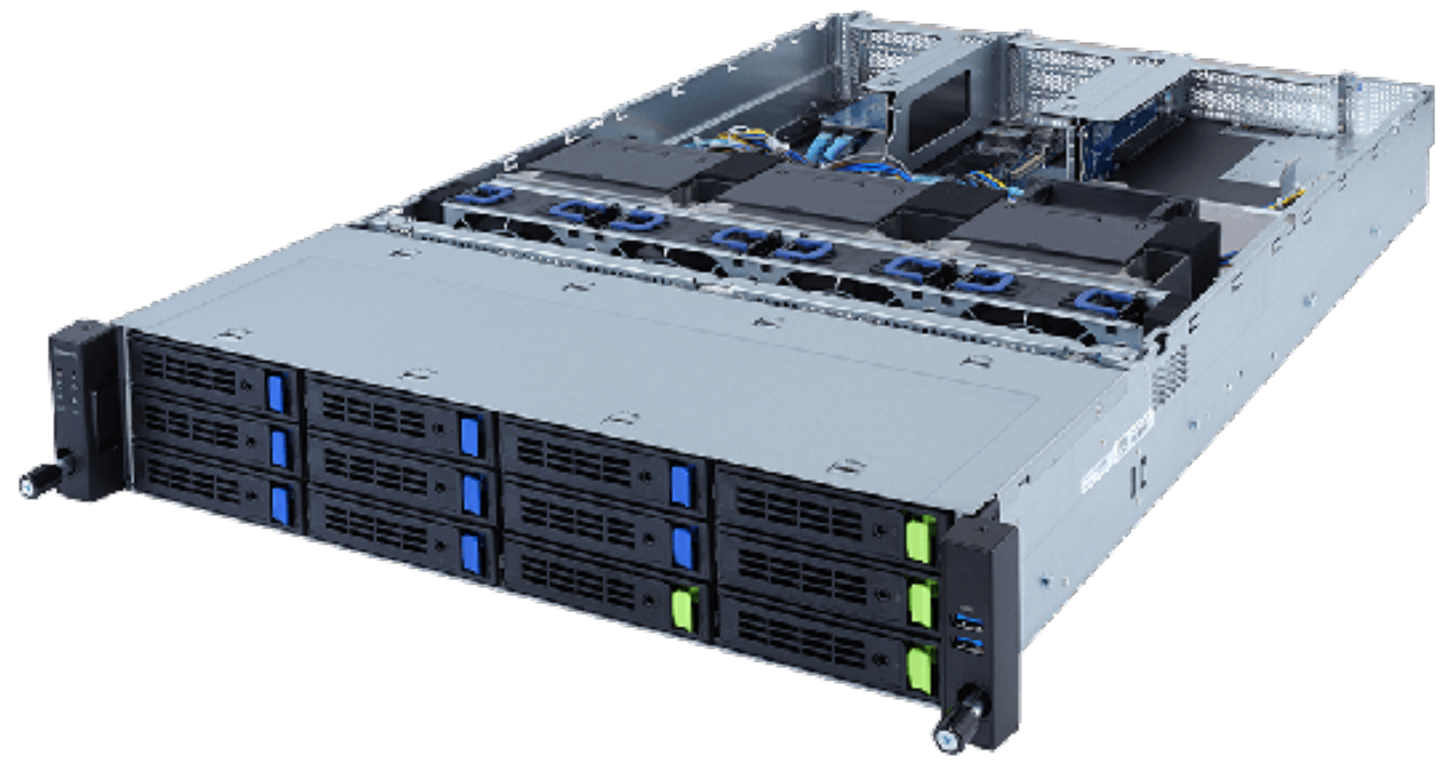
Description	Users Institutions	Admins	Users
Deep Learning-Based Rip Current Detection: In this project, we train fully supervised deep learning object detectors to detect rip currents.	ucsc.edu	Akila Udakara De Silva	

Two kinds of Nautilus Nodes

- Built on top of PRP 10-100Gbps networks
- Standardized hardware profiles
  - 8-GPU Servers (FIONA8s)
  - High-density Storage Nodes
  - NVMe and SSDs
  - 10Gbps NIC for GPUs
  - Dual 100 Gbps NIC for storage

GPU Node

GIGABYTE


Storage Node

Software Tools

Cookies

An Analogy for Nautilus

- The ingredients you choose are you code. You can adjust them to suit your needs or taste
- The mixer (or spoon and bowl) are your development tools (e.g. Docker or VIM)
- The YAML file is the recipe. How you will mix your ingredients together
- kubectl controls the oven
- Nautilus is your oven. It has many features to help you make your cookies delicious.

Using, Creating and Deploying Containerized Software

Docker, Docker Hub, YAML and Kubectl

- Docker (or other containerization software) is used to create images. Common practice is to develop inside Docker, with the container running while you make changes to your code (aka DevOps)
- Docker Hub contains thousands of pre-built images (what you need may already be available)
- Once you know what software you want to use, YAML provides the “recipe” for your deployment
- Kubectl is the tool to launch your deployments

Let’s examine Docker…

Docker and Docker Hub

Code Reuse at https://hub.docker.com
Code Development using Docker https://docs.docker.com/get-started/overview/

We know that…

- Kubernetes is an orchestration framework for deploying containerized software. It is naive about the actual software.
- In order for you to develop Services, you will need to use or create software to deploy
- Most people can simply re-use software by referencing a pre-built Docker image
- Users customize existing Docker images with additional software for their purpose
- There are many thousands of these images available on Docker Hub
- Users can create their own software containers using Docker on their local computer

Container Supply Chain

aka DevOps

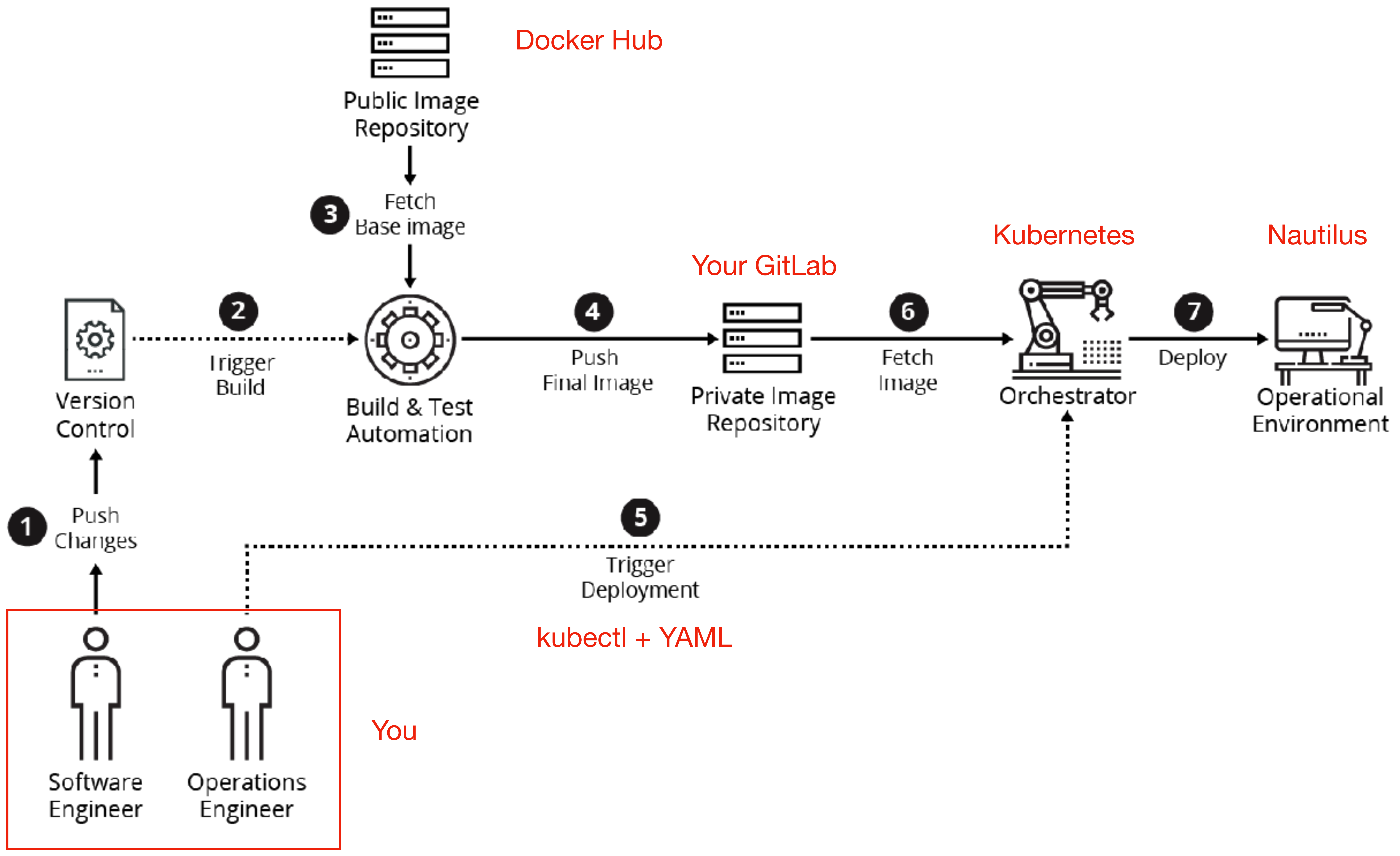


Figure 4: Model Container Supply Chain

From: CMU's Software Engineering Institute "7 Quick Steps to Using Containers Securely"

```yaml
kind: Pod
metadata:
  name: test-pod
spec:
  containers:
  - name: mypod
    image: centos:centos7
    resources:
      limits:
        memory: 100Mi
        cpu: 100m
      requests:
        memory: 100Mi
        cpu: 100m
```

YAML: Yet Another Markup Language

Code is what you will run…

Using YAML and kubectl is *how* you will run it

What is YAML?

