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CORE LAB

Kubeflow *as-a-service* on HPC clusters – first experience

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KAUST Supercomputing Core Lab

- Shaheen 2 (Flagship)
    - Cray XC40: 6174 nodes (Intel Haswell 32 cores 128GB)
- Ibex cluster:
    - Heterogeneous CPU (Intel/AMD): > 22K cores (250GB-3TB memory)
    - Heterogeneous GPU (NVIDIA): > 600 GPUs
- Shaheen 3 (Flagship refresh – Coming Soon)
    - HPE Cray EX4000: CPUs + GPUs

SLURM Everywhere

User Personas – by jobtypes

- SLURM batch jobs
  - Large scale HPC (CFD, CompChem, Earth Sci, GeoSci, Bioscience, Datascience)
  - Singleton, arrays, dependency, burst buffer
  - Client/Server (Dask, Ray)
- SLURM Interactive jobs
  - Datascience on GPUs – model development
  - Jupyter, VS Code

Motivation

- Ease-of-use for Interactive computing
- Enable resilient + reproducible workflows
- Cross-platform portability -- workstation/cloud/HPC cluster

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Kubeflow

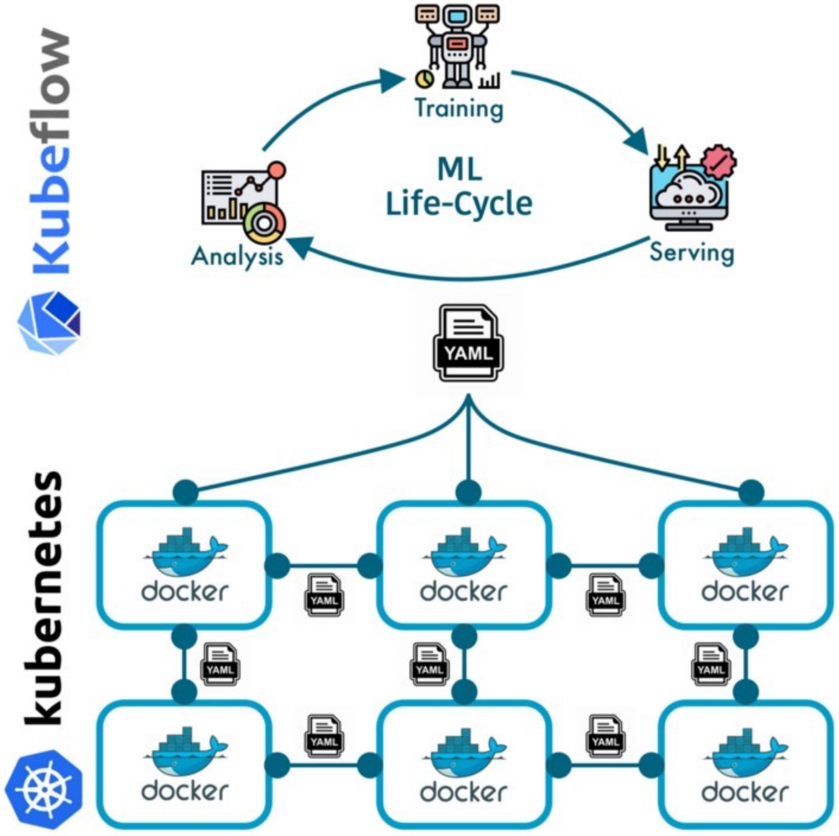
Kubeflow

Kubeflow is a framework for developing data science models and workflows

Depends on Kubernetes and abstract its use through a GUI

Kubeflow *as a service* provides:

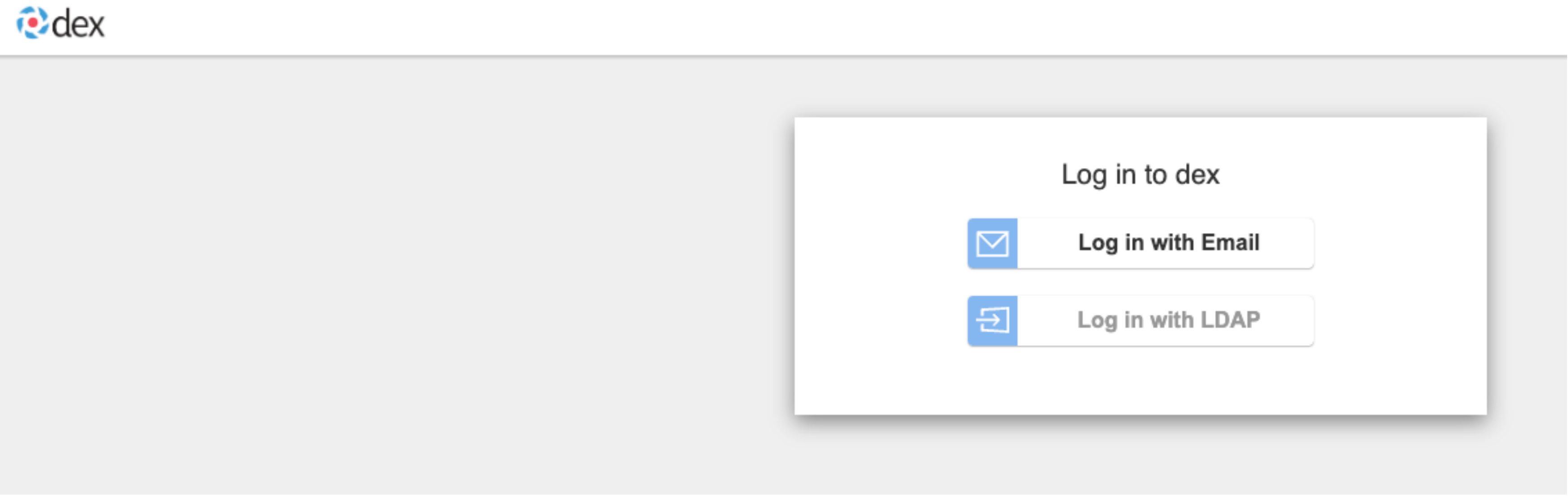
- Interactive notebooks
- Kubeflow pipelines – create reproducible workflows
- Katib – hyperparameter optimization experiments
- Kserve – model serving platform



