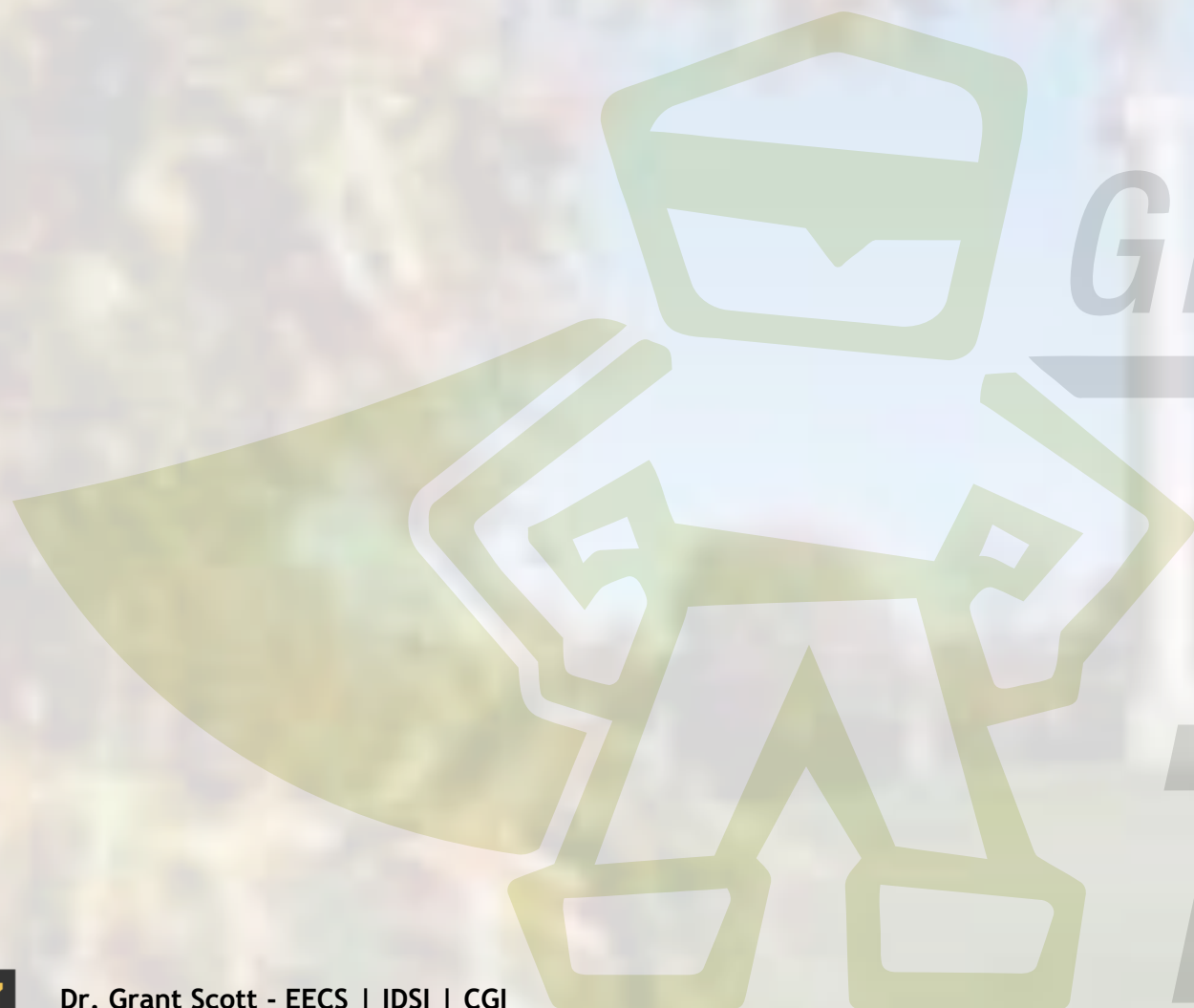


# *Setting Up Research Jobs in the PRP Nautilus Hyper-Cluster*

Grant Scott, Anes Ouadou, and Chenhan Zhao

Great Plains Network Annual Meeting

June 3, 2022



# *GREATPLAINS*

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# *CYBER*

# *TEAM*

## Workshop Outcome:

You will be able to train a deep learning  
neural network using Kubernetes and  
GPU resources on Nautilus

... and other scientific computing processes

**This workshop creation and delivery was supported  
by the National Science Foundation (NSF)**

**NSF Award #1925681 - CC\* Team: Great Plains Regional CyberTeam**



# Workshop Agenda

1. Introductions
2. Getting logged into Nautilus and Setup
3. Overview of Kubernetes Concepts
4. Accessing JupyterLab in Nautilus, configuring KubeCtl
5. Preliminary Pod Control
6. Setting Up Persistent Storage for Data Input and Output
7. Launching Training using a Customized Container Image