- A human-readable data-serialization language
- Commonly used for configurations
- Similar to eXtensible Markup Language, but with fewer syntax conventions
- Python-style indentation to reflect hierarchy and order-of-operations
- Encodes strings, integers, floats and arrays
- Most Nautilus users modify example YAML files
- Used to request resources, deploy services and code (in containers)

Sample YAML File

for a generic pod

```yaml
apiVersion: v1
kind: Pod
metadata:
  name: test-pod
spec:
  containers:
  - name: mypod
    image: centos:centos7
    resources:
      limits:
        memory: 100Mi
        cpu: 100m
      requests:
        memory: 100Mi
        cpu: 100m
    command: ["sh", "-c", "echo 'Im a new pod' && sleep infinity"]
```

Using Nautilus

Account setup
Namespace
Software
Deployment
Getting Help

Nautilus Access Levels

There are three levels of access to Nautilus

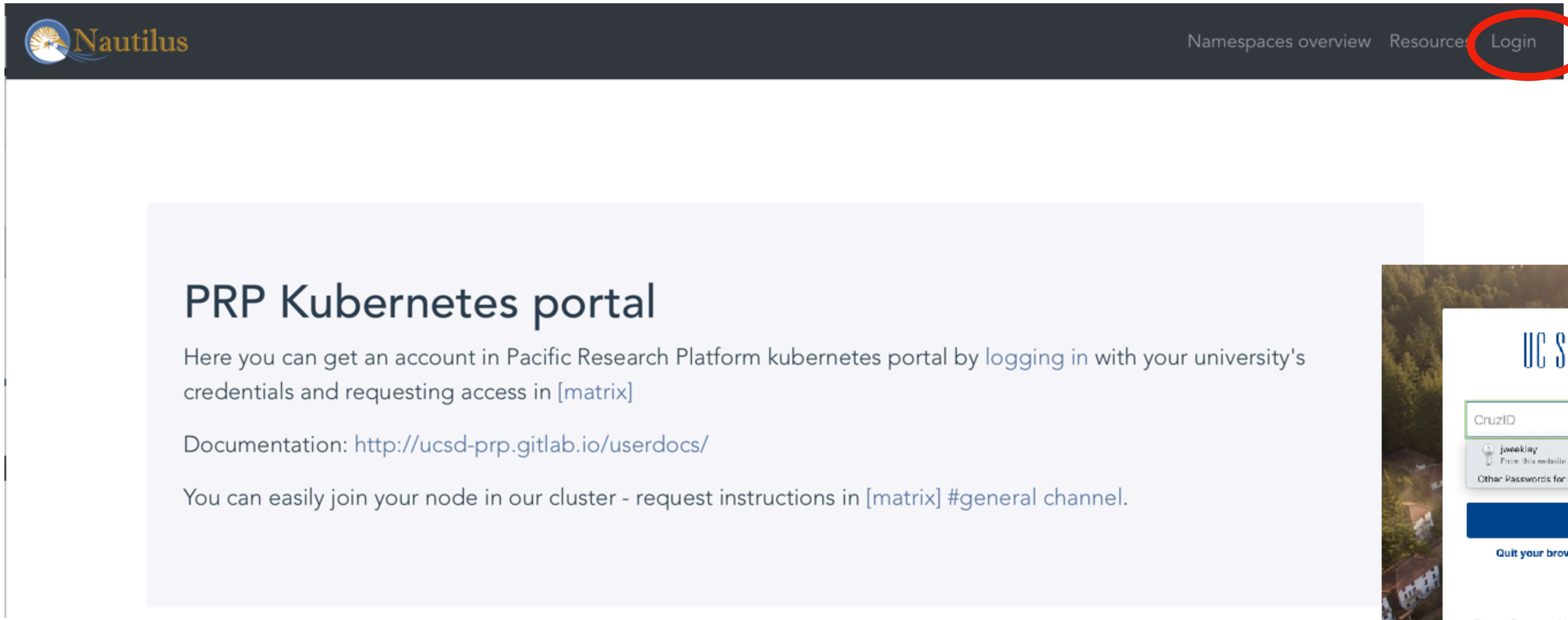
Guest

User

Admin

Logging in for the First Time

Using CI Login and Your Institutional Credentials

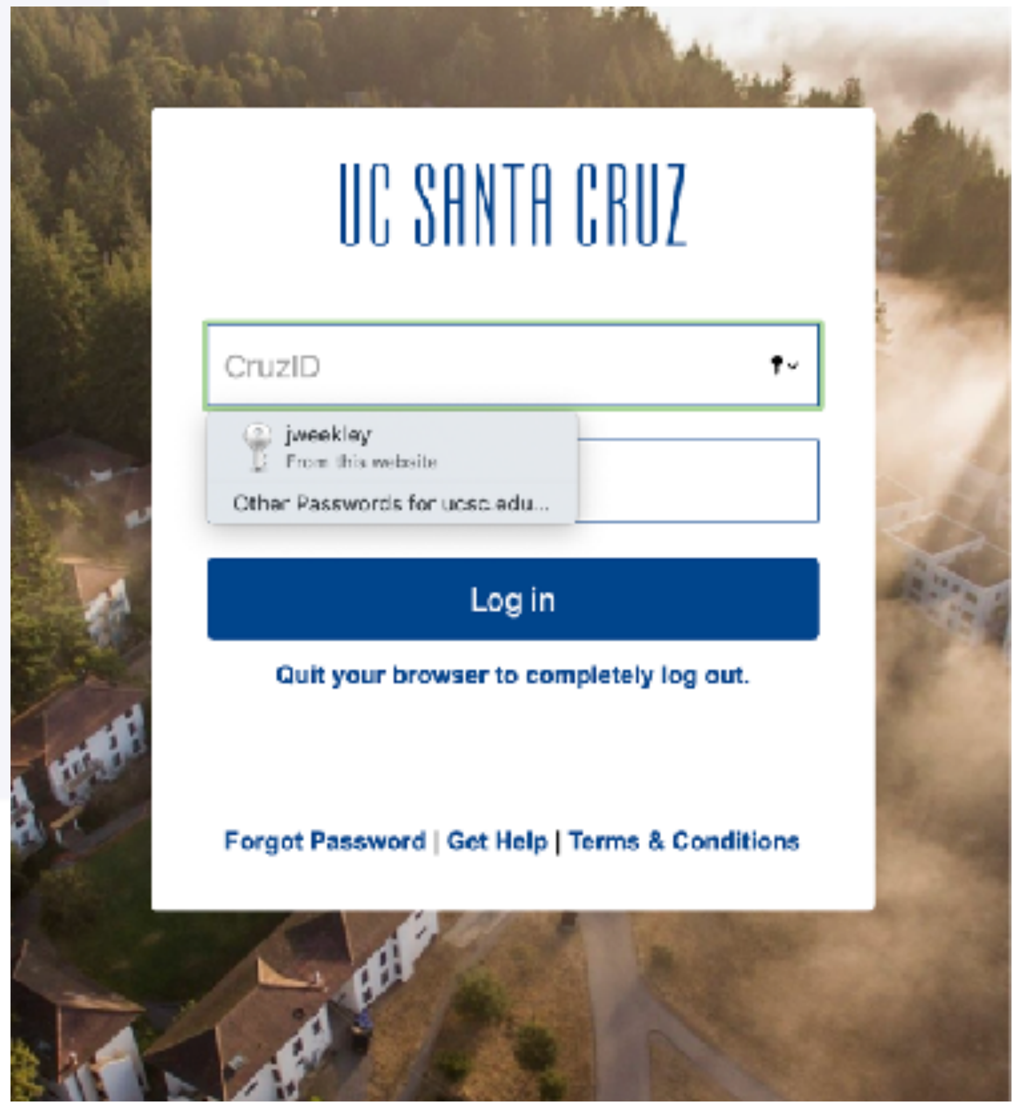


PRP Kubernetes portal

Here you can get an account in Pacific Research Platform kubernetes portal by logging in with your university's credentials and requesting access in [matrix]

Documentation: http://ucsd-prp.gitlab.io/userdocs/

You can easily join your node in our cluster - request instructions in [matrix] #general channel.