Functionality tested so far …

- Interactive computing
- Distributed training

Kubeflow Authentication



dex

Log in to dex

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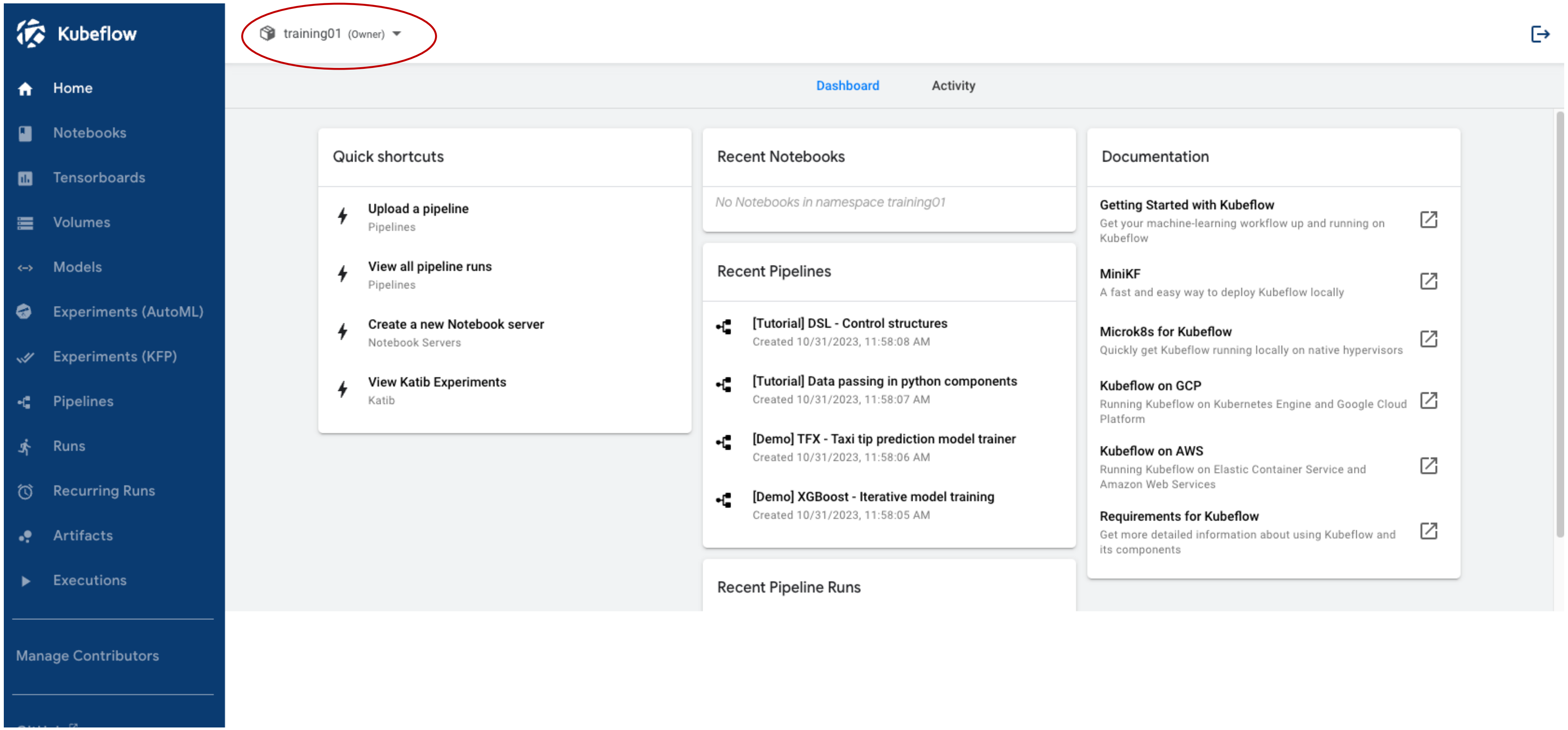
Main dashboard



Quick shortcuts

- Upload a pipeline
  Pipelines
- View all pipeline runs
  Pipelines
- Create a new Notebook server
  Notebook Servers
- View Katib Experiments
  Katib

Recent Notebooks

No Notebooks in namespace training01

Recent Pipelines

- [Tutorial] DSL - Control structures
  Created 10/31/2023, 11:58:08 AM
- [Tutorial] Data passing in python components
  Created 10/31/2023, 11:58:07 AM
- [Demo] TFX - Taxi tip prediction model trainer
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- [Demo] XGBoost - Iterative model training
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Recent Pipeline Runs