# Introductions

**Grant Scott**

**Chenhan  
Zhao**



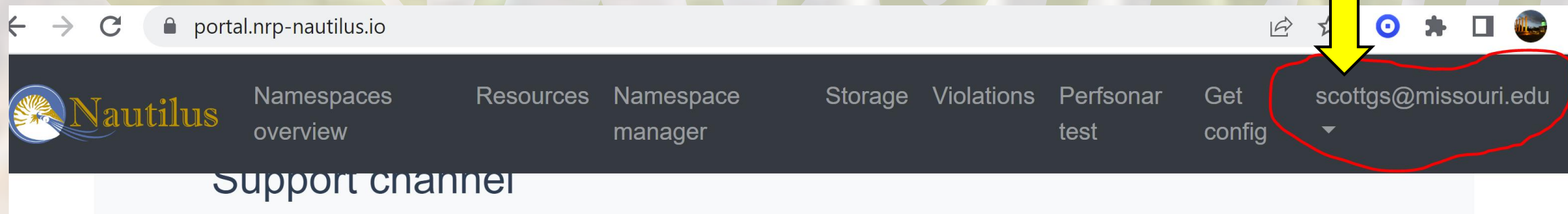
**Anes  
Ouadou**

# Getting your account linked to the Workshop Namespace

- ▶ Access the link below and follow the steps to authenticate into Nautilus

<https://ucsd-prp.gitlab.io/userdocs/start/get-access/>

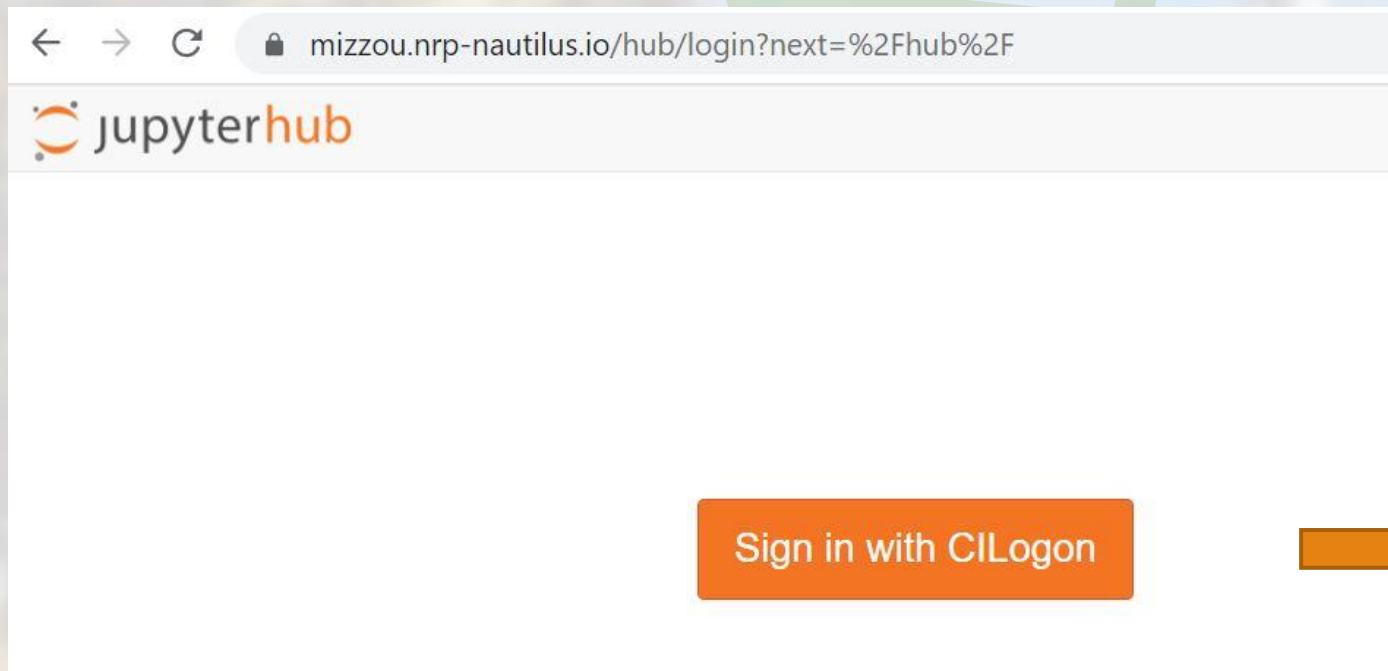
- ▶ Once you follow the instructions down to step 6, post into the GPN Slack, Channel **#gpn-nautilus-kubernetes-workshop** your User ID so Chenhan can pull you into our namespace as a User.






# Getting logged into Nautilus

## <https://mizzou.nrp-nautilus.io/>




**CILogon**

Nautilus requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon username
- Your name
- Your email address
- Your username and affiliation from your identity provider

Select An Identity Provider:

A. T. Still University  
AAF Virtual Home  
AAI@EduHr Single Sign-On Service  
Aalto University

Search:

Remember this selection: ☐

**Log On**

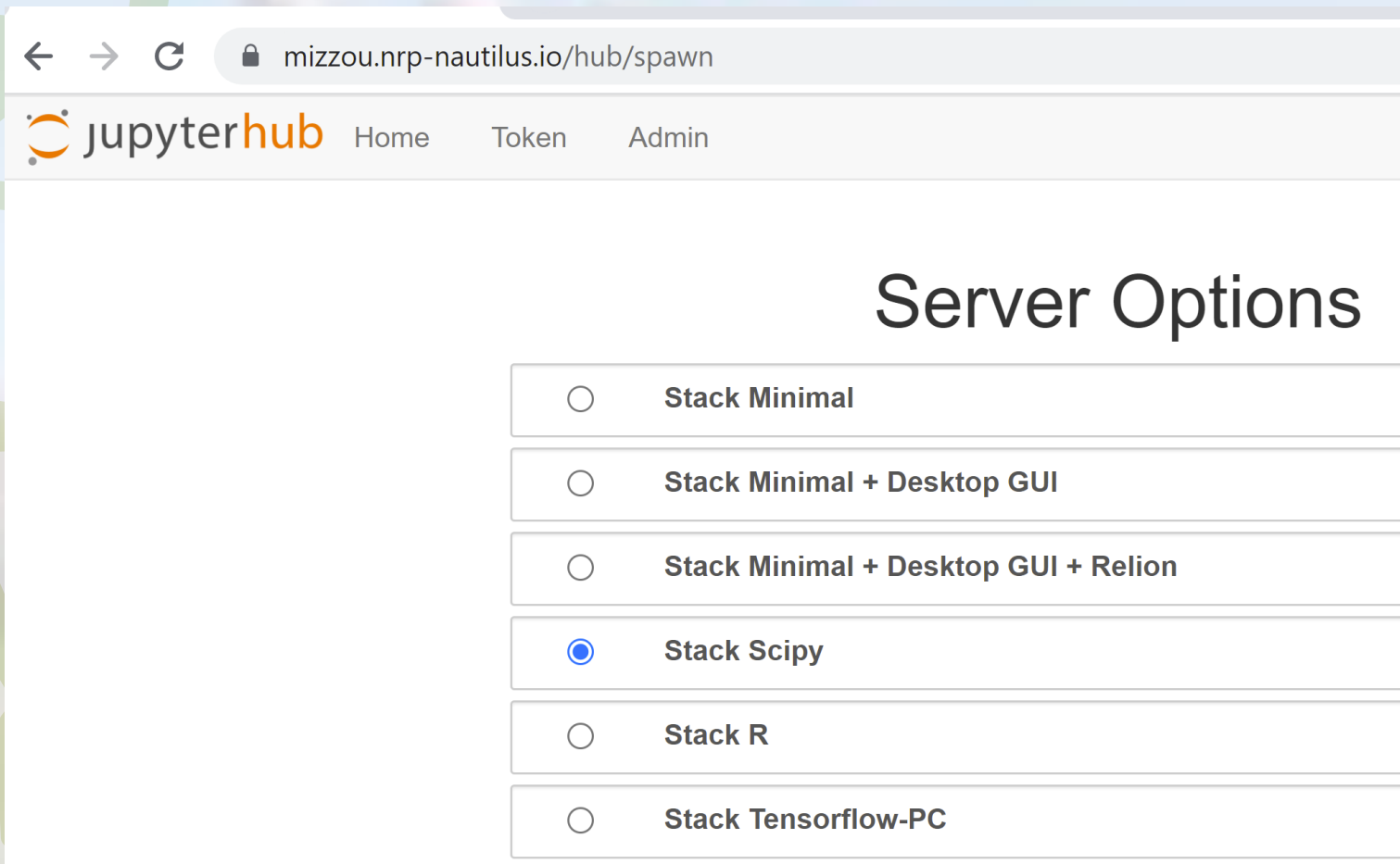
By selecting "Log On", you agree to [CILogon's privacy policy](#).



# Nautilus Jupyter Lab

## <https://mizzou.nrp-nautilus.io/>

- ▶ Jupyter Hub / Lab running on a Kubernetes cluster in Nautilus
- ▶ Use the CILogon to access any institution or use your Github.com credentials
- ▶ Use the Scipy or Datascience Stack, and click the lower **Start** button

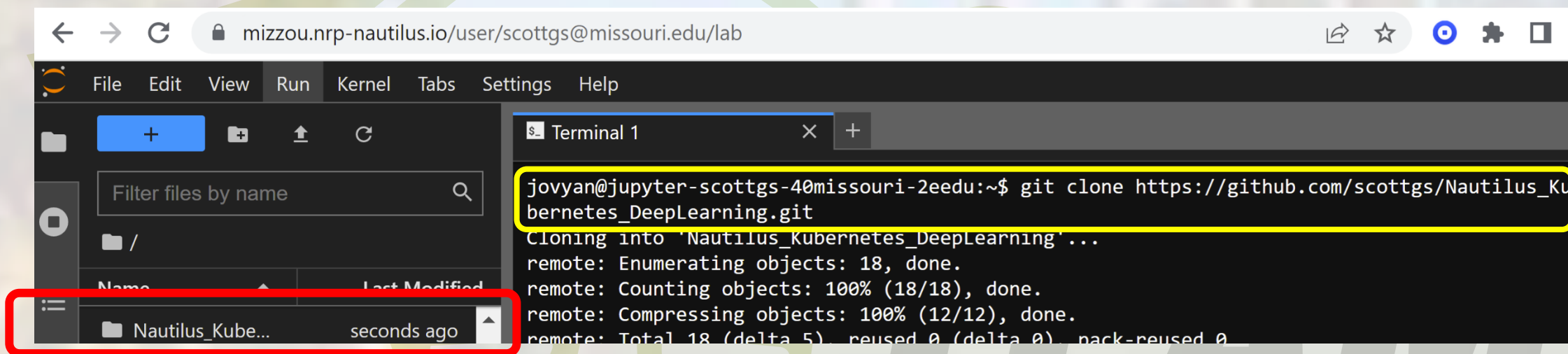
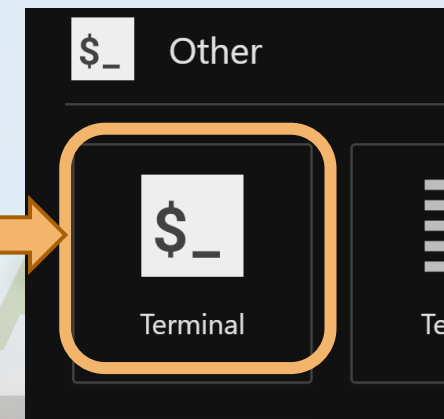


The screenshot shows a web browser at the URL `mizzou.nrp-nautilus.io/hub/spawn`. The page header includes the Jupyter Hub logo and navigation links for Home, Token, and Admin. The main content area is titled "Server Options" and displays a list of six server configurations, each with a radio button for selection:

- ☐ Stack Minimal
- ☐ Stack Minimal + Desktop GUI
- ☐ Stack Minimal + Desktop GUI + Relion
- ☒ Stack Scipy
- ☐ Stack R
- ☐ Stack Tensorflow-PC

# Pulling Down Workshop Content

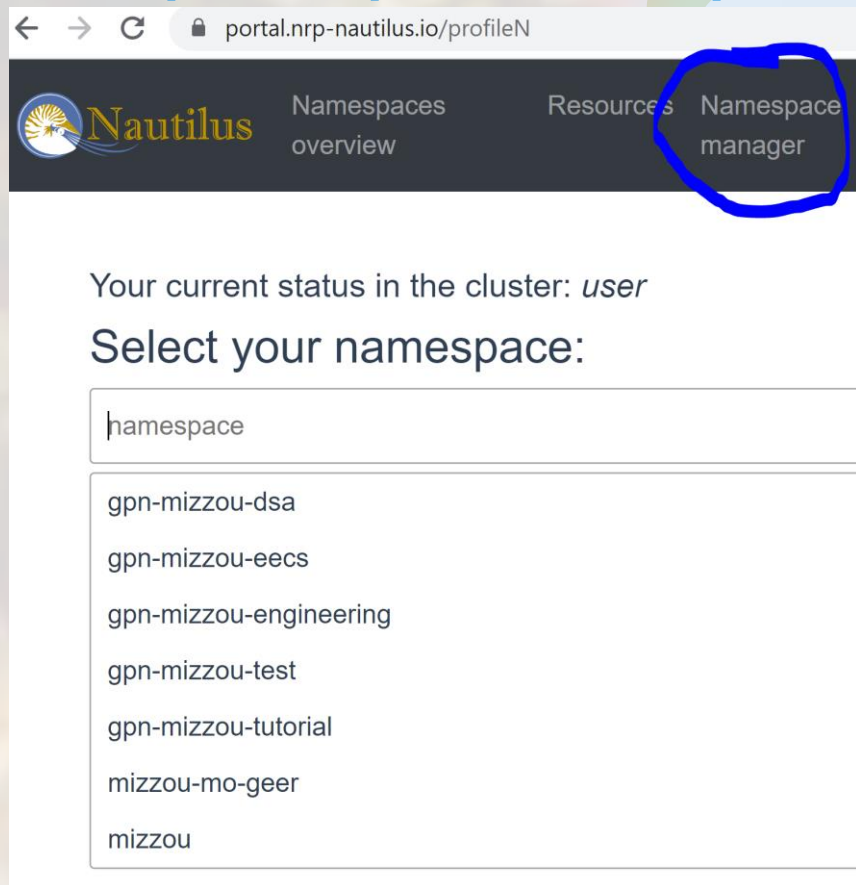
- ▶ We are cloning workshop content from Github.com
- ▶ Open a Terminal
- ▶ Clone Github.com/scottgs/Nautilus\_Kubernetes\_DeepLearning



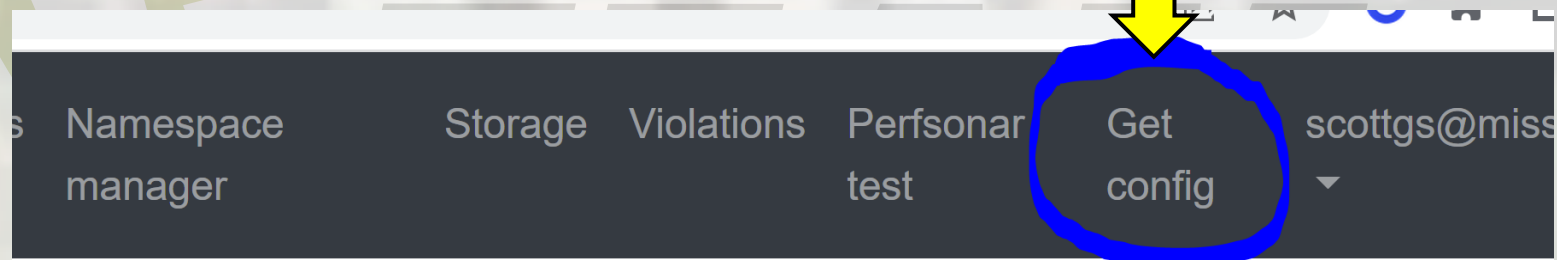
**`git clone https://github.com/scottgs/Nautilus_Kubernetes_DeepLearning.git`**

