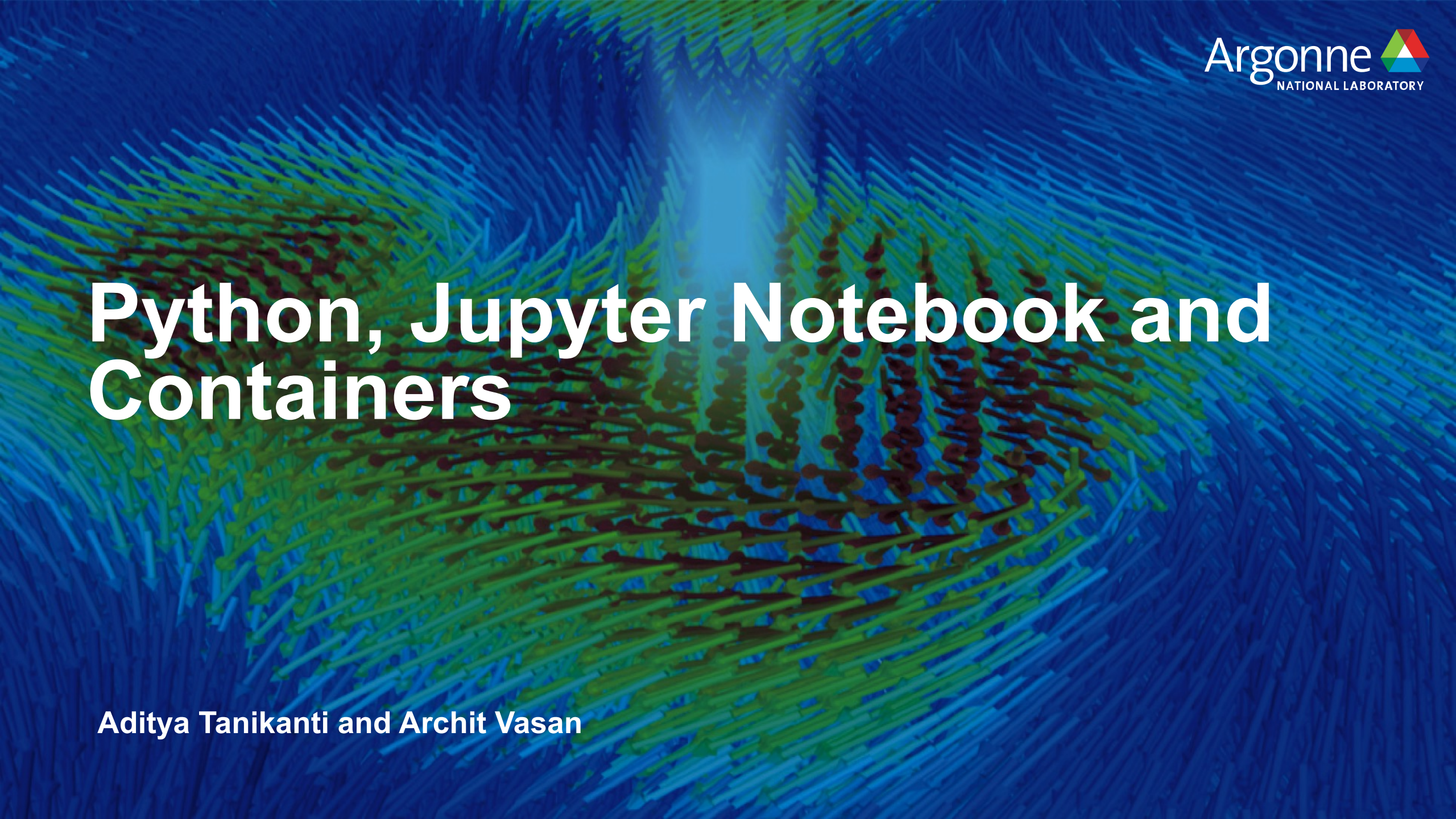

October 10-12, 2023
ALCF Hands-on HPC Workshop



Python, Jupyter Notebook and Containers

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Outline

- Using Python on Polaris
  - Managing conda environments
  - Running python and multi-rank jobs
- Using Jupyter Notebooks on Polaris
  - Creating a new notebook and running programs
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Using Python on Polaris