Documentation

- Getting Started with Kubeflow
  Get your machine-learning workflow up and running on Kubeflow
- MiniKF
  A fast and easy way to deploy Kubeflow locally
- Microk8s for Kubeflow
  Quickly get Kubeflow running locally on native hypervisors
- Kubeflow on GCP
  Running Kubeflow on Kubernetes Engine and Google Cloud Platform
- Kubeflow on AWS
  Running Kubeflow on Elastic Container Service and Amazon Web Services
- Requirements for Kubeflow
  Get more detailed information about using Kubeflow and its components

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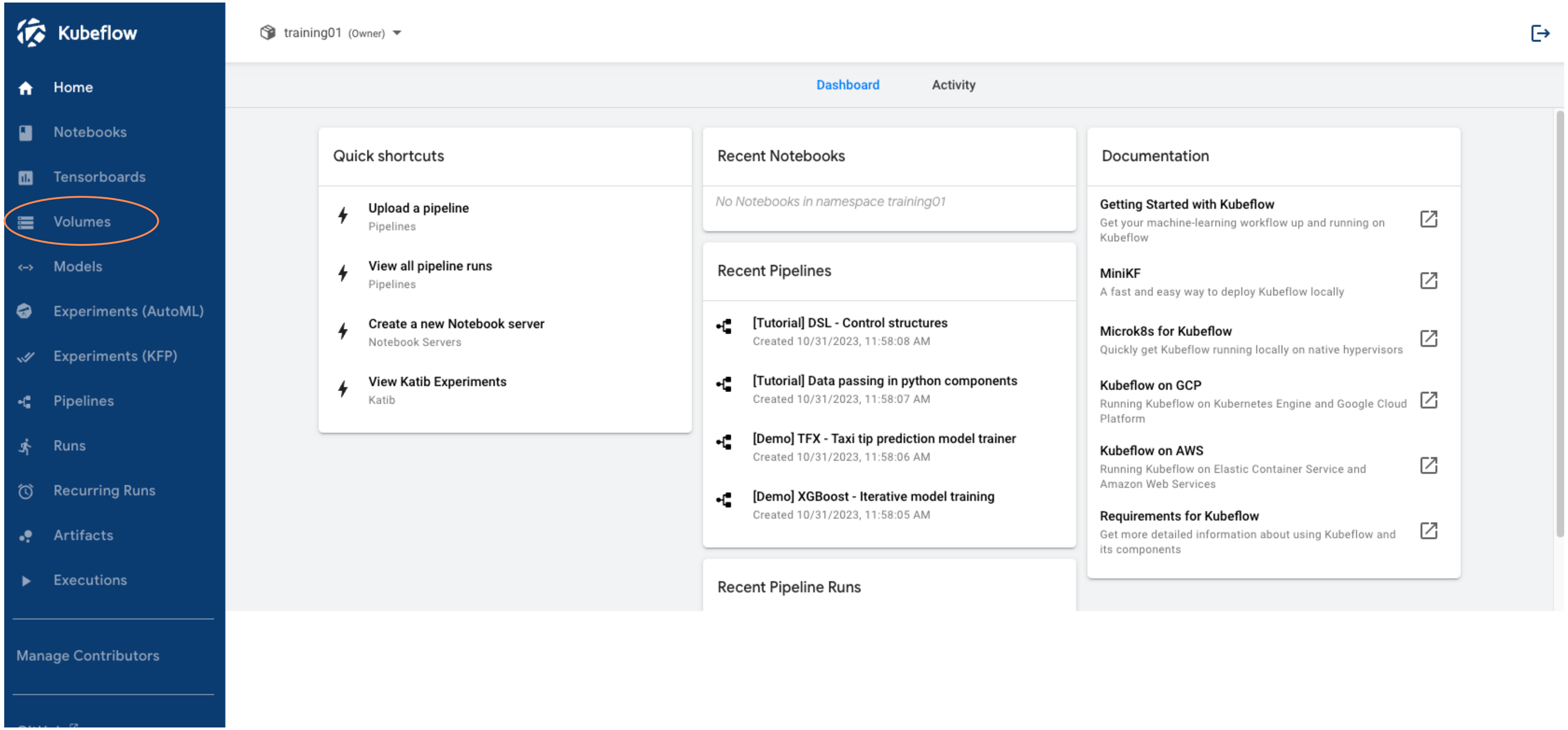
Persistent Volume -- attachable