Quit your browser to completely log out.

Forgot Password | Get Help | Terms & Conditions

Guest Level

Once you’ve logged in for the first time, you are a “Guest”

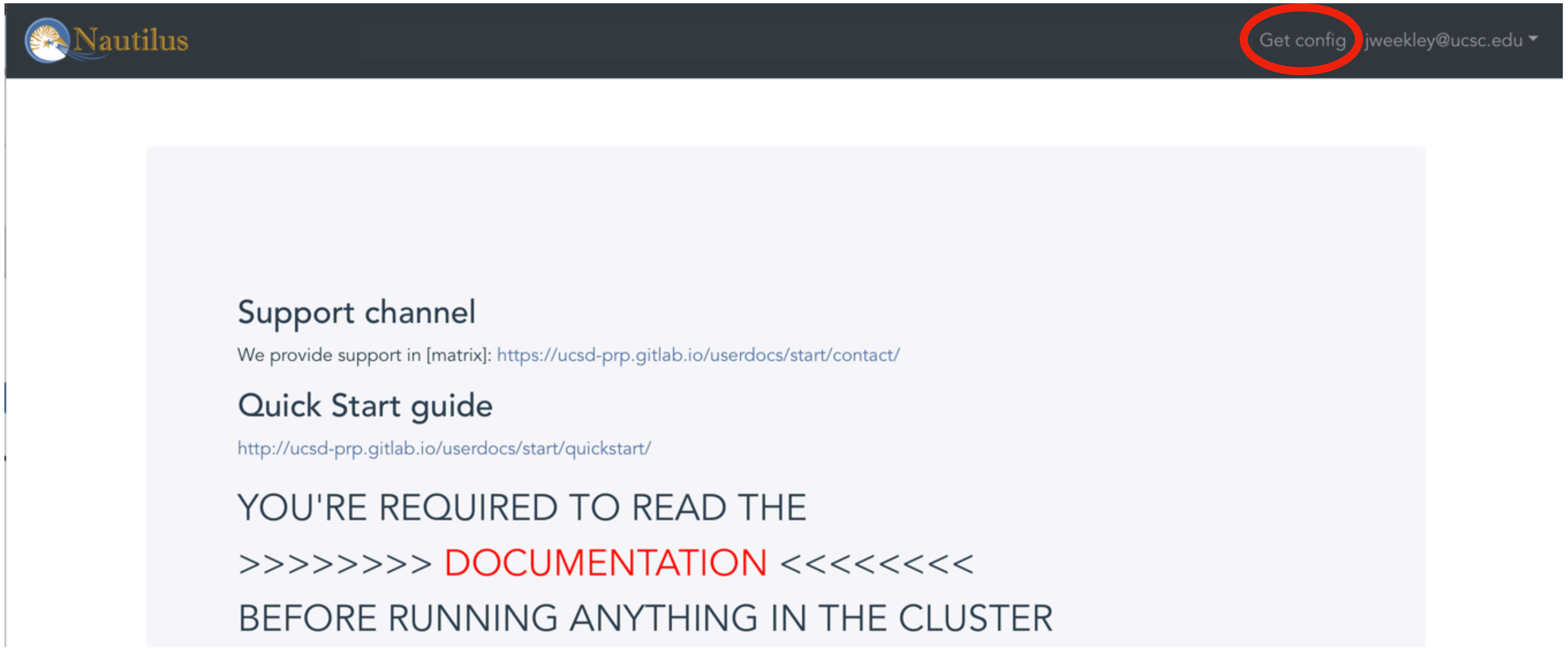
Guests have credentials but no privileges. Before you can access resources, you must be validated.

At this stage, you merely get your system configured to use Nautilus

Required Software and Configuration

Kubectl and Nautilus Configuration File

Logged in with my
Institutional Credential



Support channel

We provide support in [matrix]: https://ucsd-prp.gitlab.io/userdocs/start/contact/