Logging in to interactive nodes

- If you are an ALCF user, login to Polaris via:

```
ssh user@polaris.alcf.anl.gov
```

- Else, check:
  https://alcf.anl.gov/support-center/get-started
  - Request an interactive node:

```
qsub -I -A fallws23single -l select=1 -l walltime=01:00:00
-l filesystems=home:grand:eagle -q debug
```

  - **-I** : interactive node
  - **-A fallws23single** : fallws23single is the allocation
  - **-l select=1** : request 1 compute node
  - **-l walltime=01:00:00** : request for 1 hour
  - **-l filesystems=home:grand:eagle** : request to use these filesystems
  - **-q debug**: request to use debug queue

Managing conda environments

- Polaris uses modules to control loading of software environments
- There are prebuilt environments containing GPU-supported builds of torch, tensorflow, jax, etc.
- To use these:

```
module load conda/2023-10-04
conda activate
```

- To use an older conda version search for available conda environments and load that version:

```
module avail conda
module load conda/2022-09-08
conda activate
```

Managing conda environments

- If you need more flexibility to install your own packages (e.g. using conda iinstall, pip install)
  - Clone the base conda environment:

```
module load conda/2023-10-04
conda activate
conda create –clone base –prefix /path/to/envs/base-clone
conda activate /path/to/envs/base-clone
```

  - Note: make sure to change /path/to/envs/base-clone to where you want to install the environment
    - Also, to ensure proper functioning of your environment, install within an interactive job not on login node

Running python

- To run a single rank python job simply activate your conda environment and then run your process

```
module load conda/2023-10-04
conda activate
python example_script.py
```

- If you need additional packages for your application, activate your created conda environment and install via pip/conda

```
module load conda/2023-10-04
conda activate /path/to/envs/base-clone
pip install example_module
python example_script.py
```

Running multi-rank jobs

- Polaris has 64 CPUS and 4 A100 GPUs on each compute node.
- To parallelize across these, use MPI:

```
module load conda/2023-10-04
conda activate
mpiexec –n NPROC –ppn PROC_PER_NODE yourrun
```

- To use MPI with python, use the mpi4py module:

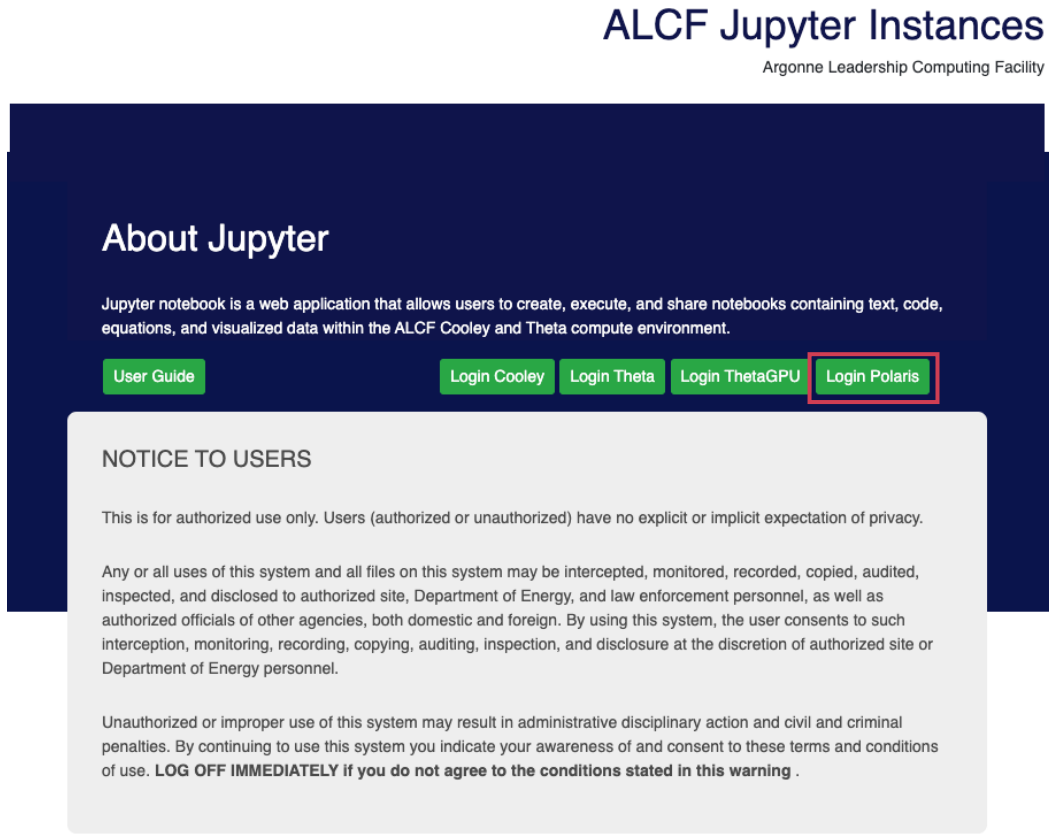
```
from mpi4py import MPI
comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()
print(f'My rank is {rank} of {size} total ranks')
```