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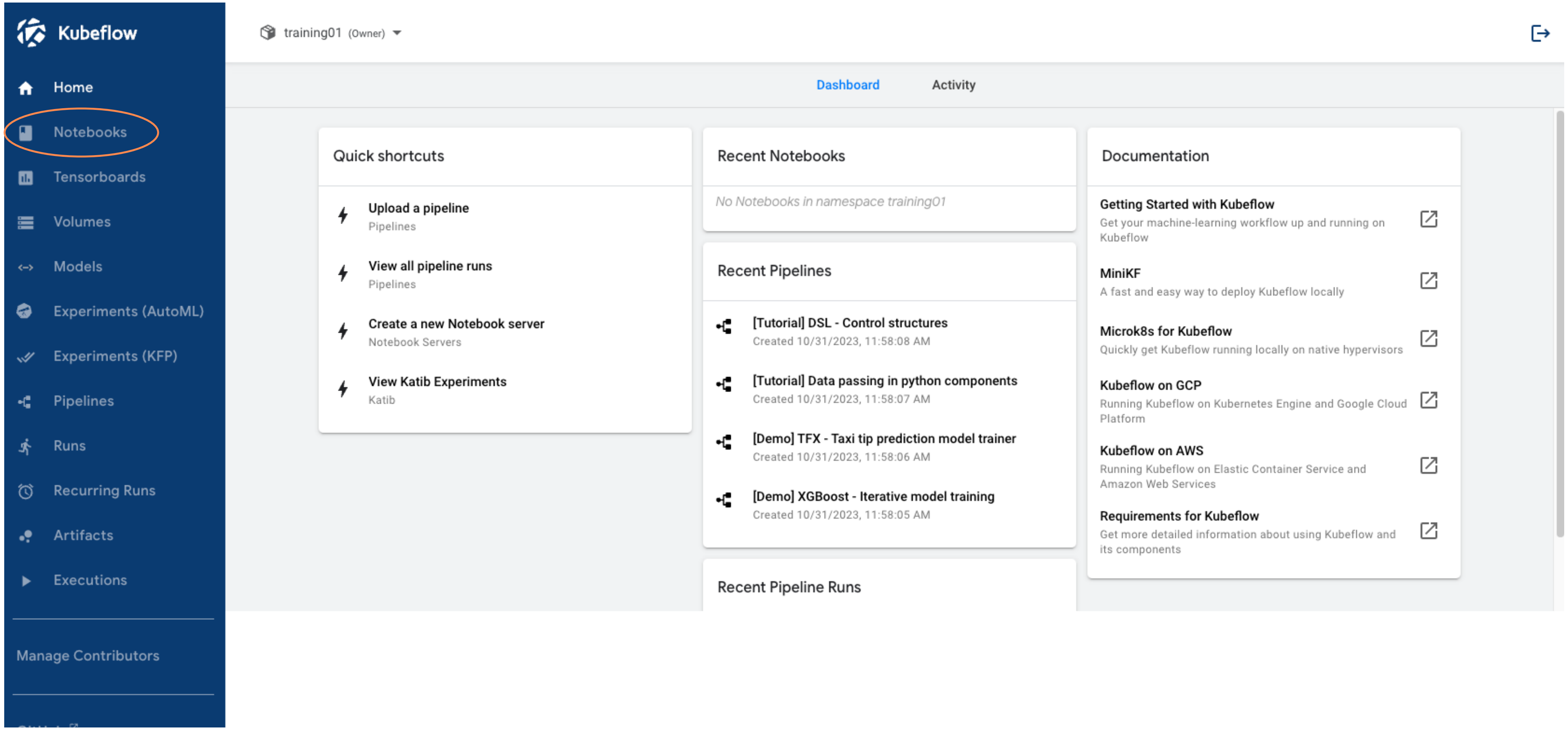
Creating Notebook



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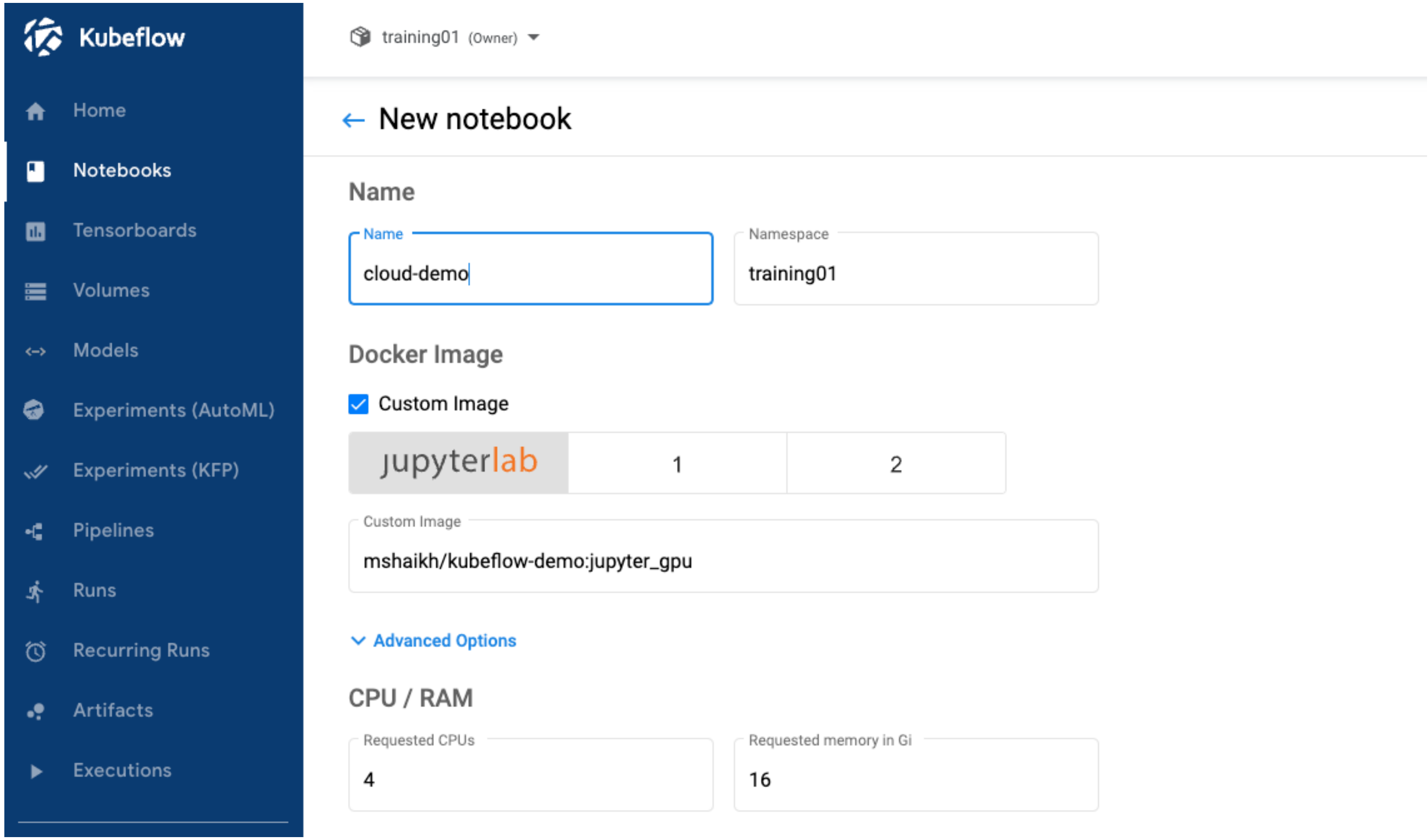