# Confirming Nautilus Namespace

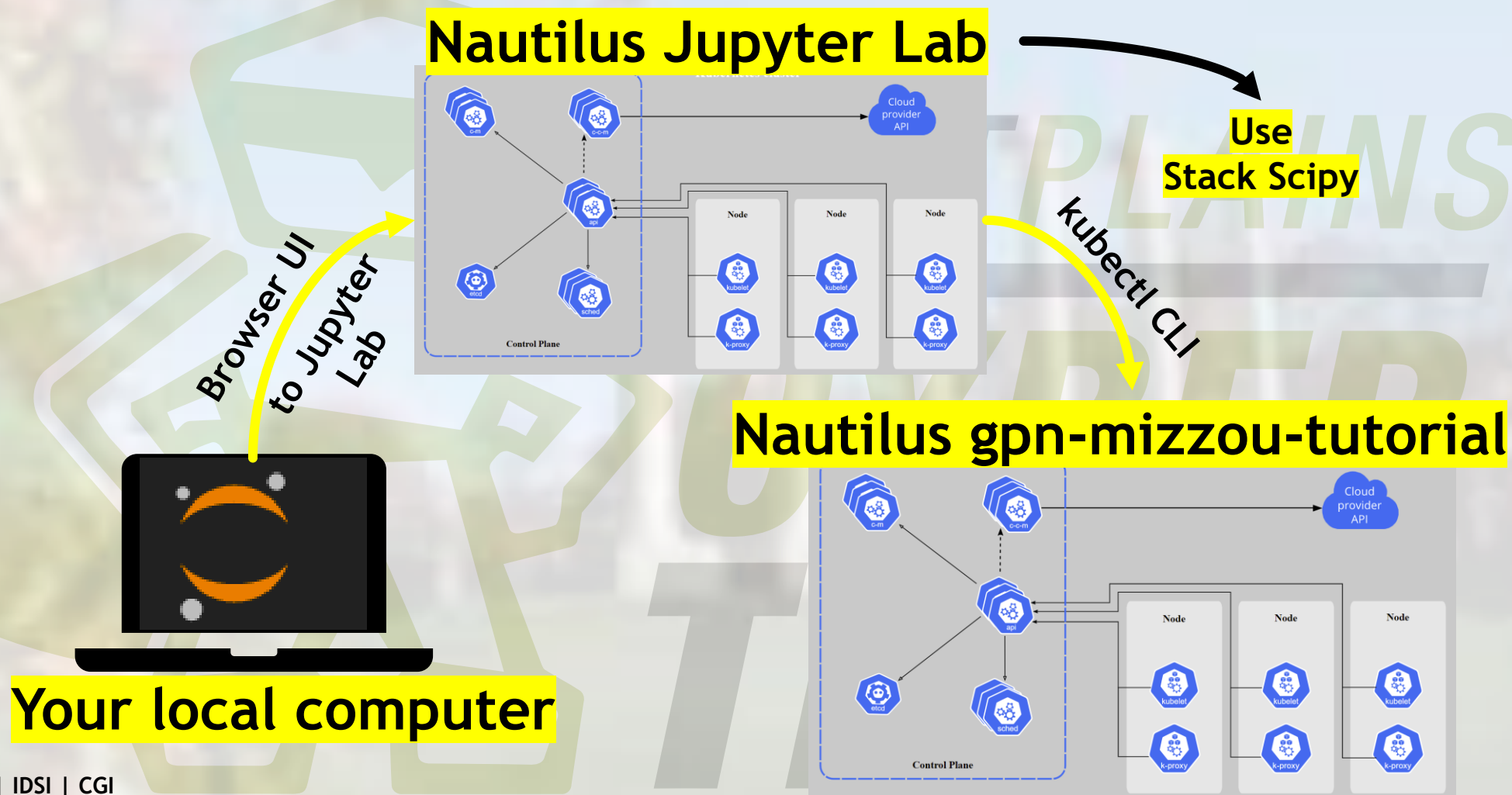
<https://portal.nrp-nautilus.io/profileN>



- ▶ Going back to our Nautilus Namespace setup, after a checkmark from Chenhan
- ▶ Select the Namespace Manager
- ▶ Once it loads, select the **gpn-mizzou-tutorial**
- ▶ Then download your Nautilus Configuration file