- This program creates an MPI World, gets number of ranks (size), and specific rank.
- It then outputs the rank id across all processes.

Using Jupyter Notebooks on Polaris

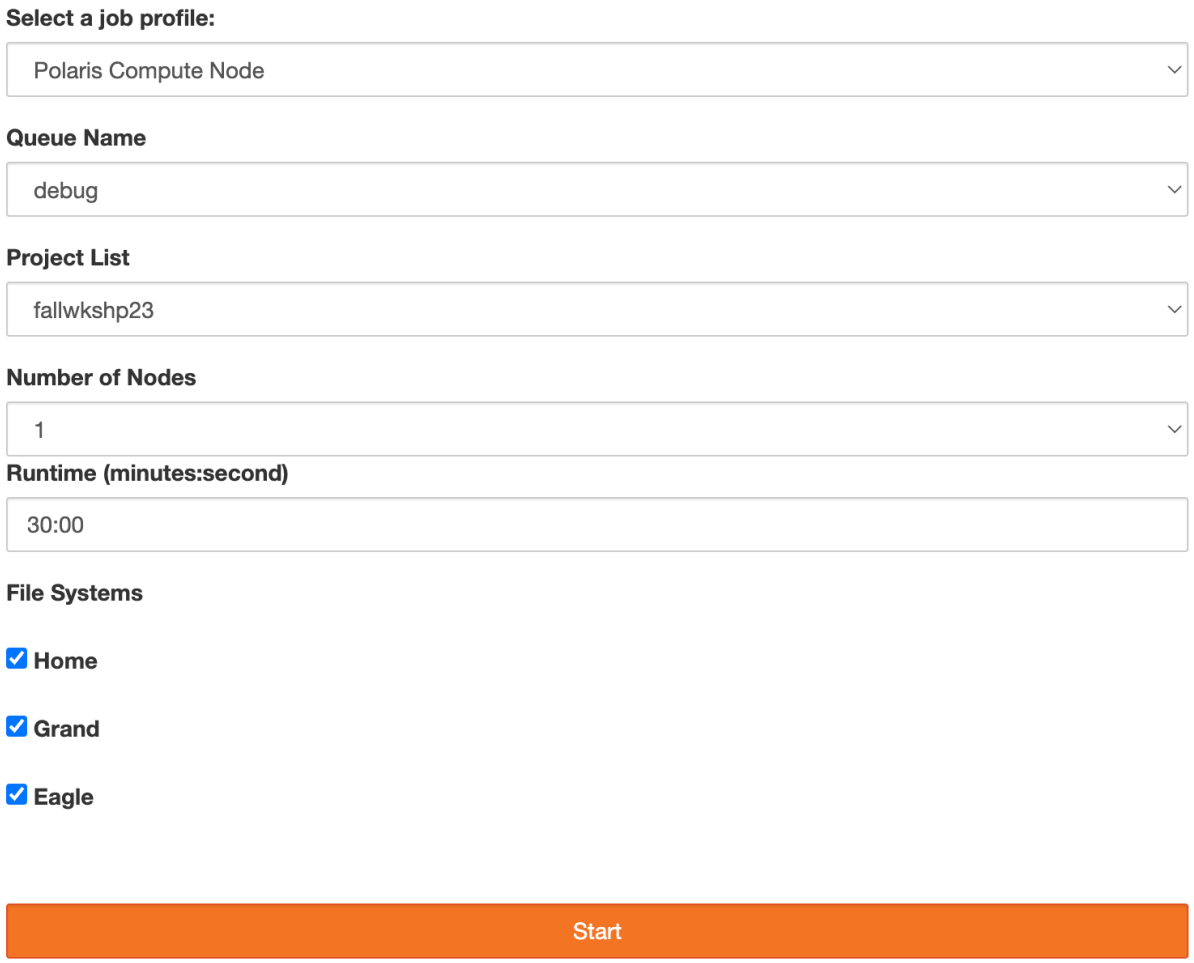
Logging in

- Access JupyterHub at: https://jupyter.alcf.anl.gov/