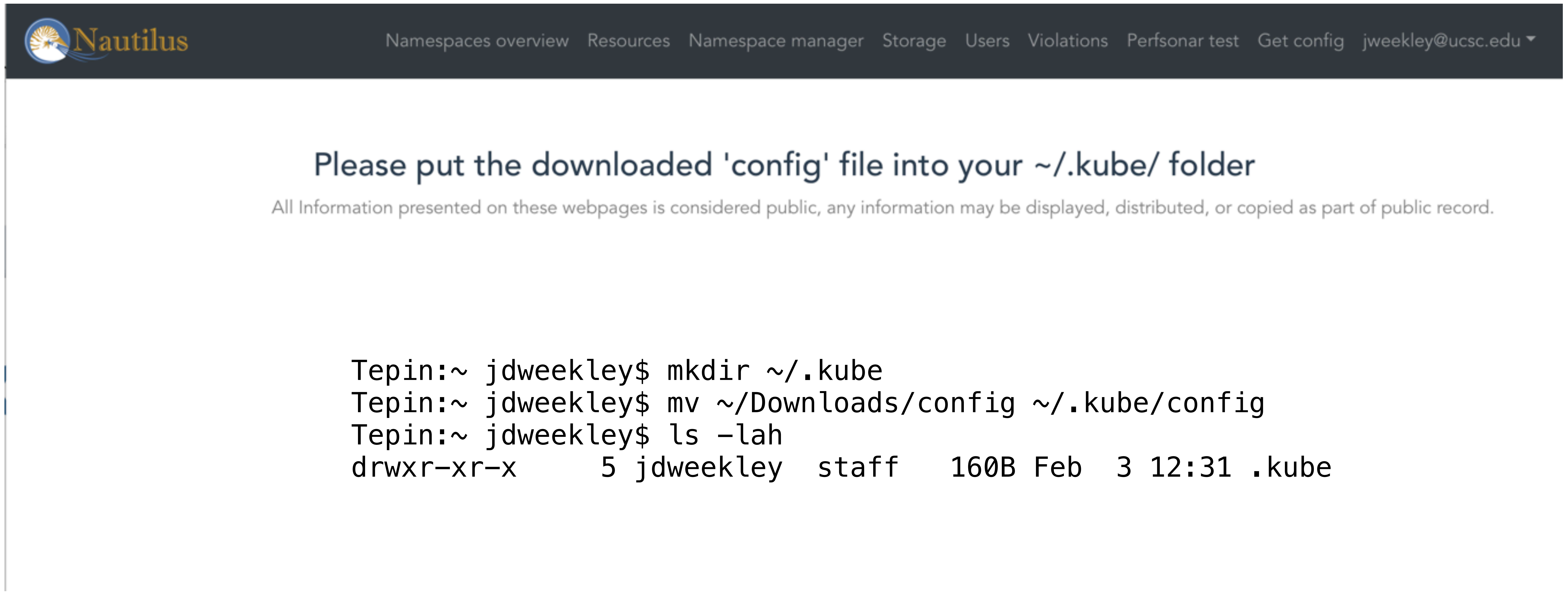
Quick Start guide

http://ucsd-prp.gitlab.io/userdocs/start/quickstart/

YOU'RE REQUIRED TO READ THE
>>>>>>>>> DOCUMENTATION <<<<<<<<<
BEFORE RUNNING ANYTHING IN THE CLUSTER

Download Configuration File

You may need to login again - be sure to use the same credentials



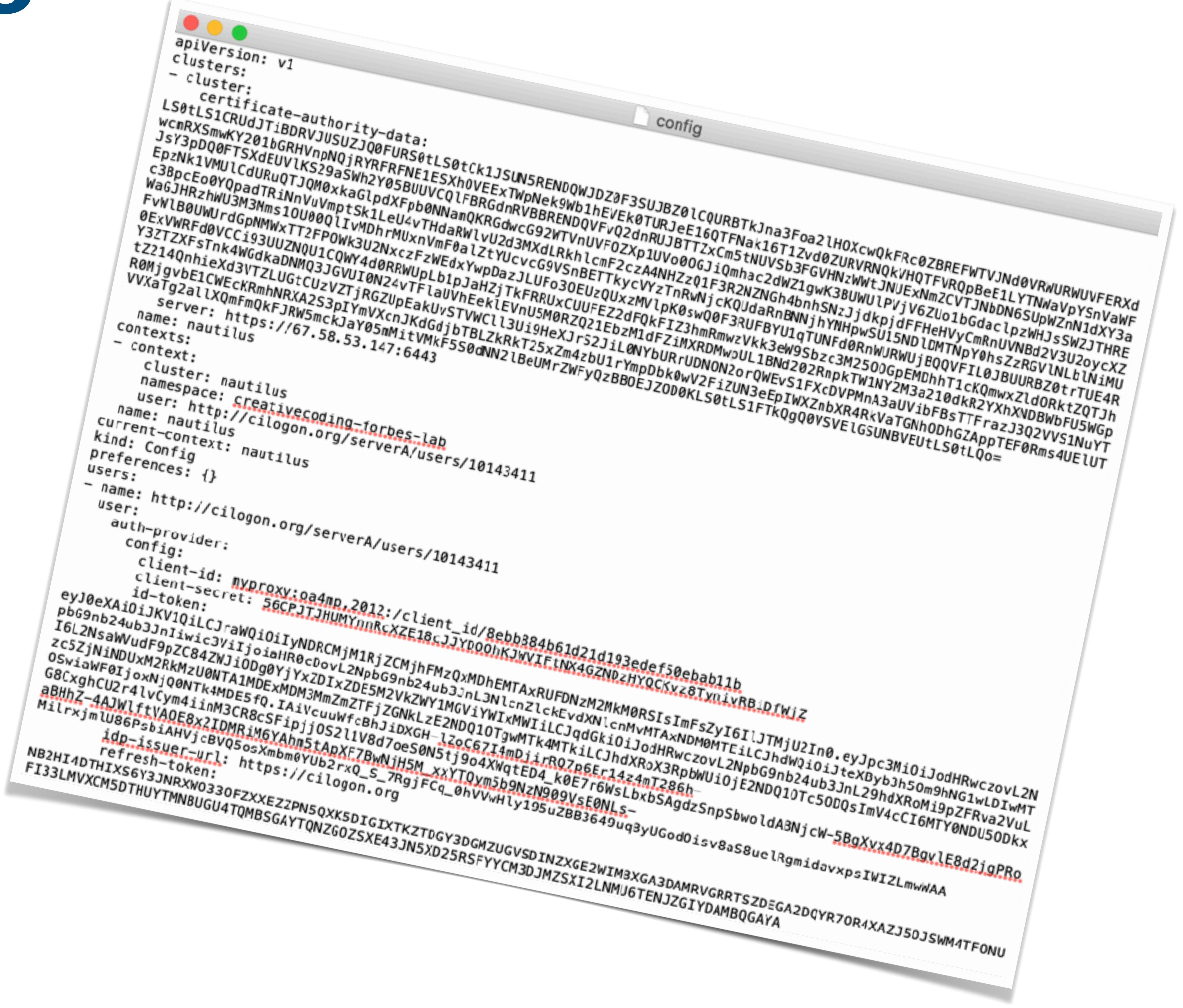
Please put the downloaded 'config' file into your ~/.kube/ folder

All Information presented on these webpages is considered public, any information may be displayed, distributed, or copied as part of public record.

```
Tepin:~ jdweekley$ mkdir ~/.kube
Tepin:~ jdweekley$ mv ~/Downloads/config ~/.kube/config
Tepin:~ jdweekley$ ls -lah
drwxr-xr-x     5 jdweekley  staff   160B Feb  3 12:31 .kube
```

In your home directory, create a hidden folder, where you will place the downloaded configuration file

The Configuration File



```
apiVersion: v1
clusters:
- cluster:
    certificate-authority-data:
LS0tLS1CRUdJTiBDRVJUSUZJQ0FURS0tLS0tCk1JSUN5RENDQWJDZ0F3SUJBZ0lCQURBTkJna3Foa2lHOXcwQkFRc0ZBREFWTVJNd0VRWURWUVFERXd
wcmRXSmwKY201bGRHVnpNQjRYRFRFNE1ESXh0VEExTWpNek9Wb1hEVEk0TURJeE16QTFNak16T1Zvd0ZURVRNQkVHQTFVRQpBeE1LYTNWaVpYSnVaWF
JsY3pDQ0FTSXdEUVlKS29aSWh2Y05BUUVCQlFBRGdnRVBBRENDQVFvQ2dnRUJBTTZxCm5tNUVSb3FGVHNzWWtJNUExNmZCVTJNbDN6SUpWZnN1dXY3a
EpzNk1VMUlCdURuQTJQM0xkaGlpdXFpb0NNamQKRGdwcG92WTVnUVFOZXp1UVo0OGJiQmhac2dWZ1gwK3BUWUlPVjV6Zlo1bGdaclpzWHJsSWZJTHRE
c3BpcEo0YQpadTRiNnVuVmptSk1LeU4vTHdaRWlvU2d3MXdLRkhlcmF2czA4NHZzQ1F3R2NZNGh4bnhSNzJjdkpjdFFHeHVyCmRnUVNBd2V3U2oycXZ
WaGJHRzhWU3M3Mms1OU00QlIvMDhrMUxnVmF0alZtYUcvcG9VSnBETTkycVYzTnRwNjcKQUdaRnBNNjhYNHpwSU15NDlDMTNpY0hsZzRGVlNLblNiMU
FvWlB0UWUrdGpNMWxTT2FPOWk3U2NxczFzWEdxYwpDazJLUFo3OEUzQUxzMVlpK0swQ0F3RUFBYU1qTUNFd0RnWURWUjBQQVFIL0JBUURBZ0trTUE4R
0ExVWRFd0VCCi93UUZNQU1CQWY4d0RRWUpLb1pJaHZjTkFRUUxCUUFEZ2dFQkFIZ3hmRmwzVkk3eW9Sbzc3M25OOGpEMDhhT1cKQmwxZldORktZQTJh
Y3ZTZXFsTnk4WGdkaDNMQ3JGVUI0N24vTFlaUVhEeklEVnU5M0RZQ21EbzM1dFZiMXRDMwpUL1BNd202RnpkTW1NY2M3a210dkR2YXhXNDBWbFU5WGp
tZ214QnhieXd3VTZLUGtCUzVZTjRGZUpEakUvSTVWCll3Ui9HeXJrS2JiL0NYbURrUDNON2orQWEvS1FXcDVPMnA3aUVibFBsTTFrazJ3Q2VVS1NuYT
R0MjgvbE1CWEcKRmhNRXA2S3pIYmVXcnJKdGdjbTBLZkRkT25xZm4zbU1rYmpDbk0wV2FiZUN3eEpIWXZmbXR4RkVaTGNhODhGZAppTEF0Rms4UElUT
VVXaTg2allXQmFmQkFJRW5mckJaY05mMitVMkF5S0dNN2lBeUMrZWFyQzBBOEJZOD0KLS0tLS1FTkQgQ0VSVElGSUNBVEUtLS0tLQo=
    server: https://67.58.53.147:6443
  name: nautilus
contexts:
- context:
    cluster: nautilus
    namespace: creativecoding-forbes-lab
    user: http://cilogon.org/serverA/users/10143411
  name: nautilus
current-context: nautilus
kind: Config
preferences: {}
users:
- name: http://cilogon.org/serverA/users/10143411
  user:
    auth-provider:
      config:
        client-id: myproxy:oa4mp,2012:/client_id/8ebb384b61d21d193edef50ebab11b
        client-secret: 56CPJTJHUMYnnRcXZE18cJJYDOOhKJWVIFtNX4GZNDzHYQCKvz8TynivRBiDfWjZ
        id-token:
eyJ0eXAiOiJKV1QiLCJraWQiOiIyNDRCMjM1RjZCMjhFMzQxMDhEMTAxRUFDNzM2MkM0RSIsImFsZyI6IlJTMjU2In0.eyJpc3MiOiJodHRwczovL2N
pbG9nb24ub3JnIiwic3ViIjoiaHR0cDovL2NpbG9nb24ub3JnL3NlcnZlckEvdXNlcnMvMTAxNDM0MTEiLCJhdWQiOiJteXByb3h5Om9hNG1wLDIwMT
I6L2NsaWVudF9pZC84ZWJiODg0YjYxZDIxZDE5M2VkZWY1MGViYWIxMWIiLCJqdGkiOiJodHRwczovL2NpbG9nb24ub3JnL29hdXRoMi9pZFRva2VuL
zc5ZjNiNDUxM2RkMzU0NTA1MDExMDM3MmZmZTFjZGNkLzE2NDQ1OTgwMTk4MTkiLCJhdXRoX3RpbWUiOjE2NDQ1OTc5ODQsImV4cCI6MTY0NDU5ODkx
OSwiaWF0IjoxNjQ0NTk4MDE5fQ.IAiVcuuWfcBhJiDXGH-lZoC67I4mDjirRQ7p6Er14z4mT286h-
G8CxghCU2r4lvCym4iinM3CR8cSFipjjOS2l1V8d7oeS0N5tj9o4XWqtED4_k0E7r6WsLbxbSAgdzSnpSbwoldA3NjcW-5BgXvx4D7BgvlE8d2jgPRo
aBHhZ-4AJWlftVAOE8x2IDMRiM6YAhm5tApXF7BwNjH5M_xxYTQym5b9NzN909VsE0NLs-
MilrxjmlU86PsbiAHVjcBVQ5osXmbm0YUb2rxQ_S_7RgjFCq_0hVVwHly195uZBB3649uq3yUGodOisv8aS8uelRgmidavxpsIWIZLmwWAA
        idp-issuer-url: https://cilogon.org
        refresh-token:
NB2HI4DTHIXS6Y3JNRXW033OFZXXEZZPN5QXK5DIGIXTKZTDGY3DGMZUGVSDINZXGE2WIM3XGA3DAMRVGRRTSZDEGA2DQYR7OR4XAZJ5DJSWM4TFONU
FI33LMVXCM5DTHUYTMNBUGU4TQMBSGAYTQNZGOZSXE43JN5XD25RSFYYCM3DJMZSXI2LNMJ6TENJZGIYDAMBQGAYA
```