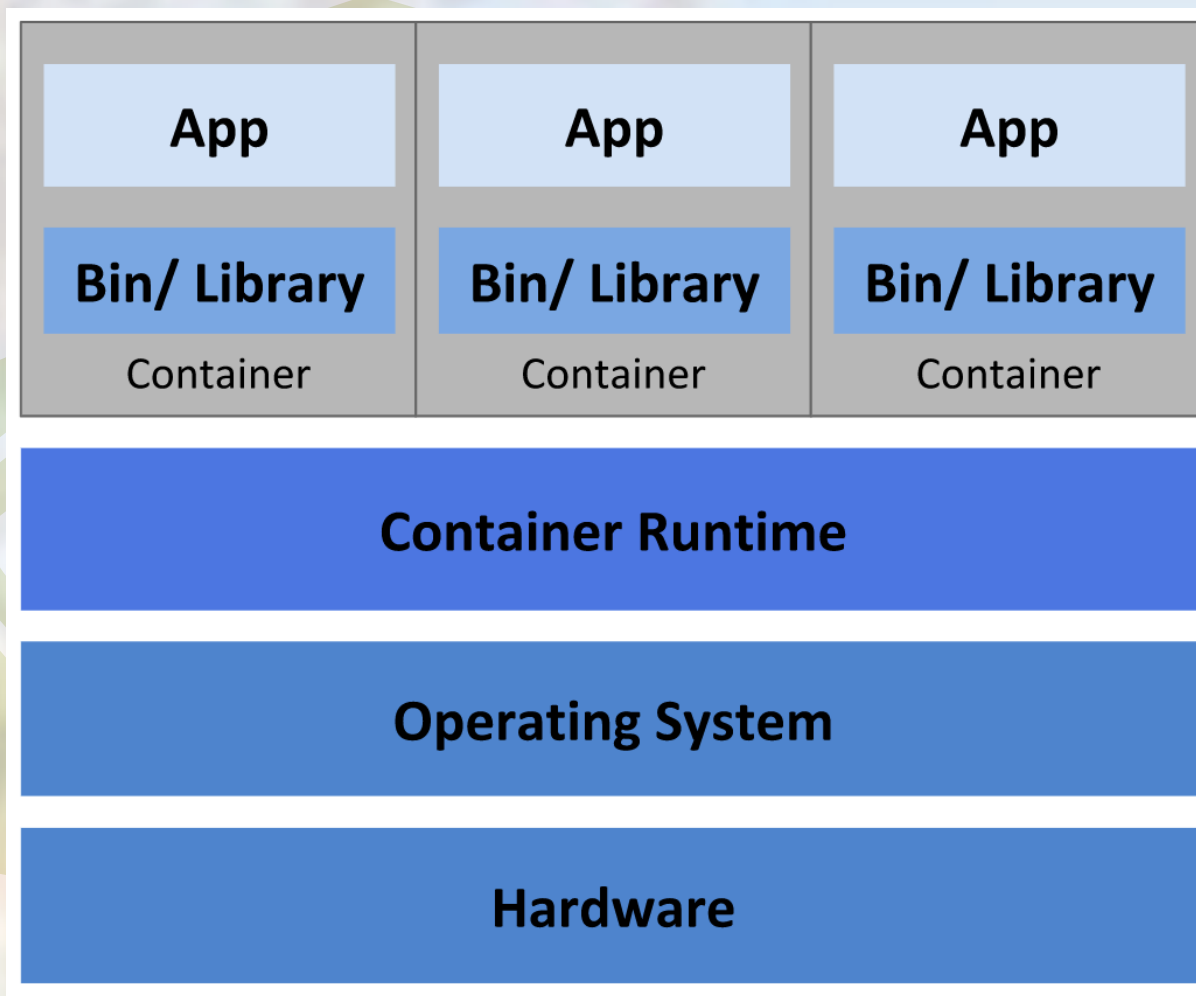


# Kubernetes - Inception Style





# Kubernetes - A foundation of Containers



# Kubernetes - Foundational Elements

- ▶ **Pods** - smallest deployable units of computing that you can create and manage in Kubernetes
- ▶ **Jobs** - creates one or more Pods and will continue to retry execution of the Pods until a specified number of them successfully terminate
- ▶ **Persistent Storage** - piece of storage in the cluster that has been provisioned by an administrator or dynamically provisioned using Storage Classes

# kubectl - CLI for Kubernetes

- ▶ Allows you to run commands against Kubernetes clusters. You can use kubectl to deploy applications, inspect and manage cluster resources, and view logs
- ▶ Can control remote Kubernetes clusters from any number of environments (Linux, Windows, or Mac)

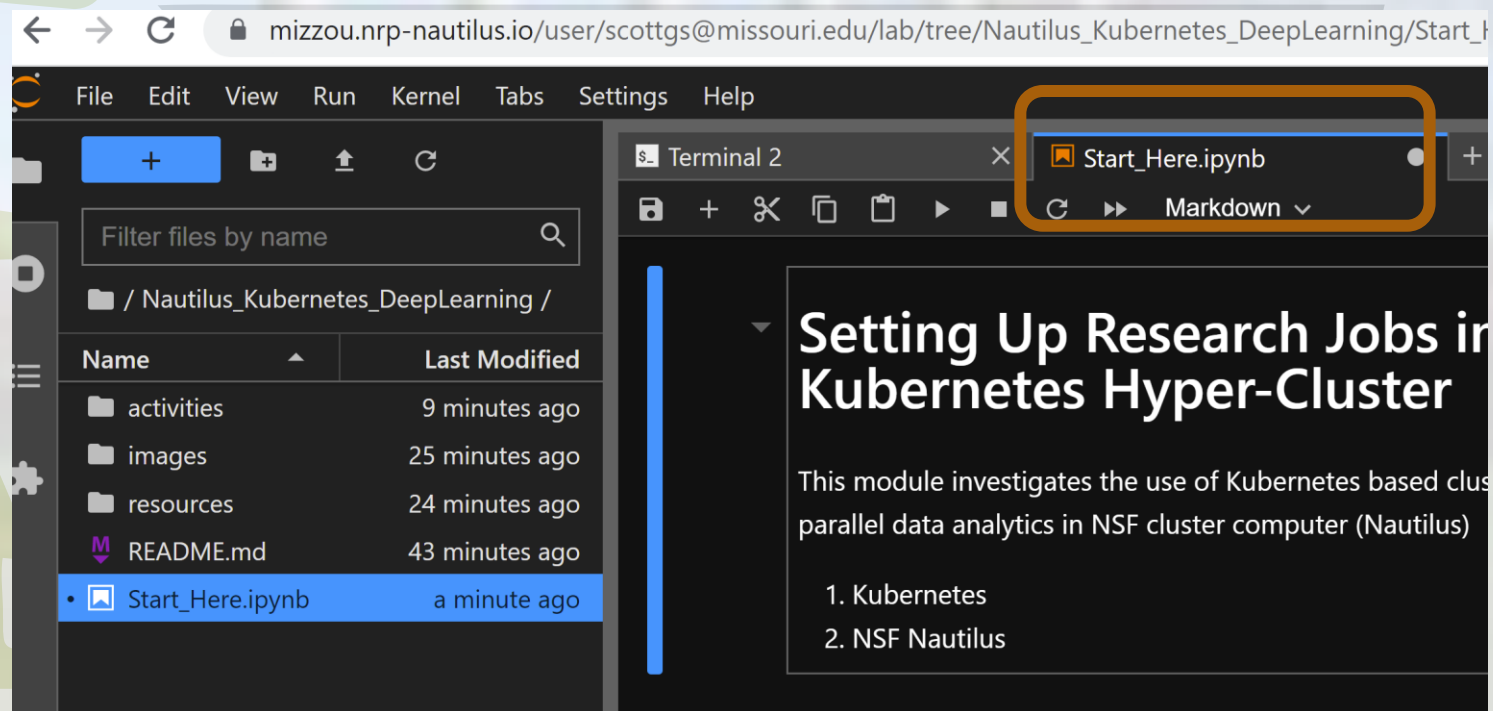
# Hands-On Activities - *Setup and Test kubectl*

- ▶ Using Kubernetes tools on Nautilus Jupyter Lab
- ▶ Attaching persistent storage to Pods
- ▶ Launch Deep Learning Training on Kubernetes