- Select **Login Polaris** and use ALCF credentials + Multi-factor Authentication to login



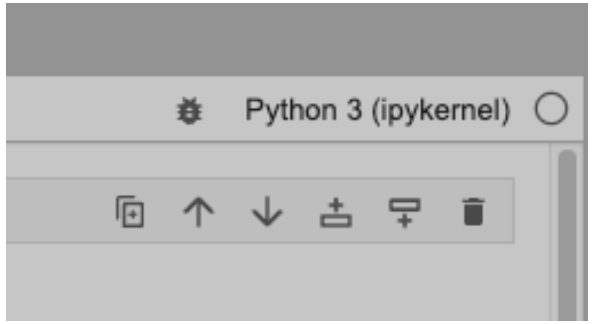
Starting a new server

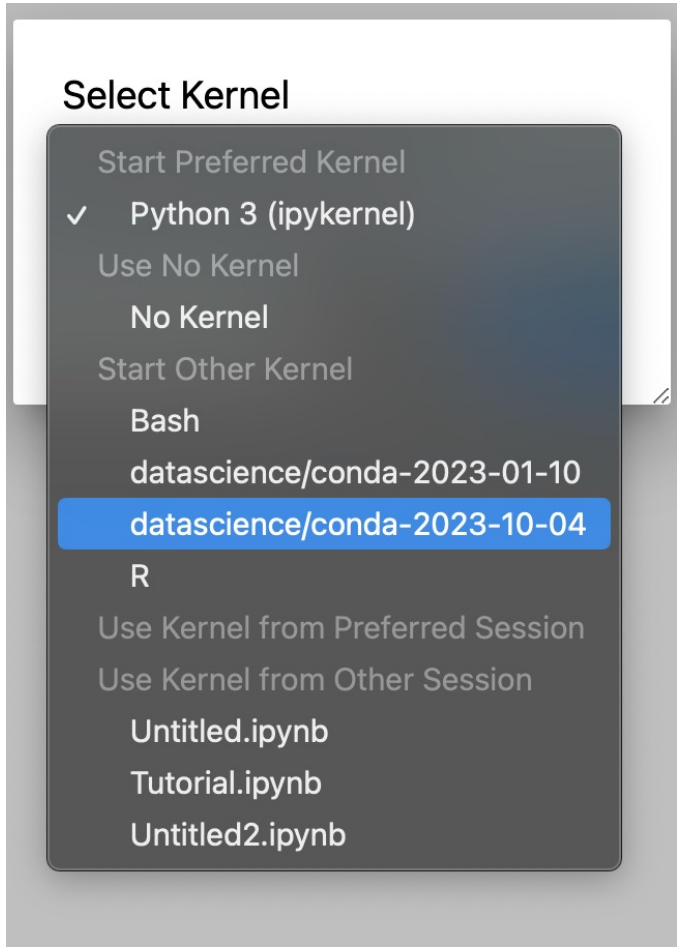
- You want to setup your server Job Options as follows.
- Pressing start will submit to the batch queue