Contains credentials and configurations that link your local computer to the cluster

Access Levels

Guest

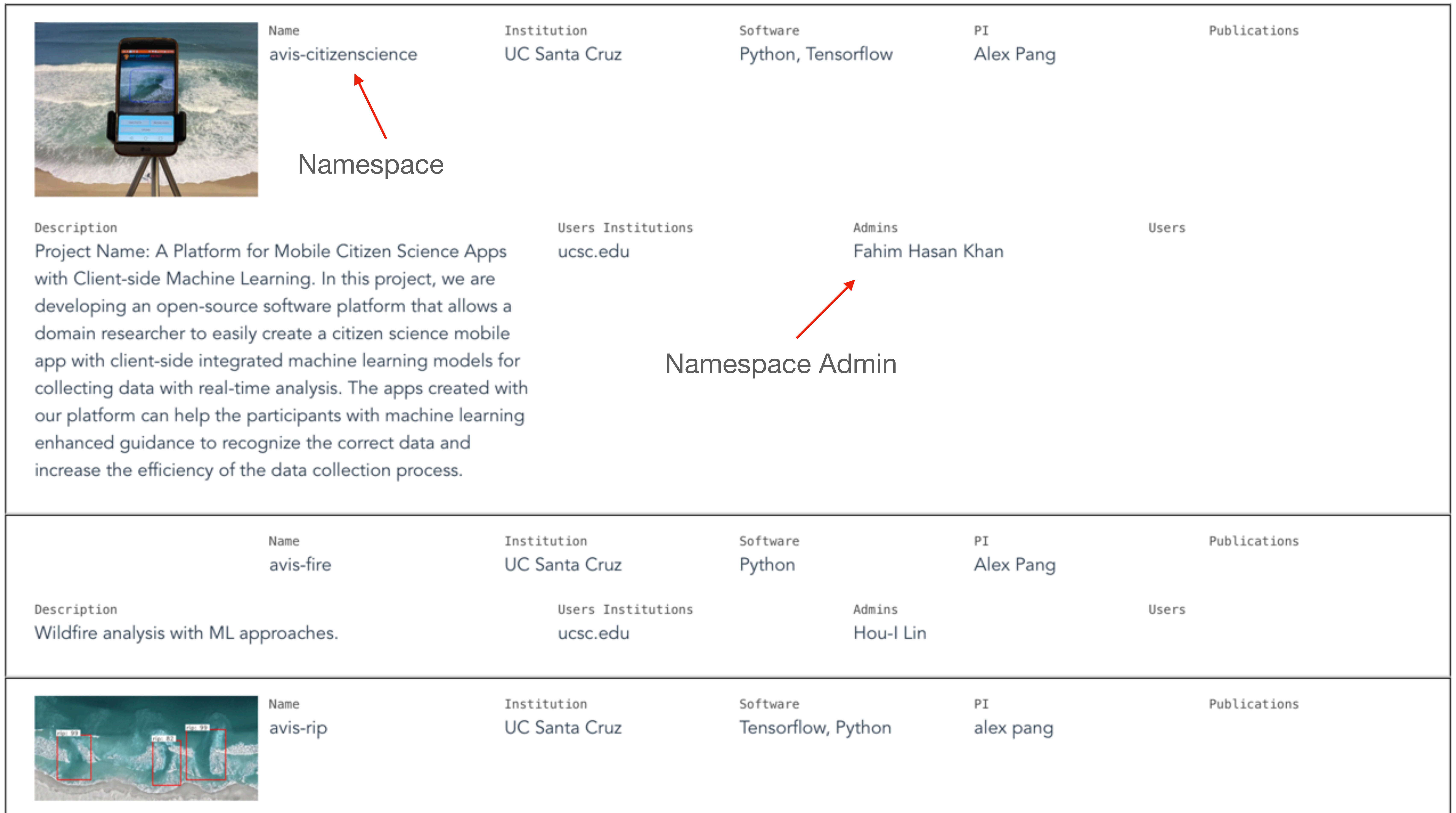
User

Admin

User Level

Guests navigate to Nautilus' Matrix Chat #Nautilus Support channel to be promoted from Guest to User.

Users may then join an existing namespace by submitting a request to the namespace admin



Name	Institution	Software	PI	Publications
avis-citizenscience	UC Santa Cruz	Python, Tensorflow	Alex Pang	

Description	Users Institutions	Admins	Users
Project Name: A Platform for Mobile Citizen Science Apps with Client-side Machine Learning. In this project, we are developing an open-source software platform that allows a domain researcher to easily create a citizen science mobile app with client-side integrated machine learning models for collecting data with real-time analysis. The apps created with our platform can help the participants with machine learning enhanced guidance to recognize the correct data and increase the efficiency of the data collection process.	ucsc.edu	Fahim Hasan Khan	

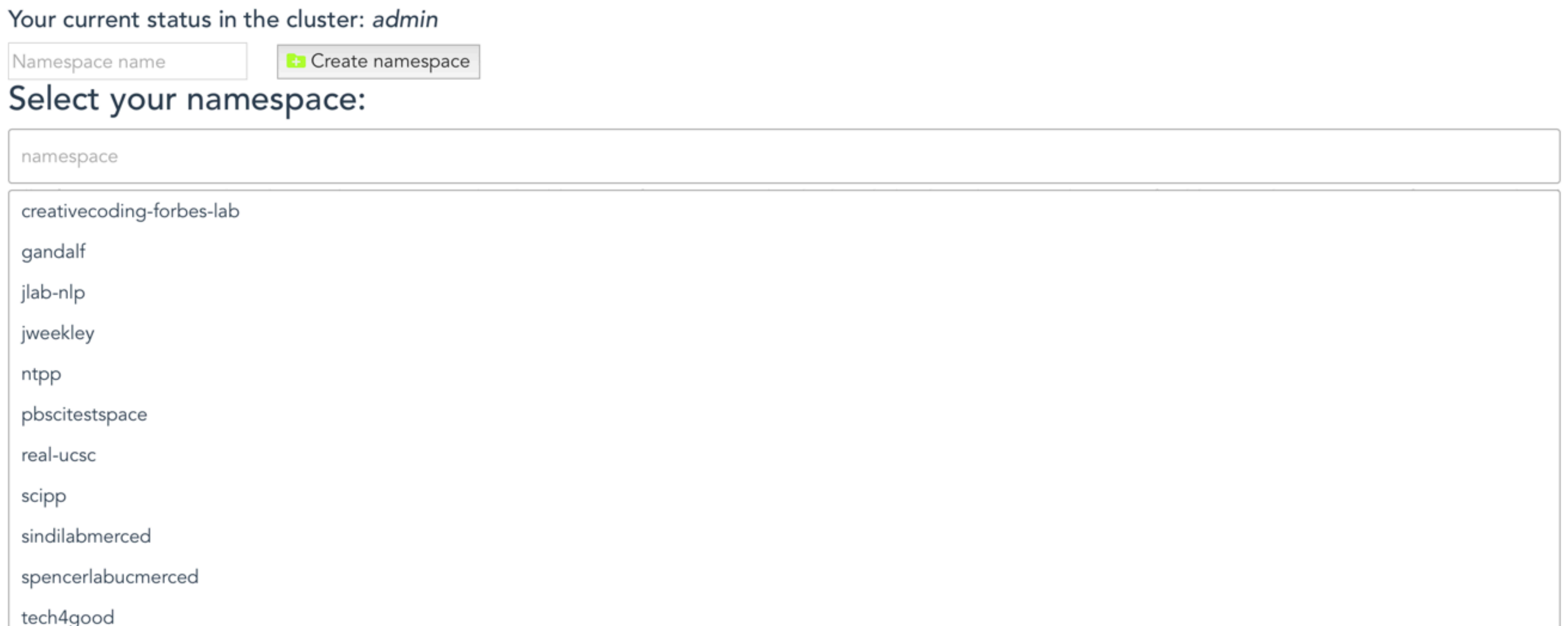
Name	Institution	Software	PI	Publications
avis-fire	UC Santa Cruz	Python	Alex Pang	