# Hands-On Activities - *Setup and Test kubectl*

- ▶ In prior steps, the github repository for this workshop was cloned into your Jupyter Lab environment
- ▶ Navigate to the workshop folder
- ▶ Click on the Start\_Here notebook
- ▶ New tab opens



# Set Up Kubernetes - *Setup and Test kubectl*

## Finish Preparation of Kubernetes

1. Create a Kubernetes configuration directory
2. Upload the config file you got from the Nautilus Portal to Jupyter Lab (home folder)
3. Move into place
4. Install the Kubernetes CLI

```
mkdir ~/.kube
```

```
mv config ~/.kube/
```

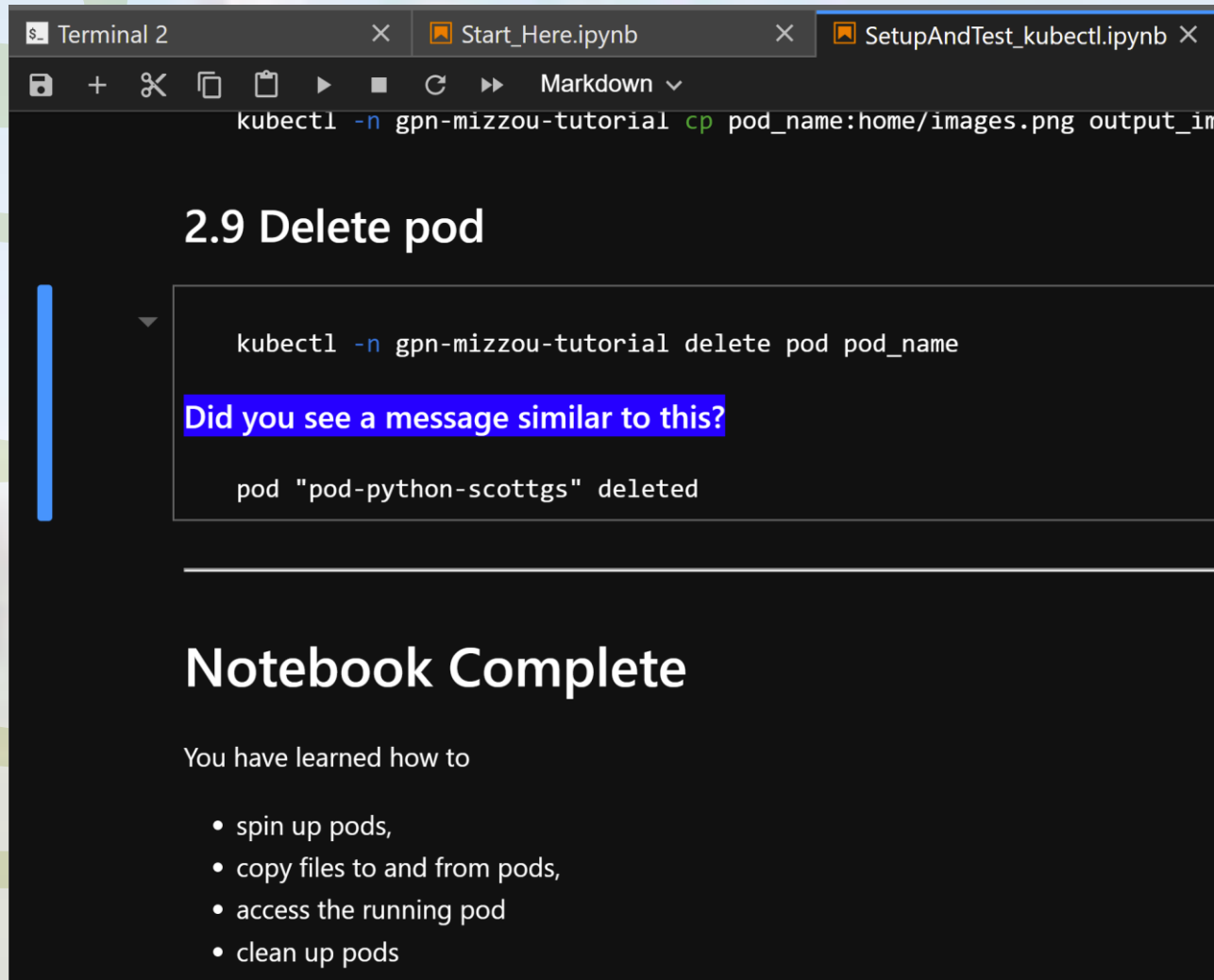
Follow steps on:

<https://kubernetes.io/docs/tasks/tools/install-kubectl-linux/#install-using-native-package-management>

# Set Up Kubernetes - *Setup and Test kubectl*

## Work through step 2 of the notebook

1. Create a pod
2. Copy files to the pod
3. Access the running pod
4. Install software
5. Run script
6. Copy files from the pod
7. Remove the pod



The screenshot shows a Jupyter Notebook interface with three tabs: 'Terminal 2', 'Start\_Here.ipynb', and 'SetupAndTest\_kubectl.ipynb'. The 'Terminal 2' tab is active, displaying a terminal window with the command `kubectl -n gpn-mizzou-tutorial cp pod_name:home/images.png output_im`. The notebook content is visible in the background, showing a section titled '2.9 Delete pod' with a code block containing `kubectl -n gpn-mizzou-tutorial delete pod pod_name`. Below the code block, there is a highlighted text box that says 'Did you see a message similar to this?' followed by the output `pod "pod-python-scottgs" deleted`. The notebook also has a section titled 'Notebook Complete' with a summary of what was learned.

```
kubectl -n gpn-mizzou-tutorial cp pod_name:home/images.png output_im
```