Creating new notebook

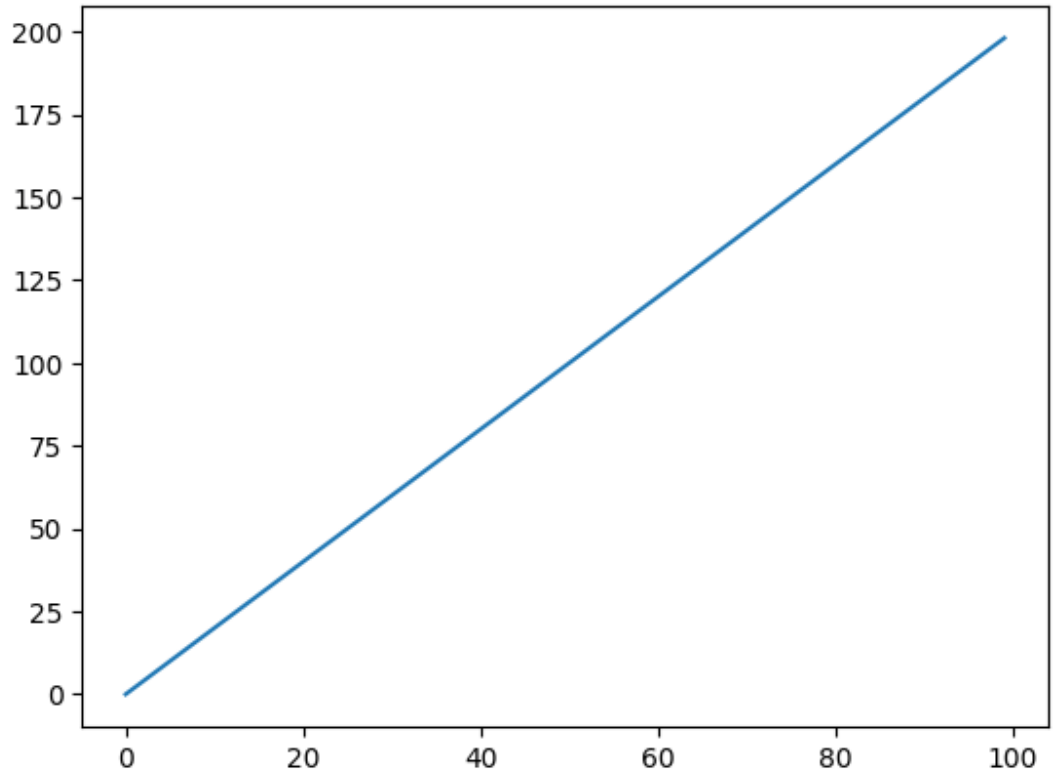
- Once the job begins start a new notebook.
- To use a conda environment with several necessary python modules, change kernel to datascience/conda-2023-10-04