training01 (Owner)

← New notebook

Name

Name: cloud-demo

Namespace: training01

Docker Image

☑ Custom Image

jupyterlab	1	2

Custom Image: mshaikh/kubeflow-demo:jupyter_gpu

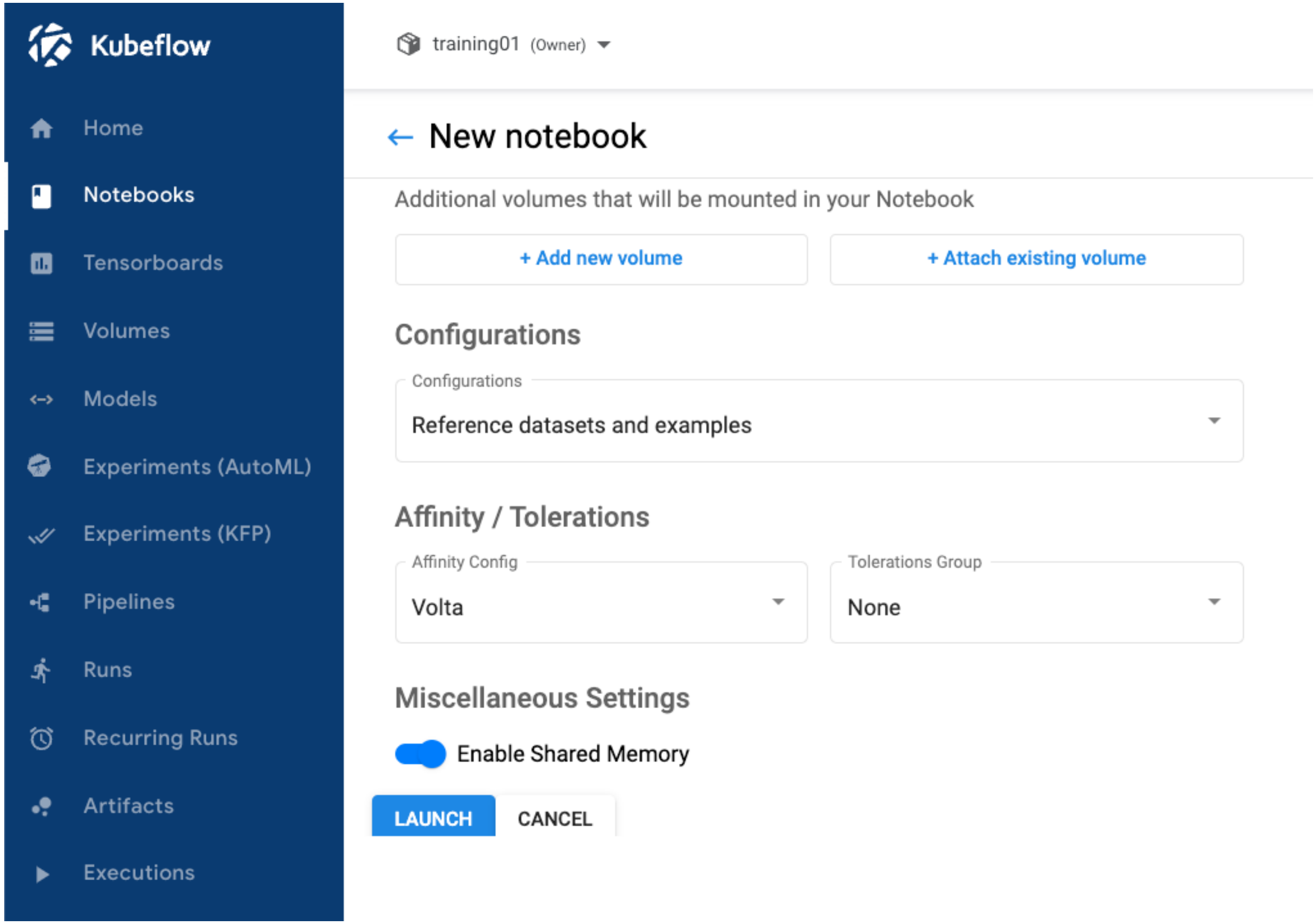
Advanced Options

CPU / RAM

Requested CPUs: 4

Requested memory in Gi: 16

Creating Notebook



New notebook

Additional volumes that will be mounted in your Notebook

Configurations

Configurations: Reference datasets and examples

Affinity / Tolerations

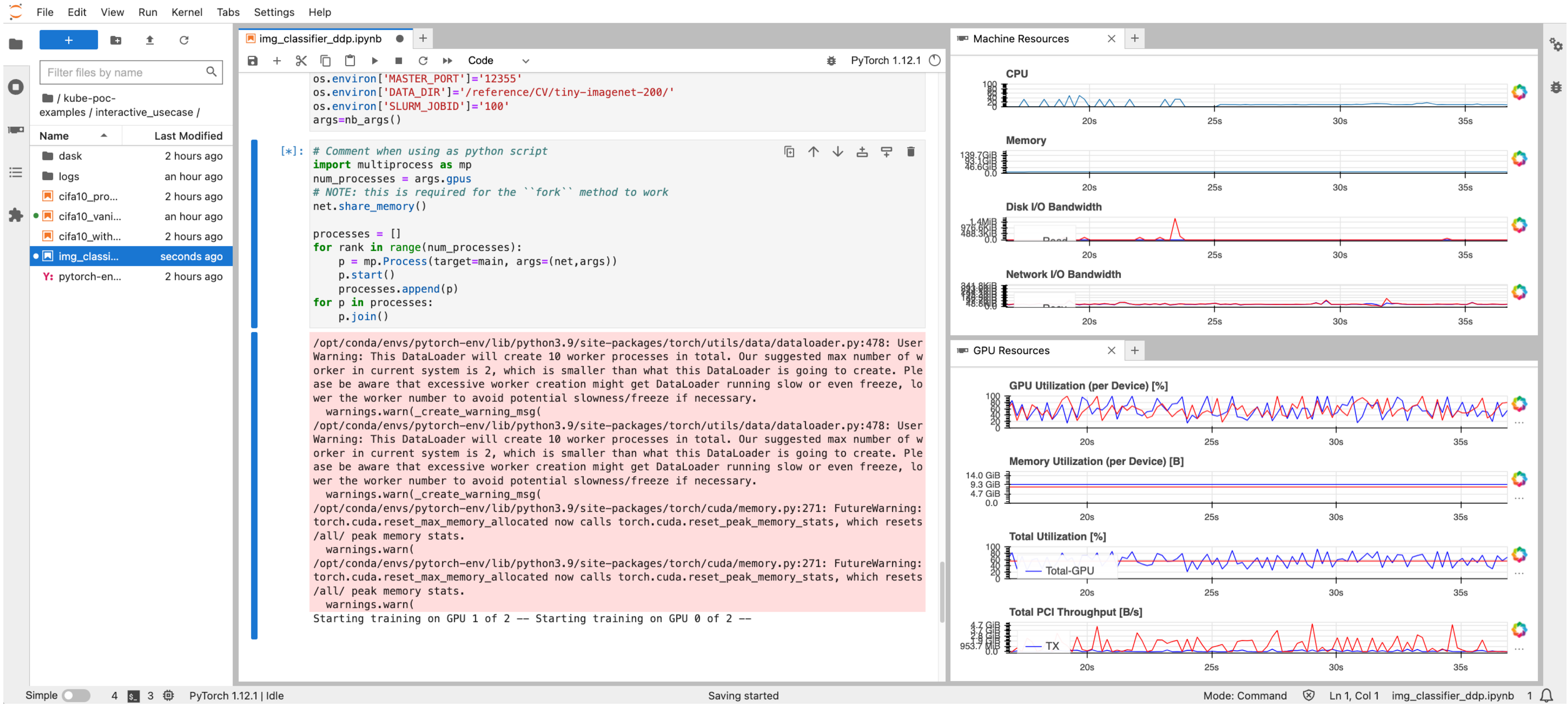
Affinity Config: Volta

Tolerations Group: None

Miscellaneous Settings

Enable Shared Memory

Creating Notebook



Name	Last Modified
dask	2 hours ago
logs	an hour ago
cifa10_pro...	2 hours ago
cifa10_vani...	an hour ago
cifa10_with...	2 hours ago
img_classi...	seconds ago
pytorch-en...	2 hours ago

```
os.environ['MASTER_PORT']='12355'
os.environ['DATA_DIR']='/reference/CV/tiny-imagenet-200/'
os.environ['SLURM_JOBID']='100'
args=nb_args()
```

[*]:

```
# Comment when using as python script
import multiprocess as mp
num_processes = args.gpus
# NOTE: this is required for the ``fork`` method to work
net.share_memory()

processes = []
for rank in range(num_processes):
    p = mp.Process(target=main, args=(net,args))
    p.start()
    processes.append(p)
for p in processes:
    p.join()
```

```
/opt/conda/envs/pytorch-env/lib/python3.9/site-packages/torch/utils/data/dataloader.py:478: User
Warning: This DataLoader will create 10 worker processes in total. Our suggested max number of w
orker in current system is 2, which is smaller than what this DataLoader is going to create. Ple
ase be aware that excessive worker creation might get DataLoader running slow or even freeze, lo
wer the worker number to avoid potential slowness/freeze if necessary.
  warnings.warn(_create_warning_msg(
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  warnings.warn(_create_warning_msg(
/opt/conda/envs/pytorch-env/lib/python3.9/site-packages/torch/cuda/memory.py:271: FutureWarning:
torch.cuda.reset_max_memory_allocated now calls torch.cuda.reset_peak_memory_stats, which resets
/all/ peak memory stats.
  warnings.warn(
/opt/conda/envs/pytorch-env/lib/python3.9/site-packages/torch/cuda/memory.py:271: FutureWarning:
torch.cuda.reset_max_memory_allocated now calls torch.cuda.reset_peak_memory_stats, which resets
/all/ peak memory stats.
  warnings.warn(
Starting training on GPU 1 of 2 -- Starting training on GPU 0 of 2 --
```