### 2.9 Delete pod

```
kubectl -n gpn-mizzou-tutorial delete pod pod_name
```

Did you see a message similar to this?

```
pod "pod-python-scottgs" deleted
```

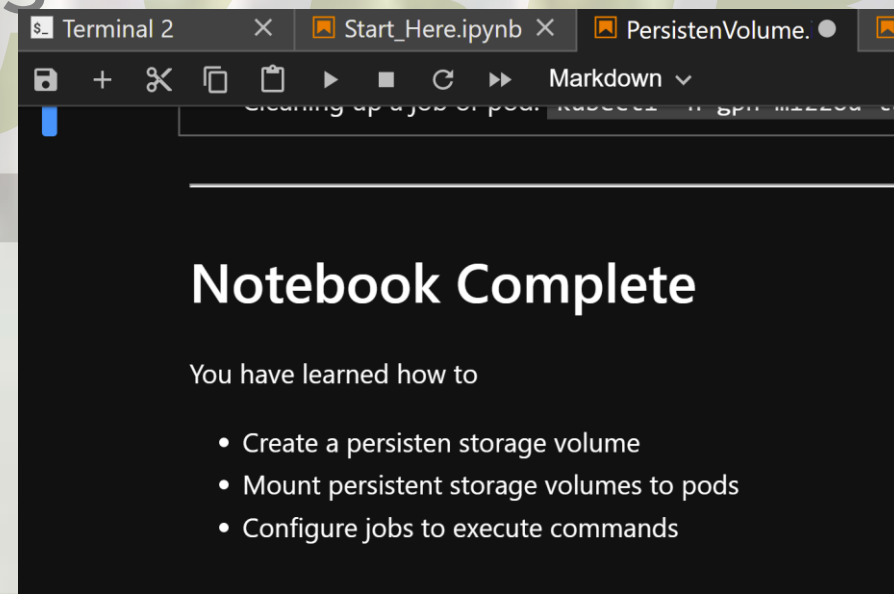
## Notebook Complete

You have learned how to

- spin up pods,
- copy files to and from pods,
- access the running pod
- clean up pods

# Hands-On Activities - Create a persistent volume

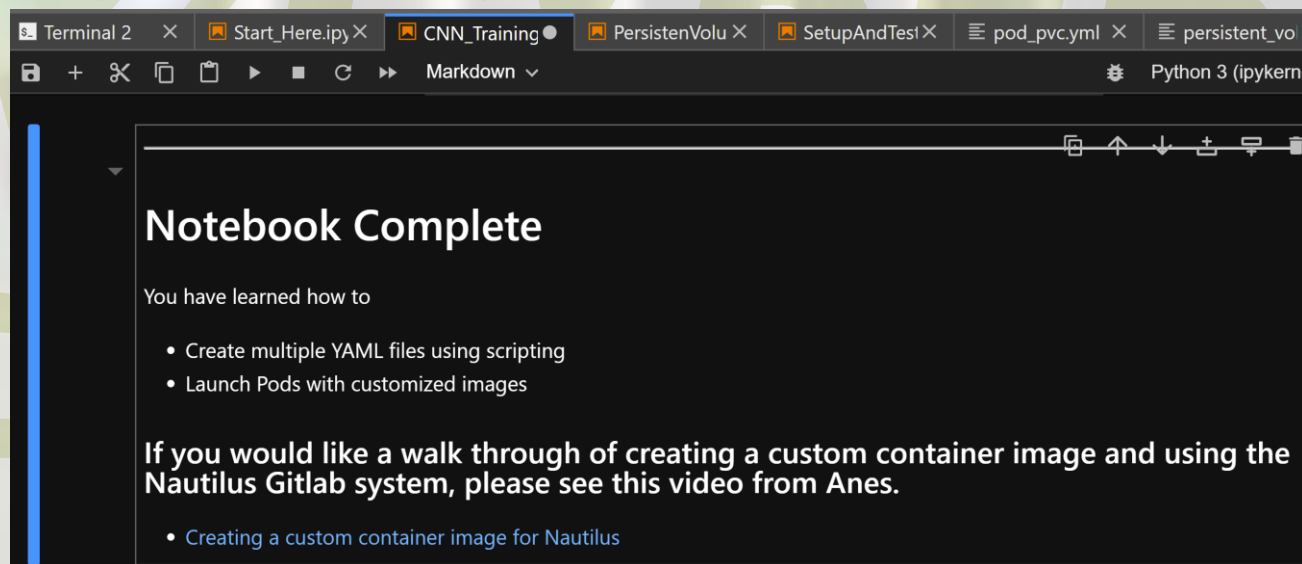
- ▶ Using Kubernetes tools on Nautilus Jupyter Lab
- ▶ **Attaching persistent storage to Pods**
- ▶ Launch Deep Learning Training on Kubernetes





# Hands-On Activities - Convolutional Neural Network on Nautilus

- ▶ Using Kubernetes tools on Nautilus Jupyter Lab
- ▶ Attaching persistent storage to Pods
- ▶ **Launch Deep Learning Training on Kubernetes**



# This completes the workshop activities!

-- We either flew through or are way behind

- ▶ You now have a taste of what setting up research tasks, deep learning in this case, on the NSF Nautilus cluster.
- ▶ This is just the tip of the iceberg!

**Thank you for working through the activities on this workshop!**

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**[NSF Award Search: Award #1925681 - CC\\* Team: Great Plains Regional CyberTeam](#)**

Questions? Post-Workshop, GPN Slack  
Channel [#gpn-nautilus-kubernetes-workshop](#)