Description	Users Institutions	Admins	Users
Wildfire analysis with ML approaches.	ucsc.edu	Hou-I Lin	

Name	Institution	Software	PI	Publications
avis-rip	UC Santa Cruz	Tensorflow, Python	alex pang	

Admin Level

- Users may request to be promoted to Admin in the chat support channel
- Admins may create namespaces, join users to them and are responsible for maintaining community standards for the users in their namespaces

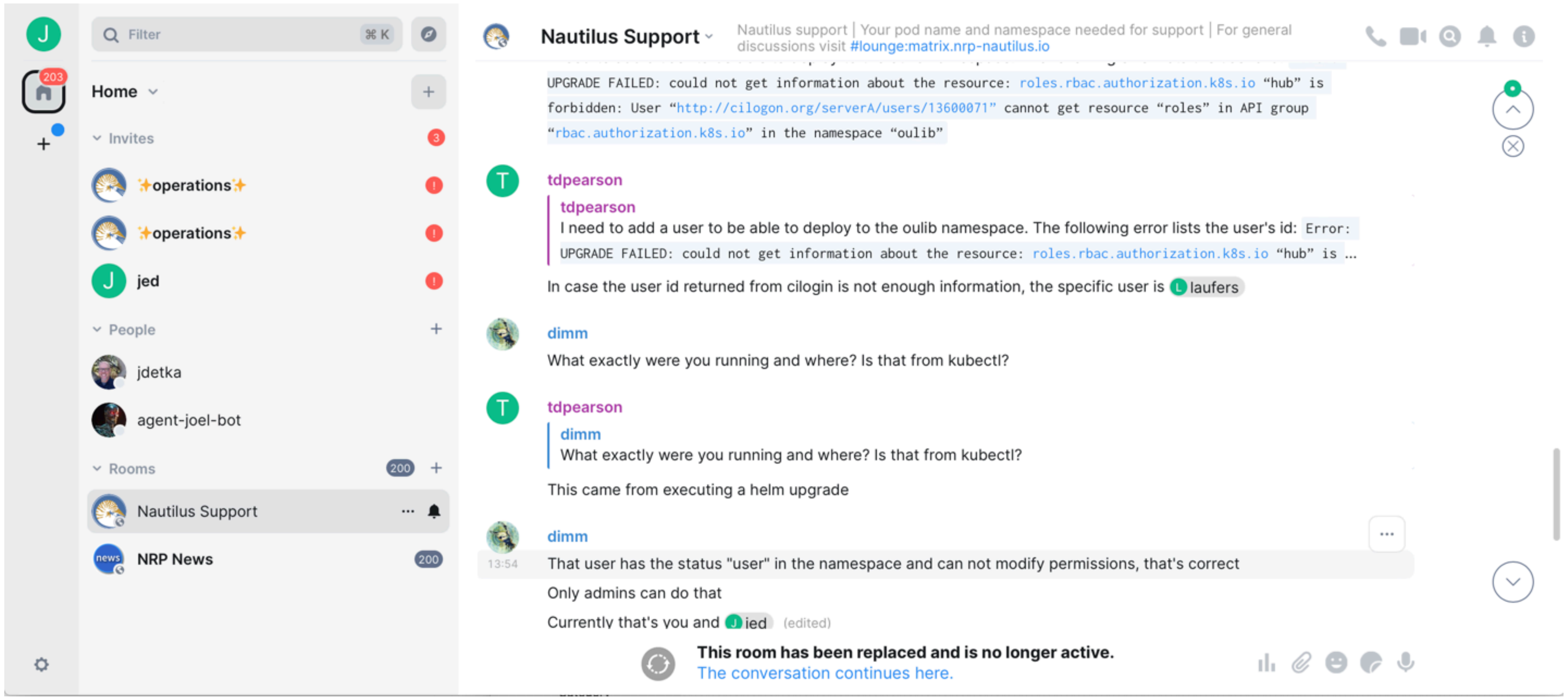

Your current status in the cluster: *admin*

Select your namespace:

creativecoding-forbes-lab
gandalf
jlab-nlp
jweekley
ntpp
pbscitestspace
real-ucsc
scipp
sindilabmerced
spencerlabucmerced
tech4good

Requesting Privileges (and Getting Help)

Via the Matrix chat at https://element.nrp-nautilus.io


Filter
⌘ K
203
Home
Invites
3
✨operations✨
✨operations✨
jed
People
jdetka
agent-joel-bot
Rooms
200
Nautilus Support
NRP News
200
Nautilus Support
Nautilus support | Your pod name and namespace needed for support | For general discussions visit #lounge:matrix.nrp-nautilus.io

```
UPGRADE FAILED: could not get information about the resource: roles.rbac.authorization.k8s.io "hub" is
forbidden: User "http://cilogon.org/serverA/users/13600071" cannot get resource "roles" in API group
"rbac.authorization.k8s.io" in the namespace "oulib"
```

tdpearson

> **tdpearson**
> I need to add a user to be able to deploy to the oulib namespace. The following error lists the user's id: `Error:`
> `UPGRADE FAILED: could not get information about the resource: roles.rbac.authorization.k8s.io "hub" is ...`

In case the user id returned from cilogin is not enough information, the specific user is laufers

dimm

What exactly were you running and where? Is that from kubectl?

tdpearson

> **dimm**
> What exactly were you running and where? Is that from kubectl?

This came from executing a helm upgrade

dimm

13:54 That user has the status "user" in the namespace and can not modify permissions, that's correct

Only admins can do that

Currently that's you and jed (edited)

This room has been replaced and is no longer active.
The conversation continues here.

All requests for assistance are done in Matrix

Nautilus

Controlling the Cluster from your Desktop

Review of what we’ve done so far…

- We have access to Nautilus and we’ve been promoted to User (to join someone else’s namespace) or we’ve created our own namespace as Admin
- We have installed Docker so we can build or modify images (i.e. containers)
- We have access to a private repo
- We have installed our config file so the cluster knows who we are

How do we actually control the cluster?

Installing Kubectl

In order to use your config file to control the cluster, you will need to install this tool

The Kubernetes command-line tool, kubectl, allows you to run commands against Kubernetes clusters. You can use kubectl to deploy applications, inspect and manage cluster resources, and view logs. For more information including a complete list of kubectl operations, see the kubectl reference documentation.

Installation instructions can be found here:

https://kubernetes.io/docs/tasks/tools/

Structure of kubectl

Users interface with a Kubernetes-controlled system using The Kubernetes command-line tool, “kubectl”

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

“command” describes the operation to perform. They are limited to these operations:

- create generates new resources from files or standard input devices
- describe retrieves details about a resource or resource group
- get fetches cluster data from various sources
- delete removes resources as directed
- apply pushes changes based on configuration files

Structure of kubectl (cont)

Users interface with a Kubernetes-controlled system using The Kubernetes command-line tool, “kubectl”

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

[TYPE] specifies the category of resource you are targeting

[NAME] this case-sensitive field specifies the name of the resource (you will name your pods, deployments, etc.) Using the NAME field restricts to operation to that named resource. Leaving it blank will apply it universally.

[Flags] the modifier [Flags] denotes any special options or requests made of a resource. This modifier can be used to over-ride defaults or environment variables.

What about my data?