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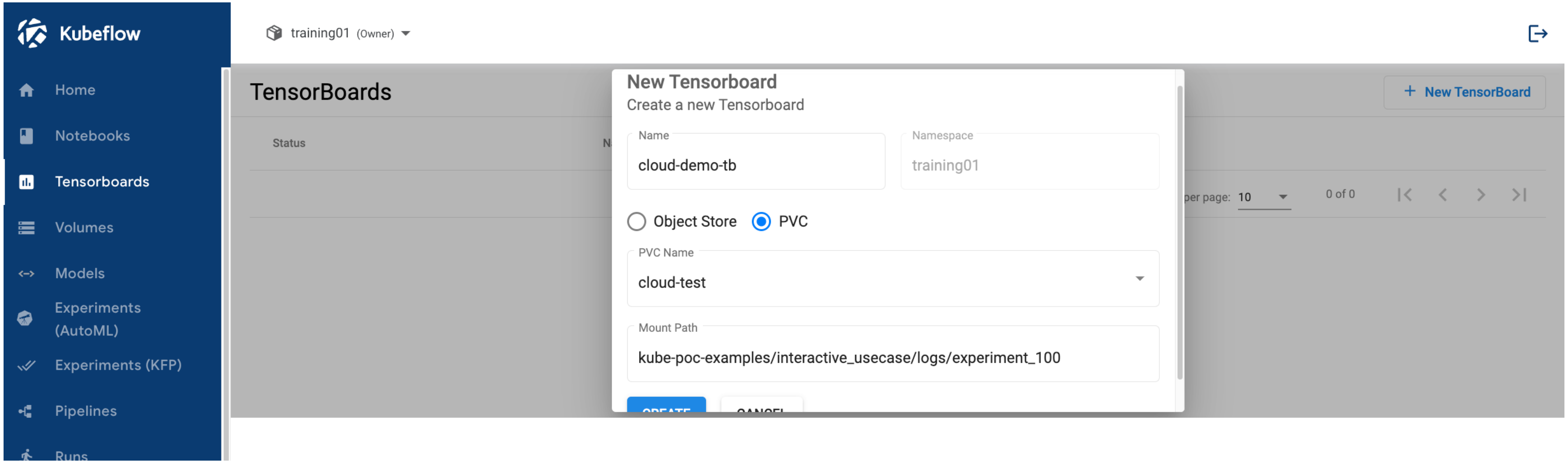
Tensorboard service



New Tensorboard
Create a new Tensorboard

Name: cloud-demo-tb

Namespace: training01

○ Object Store ● PVC

PVC Name: cloud-test

Mount Path: kube-poc-examples/interactive_usecase/logs/experiment_100

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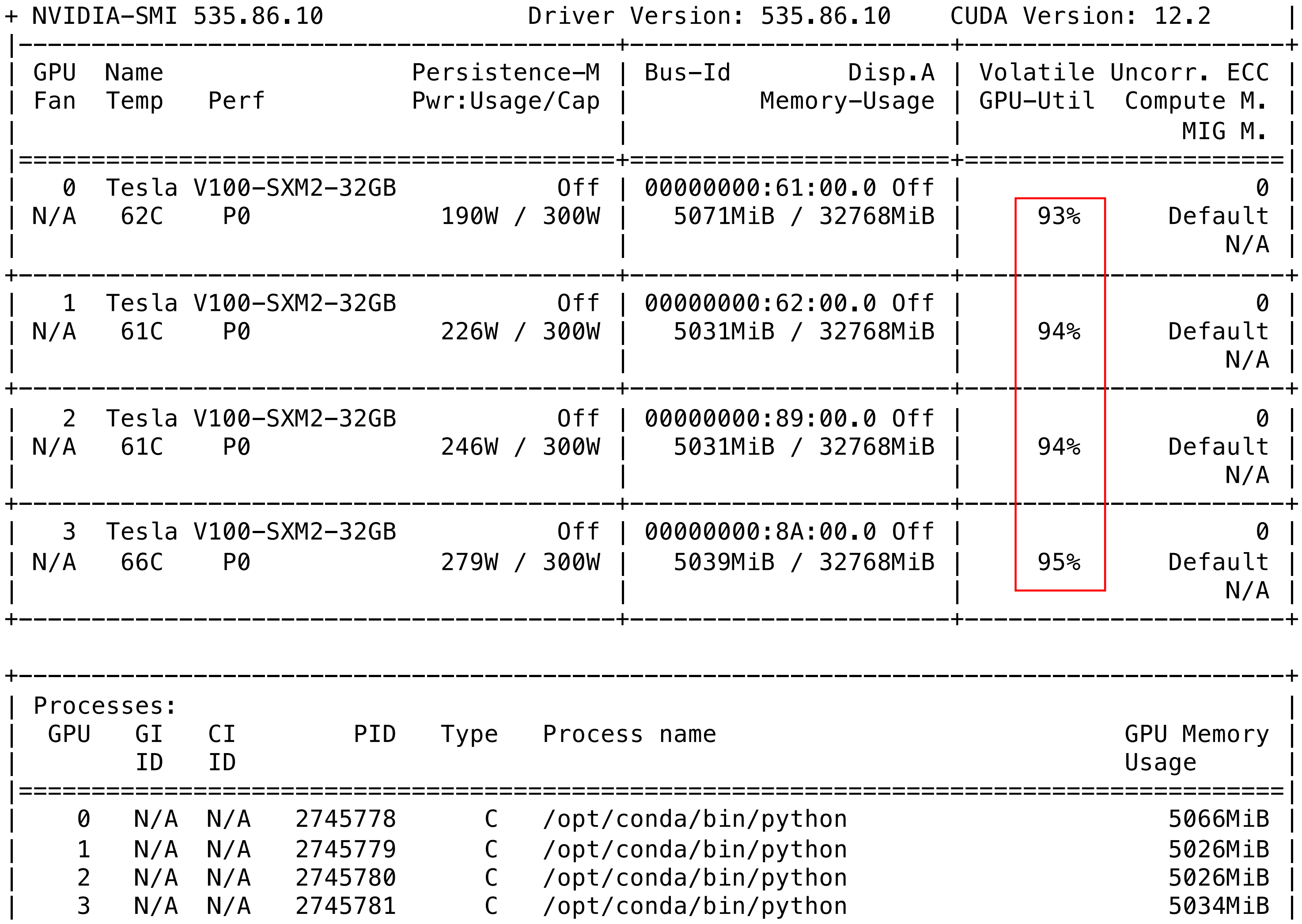
Distributed training