Simple example

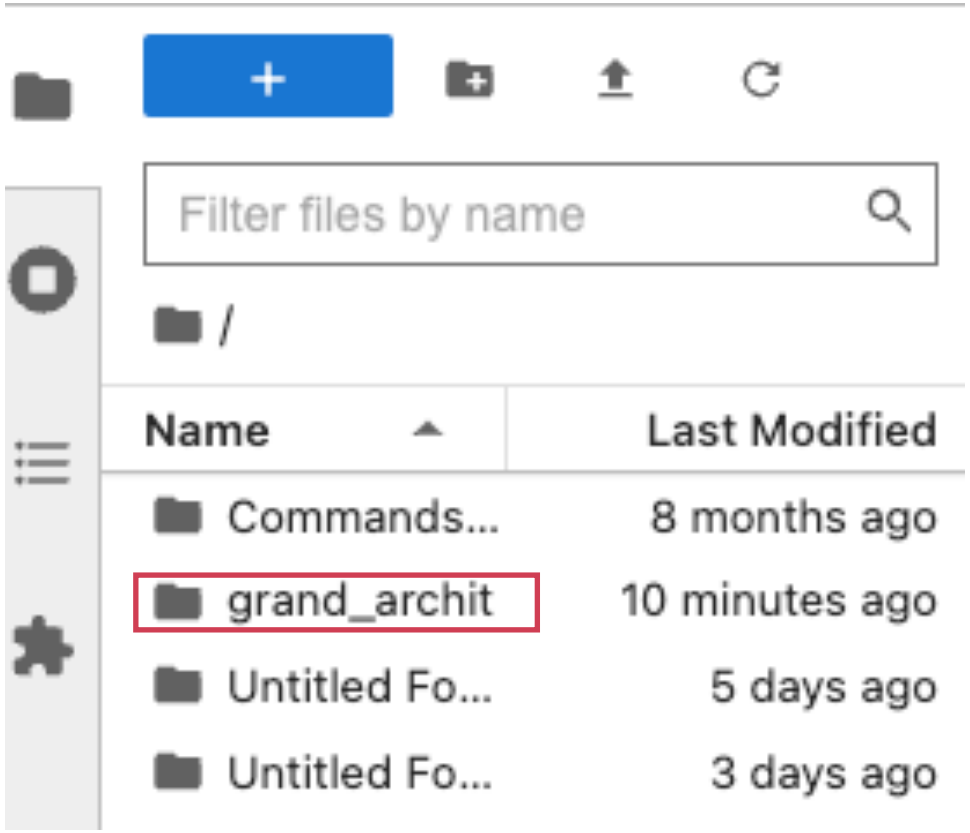
```
[1]: import numpy as np

[2]: import matplotlib.pyplot as plt

[3]: a = [i * 2 for i in range(0, 100)]

[4]: plt.plot(a)

[4]: [<matplotlib.lines.Line2D at 0x14e74c605ba0>]
```



Accessing project folders

- JupyterHub starts on your home folder
- Need to create symbolic link to access projects

```
!ln -s /grand/datascience/avasan grand_archit
```



Working with machine learning modules

- Machine learning modules Tensorflow and Pytorch are installed in datascience/conda-2023-10-04 module
- Here is how to check GPU usage on these modules:

```
import tensorflow as tf
```

```
2023-10-09 19:14:58.095004: I tensorflow/core/platform/cpu_feature_guard.cc:193] This TensorFlow binary is optimized with oneAPI Deep Neu
ral Network Library (oneDNN) to use the following CPU instructions in performance-critical operations:  SSE3 SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags.
```

```
tf.config.list_physical_devices('GPU')
```

```
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU'),
 PhysicalDevice(name='/physical_device:GPU:1', device_type='GPU'),
 PhysicalDevice(name='/physical_device:GPU:2', device_type='GPU'),
 PhysicalDevice(name='/physical_device:GPU:3', device_type='GPU')]
```

```
import torch
```

```
torch.cuda.is_available()
```