Persistent Data in K8s

- Managing storage is a distinct problem from managing compute instances
- Storage is provisioned through the *PersistentVolumeClaim,* on Nautilus comes in distinct classes and regions
- Ceph shared filesystem (CephFS) is the primary way of storing data in Nautilus which allows mounting the same volume(s) from multiple PODs in parallel

StorageClass	Filesystem Type	Region	AccessModes	Storage Type	Size
rook-cephfs	CephFS	US West	ReadWriteMany	Spinning drives with NVME meta	2.5 PB
rook-cephfs-east	CephFS	US East	ReadWriteMany	Mixed	1 PB
rook-cephfs-pacific	CephFS	Hawaii+Guam	ReadWriteMany	Spinning drives with NVME meta	384TB
beegfs	BeeGFS	US West	ReadWriteMany		2PB
rook-ceph-block (*default*)	RBD	US West	ReadWriteOnce	Spinning drives with NVME meta	2.5 PB
rook-ceph-block-east	RBD	US East	ReadWriteOnce	Mixed	1 PB
rook-ceph-block-pacific	RBD	Hawaii+Guam	ReadWriteOnce	Spinning drives with NVME meta	384 TB
seaweedfs-storage	SeaweedFS	US West	ReadWriteMany	NVME	300 TB

Other Types of Storage in Nautilus

- Local: Most nodes in the cluster have local NVME drives, which provide faster I/O than shared filesystems. These can be used for workloads that require very intensive I/O operations
- Nextcloud: access to the Nextcloud instance running on Nautilus. It's similar to other file sharing systems (Dropbox, Google Drive etc) and can be used to get data in the cluster, temporary stage the results, share data and so on
- SeaweedFS is a high-performance distributed filesystem, optimized for working with huge number of files and also huge files
- SyncThing is a tool to synchronize files collections between several devices with no single server, which creates a mesh between all devices and works well for large files collections

Moving Data

Remember: K8s pods have local addresses and are not accessible from outside

- Kubectl has a copy function:

```
kubectl -n my_namespace cp ~/tmp/file.dat my_super_pod:/tmp/file.dat
```

  This method is not suitable for large data transfers!

- Using S3 is the most scaleable way to move large data sets. Refer to the S3 Documentation for more information

- Directly manipulating from inside your pod using standard Linux tools. This allows you to move the data in as if it were another physical host. All the same rules apply. CAVEAT: once the pod goes away, so does your data.

Other considerations…

Microservices

Breaking your workflow into services, and those services into microservices may help you debug and scale

What is a Microservice?

- A microservice is an architectural design for building a distributed application.
- Microservices break an application into independent, loosely-coupled, individually deployable services.
- This architecture allows for each service to scale or update using the deployment of service proxies without disrupting other services in the application and enables the rapid, frequent and reliable delivery of large, complex applications.

Additional Applications

Some helpful applications run natively in Nautilus

Computation

- JupyterHub (West Coast)
- JupyterHub (East Coast)
- WebODM (Web Open Drone Map): Drone Images stitching
- Appwrite: Backend Server for Web, Mobile, others

Collaboration

- EtherPad: notebooks
- GitLab
- Jitsi: Video conferencing
- Nextcloud: File sharing
- Overleaf: LaTeX collaboration

Monitoring

- Traceroute tool
- PerfSONAR

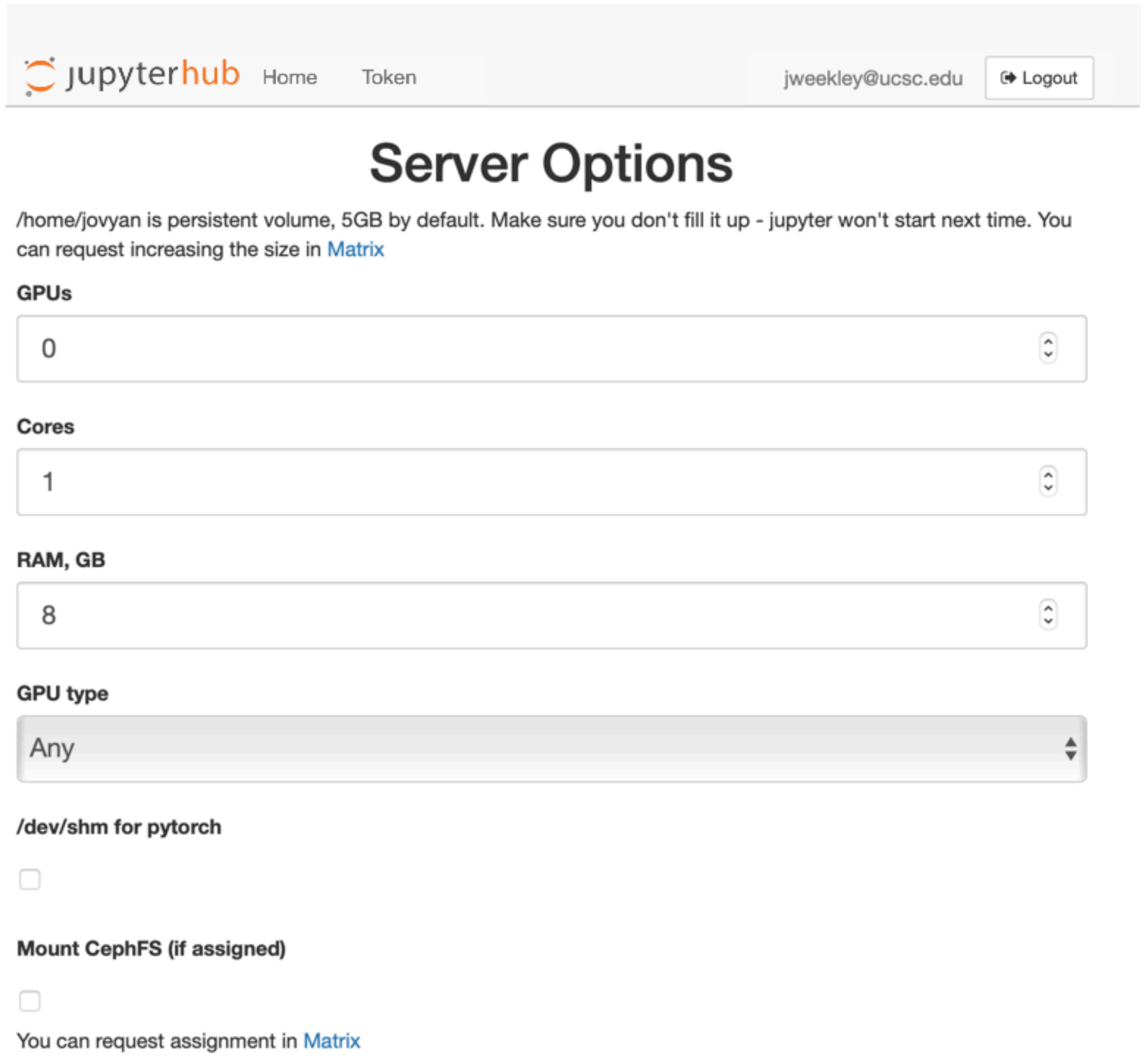
More on Jupyter Lab

Jupyter on Nautilus

A few things to know…

- New users should request access in Matrix
- Multiple GPU types available:

1060	1080
1080Ti	2080Ti
TITAN XP	Tesla K40
TITAN RTX	3090
Tesla V100	RTX A100
RTX8000	RTX A40



Server Options

/home/jovyan is persistent volume, 5GB by default. Make sure you don't fill it up - jupyter won't start next time. You can request increasing the size in Matrix

GPUs: 0

Cores: 1

RAM, GB: 8

GPU type: Any

/dev/shm for pytorch

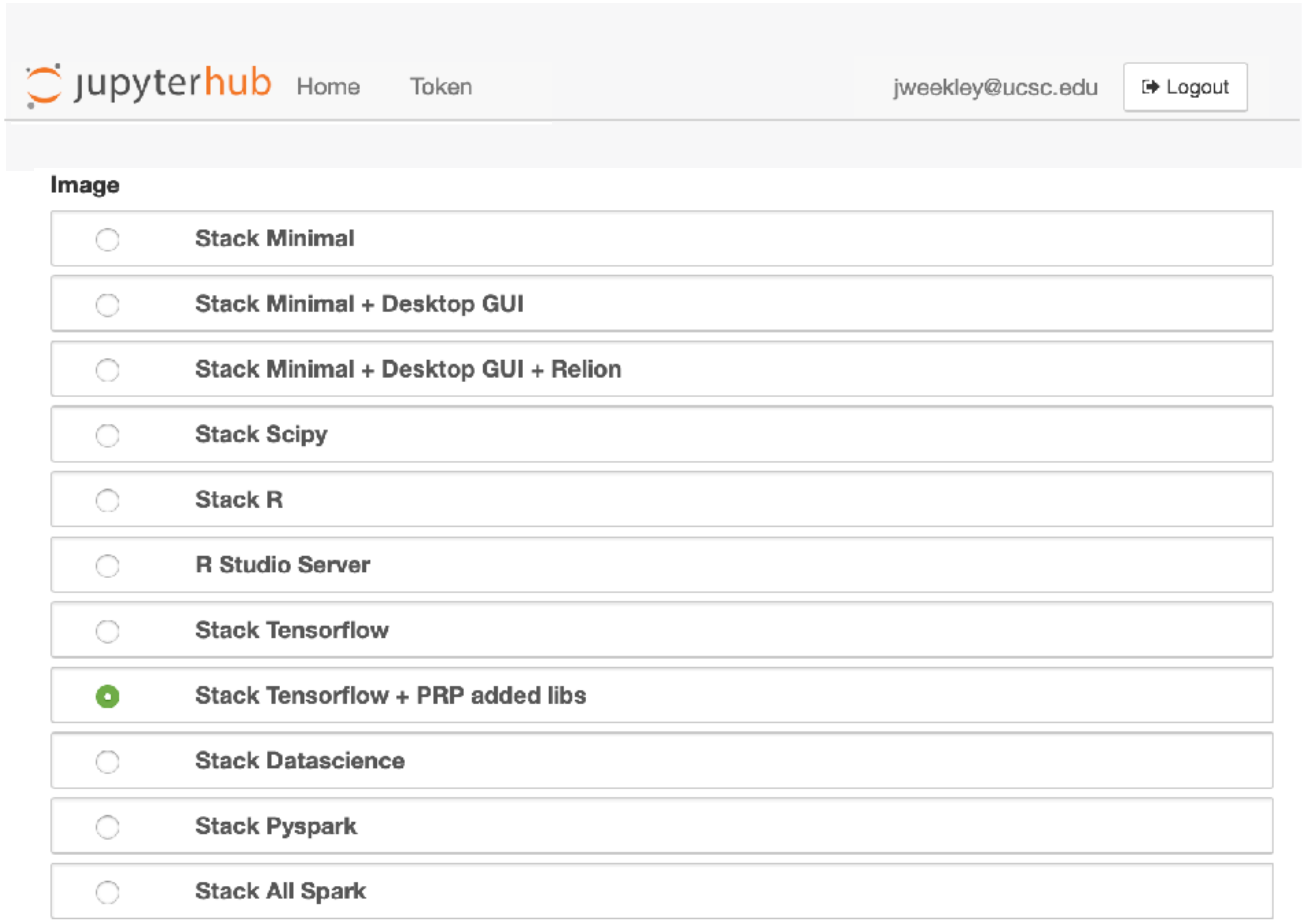
Mount CephFS (if assigned)

You can request assignment in Matrix

Jupyter on Nautilus

A few more things to know…

- Mounting of CephFS PVCs allowed
- Preconfigured, common software stacks
- Runs common iPython Notebooks
- Notebooks persist (very handy)



Image

- ○ Stack Minimal
- ○ Stack Minimal + Desktop GUI
- ○ Stack Minimal + Desktop GUI + Relion
- ○ Stack Scipy
- ○ Stack R
- ○ R Studio Server
- ○ Stack Tensorflow
- ● Stack Tensorflow + PRP added libs [✓]
- ○ Stack Datascience
- ○ Stack Pyspark
- ○ Stack All Spark

File Edit View Run Kernel Tabs Settings Help
OPEN TABS Close All
Lesson-1.ipynb
Untitled.ipynb
KERNELS Shut Down All
Lesson-1.ipynb
Untitled.ipynb
TERMINALS Shut Down All
Lesson-1.ipynb
Untitled.ipynb
Markdown
Python 3 (ipykernel)

Important note: You should always work on a duplicate of the course notebook. On the page you used to open this, tick the box next to the name of the notebook and click duplicate to easily create a new version of this notebook.

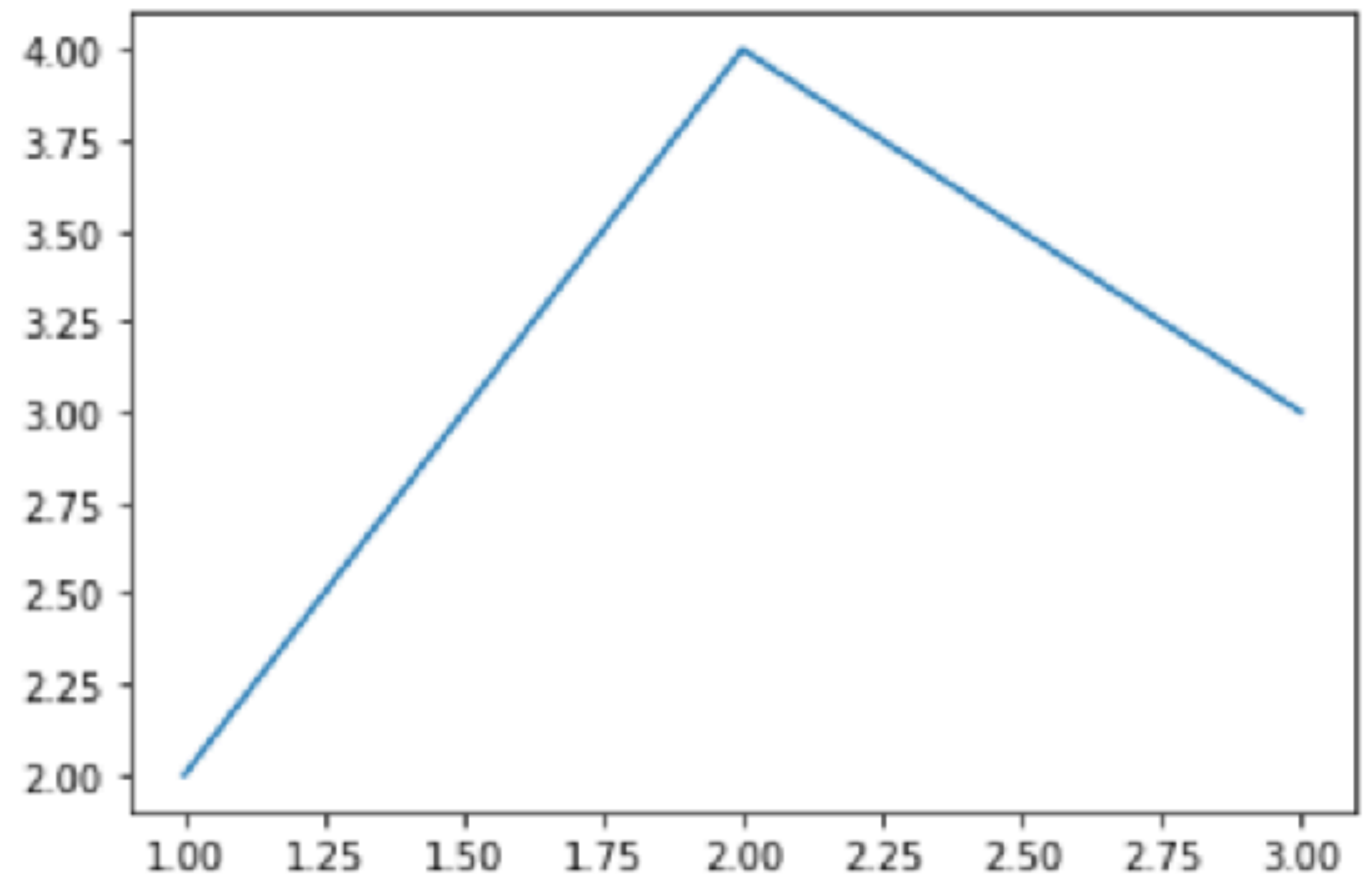
You will get errors each time you try to update your course repository if you don't do this, and your changes will end up being erased by the original course version.

```
[11]: import matplotlib.pyplot as plt
```

Welcome to Jupyter Notebooks!

```
[12]: plt.plot([1, 2, 3], [2, 4, 3])

      plt.show()
```



If you want to learn how to use this tool you've come to the right place. This article will teach you all you need to know to use Jupyter Notebooks effectively. You only need to go through Section 1 to learn the basics and you can go into Section 2 if you want to further increase your productivity.

Review

Putting it all together…

- There are software tools and configurations you'll need: Docker, kubectl, config file in ~./kube directory
- Docker can be used to build customize containers
- Docker Hub has many pre-built software containers
- Access to Nautilus is granted at three levels: guest, user and admin
- kubectl is how you interact with the cluster
- Your YAML file tells the cluster what you want it to do
- Deployments are groups of pods and services that make up your workflow
- Storage outside of your pod is available through a PersistentVolumeClaim
- Jupyter Lab is a good place to start exploring

For operational support, visit Nautilus Matrix chat

Final Q&A

Questions about this Nautilus: see Documentation

Questions about this presentation? jweekley@ucsc.edu

The End

Introduction to PRP Nautilus, Kubernetes, and Containerized Software

Jeffrey Weekley

11 FEB 2022