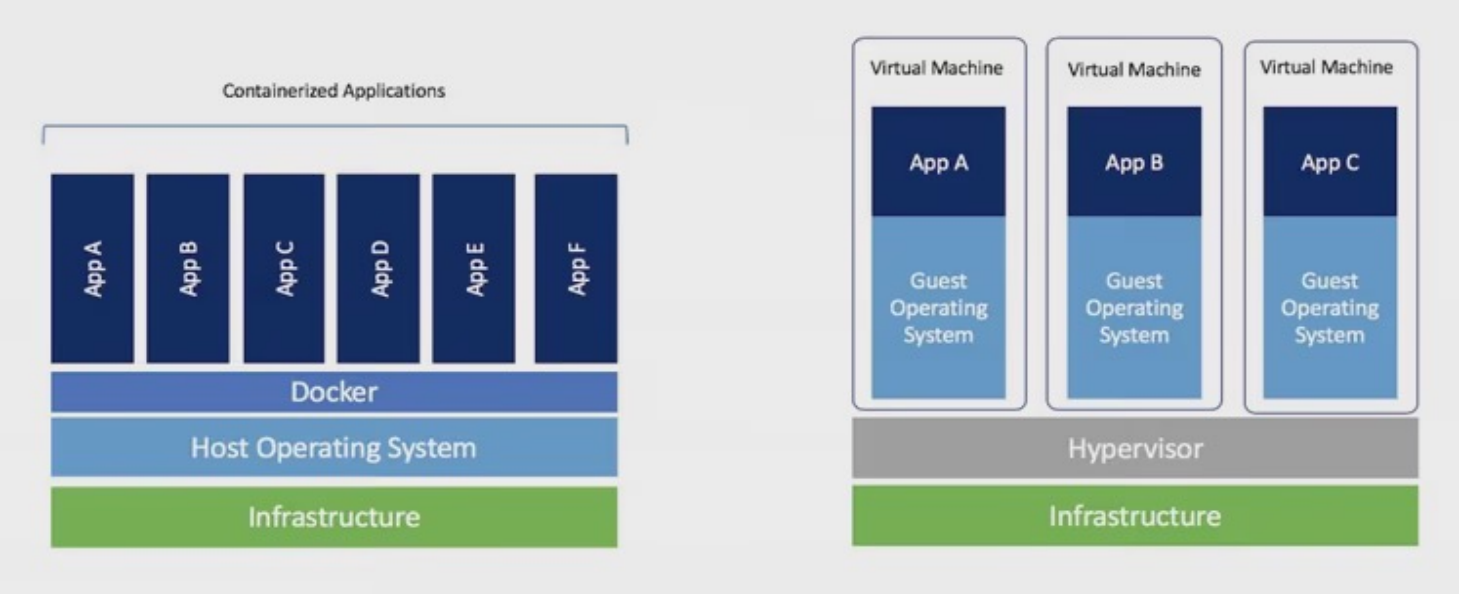
```
True
```

Containers at ALCF

Introduction to Containers

A container is a software package that wraps a software process or microservice to make it executable in all computing environments. It encapsulates an application and its dependencies into a "container". It runs natively on the operating system's kernel, sharing the kernel with other containers.

Ideally, a container can be copied from one system to another, and the contained software runs without changes to the installation. Containers are often compared to virtual machines (VMs)



Advantages of Containers:

Portability: Consistent behavior across different environments.

Lightweight: Quick startups and efficient resource use.

Isolation: Secure and conflict-free application environments.

Efficiency: Maximizes system resource utilization.

Microservices: Supports breaking apps into smaller, scalable services.

Scalability: Easily scales with tools like Kubernetes.

Version Control: Infrastructure can be tracked and managed like code.

CI/CD: Simplifies continuous deployment and integration.

Developer Productivity: Consistent local development setup.

Strong Ecosystem: Vast community and third-party tool support.

Containers at ALCF

- Several container technologies like Docker, podman, containerd. At ALCF, users must run Singularity containers. Singularity is a container technology built for supercomputers with security in mind. Singularity has now joined the Linux Foundation and has been renamed Apptainer
- Either build a singularity container from scratch or build a docker container locally on your machine and subsequently convert it to a singularity container. An example to build a docker container locally can be found in our user docs.
- We have a registry for different containers at ALCF. A walkthrough of running an MPI container on Polaris is here
- Reach out to support@alcf.anl.gov if you have any questions.

Thank you!