Trianing Opreator -- PytorchJob

```
apiVersion: "kubeflow.org/v1"
kind: "PyTorchJob"
metadata:
  name: “DDP”
  namespace: training01
spec:
  pytorchReplicaSpecs:
    Worker:
      replicas: 1
      restartPolicy: Never
      template:
        metadata:
          annotations:
            sidecar.istio.io/inject: "false"
        spec:
          affinity:
            nodeAffinity:
            requiredDuringSchedulingIgnoredDuringExecution:
             nodeSelectorTerms:
               - matchExpressions:
                 - key: nvidia.com/gpu.product
                   operator: In
                   values:
                     - "Tesla-V100-SXM2-32GB"
```

```
containers:
    - name: pytorch
      image: docker.io/mshaikh/kubeflow-demo:kf-dist-torch-vanilla
      imagePullPolicy: IfNotPresent
      command: [ "torchrun",
                 "--nnodes", "1",
                 "--nproc_per_node","4",
                 "--node_rank","0",
                 "/workspace/mnist/src/ddp.py",
                 "--batch-size","32",
                 "--num-worker","8",
                 "--epochs","4",
                 "--lr","0.001" ]
      env:
      - name: 'NCCL_DEBUG'
        value: 'INFO'
      - name: 'DATA_DIR'
        value: '/data/tiny-imagenet-200'
      - name: 'OMP_NUM_THREADS'
        value: '1'
      resources:
        limits:
          cpu: 8
          memory: '200Gi'
          nvidia.com/gpu: 4
      volumeMounts:
        - name: dshm
          mountPath: /dev/shm
  volumes:
    - emptyDir:
        medium: Memory
      name: dshm
```



```
+ NVIDIA-SMI 535.86.10              Driver Version: 535.86.10    CUDA Version: 12.2     |
|-----------------------------------------+----------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |         Memory-Usage | GPU-Util  Compute M. |
|                                         |                      |               MIG M. |
|=========================================+======================+======================|
|   0  Tesla V100-SXM2-32GB           Off | 00000000:61:00.0 Off |                    0 |
| N/A   62C    P0             190W / 300W |   5071MiB / 32768MiB |     93%      Default |
|                                         |                      |                  N/A |
+-----------------------------------------+----------------------+----------------------+
|   1  Tesla V100-SXM2-32GB           Off | 00000000:62:00.0 Off |                    0 |
| N/A   61C    P0             226W / 300W |   5031MiB / 32768MiB |     94%      Default |
|                                         |                      |                  N/A |
+-----------------------------------------+----------------------+----------------------+
|   2  Tesla V100-SXM2-32GB           Off | 00000000:89:00.0 Off |                    0 |
| N/A   61C    P0             246W / 300W |   5031MiB / 32768MiB |     94%      Default |
|                                         |                      |                  N/A |
+-----------------------------------------+----------------------+----------------------+
|   3  Tesla V100-SXM2-32GB           Off | 00000000:8A:00.0 Off |                    0 |
| N/A   66C    P0             279W / 300W |   5039MiB / 32768MiB |     95%      Default |
|                                         |                      |                  N/A |
+-----------------------------------------+----------------------+----------------------+

+---------------------------------------------------------------------------------------+
| Processes:                                                                            |
|  GPU   GI   CI        PID   Type   Process name                            GPU Memory |
|        ID   ID                                                             Usage      |
|=======================================================================================|
|    0   N/A  N/A    2745778      C   /opt/conda/bin/python                      5066MiB |
|    1   N/A  N/A    2745779      C   /opt/conda/bin/python                      5026MiB |
|    2   N/A  N/A    2745780      C   /opt/conda/bin/python                      5026MiB |
|    3   N/A  N/A    2745781      C   /opt/conda/bin/python                      5034MiB |
```

SLURM vs Kubeflow

- PyTorch DDP training
- Dataset: TinyImageNet200
- Model: ResNet50
- Nodes: 1
- GPUs per node: 4 V100 SXM2 (32GB)

- Training for 20 epochs
- Batch size: 256

SLURM		Kubeflow training opreator	
Time to solution(s)	Accuracy	Time to solution(s)	Accuracy
1939.232	48%	1881.21	48%

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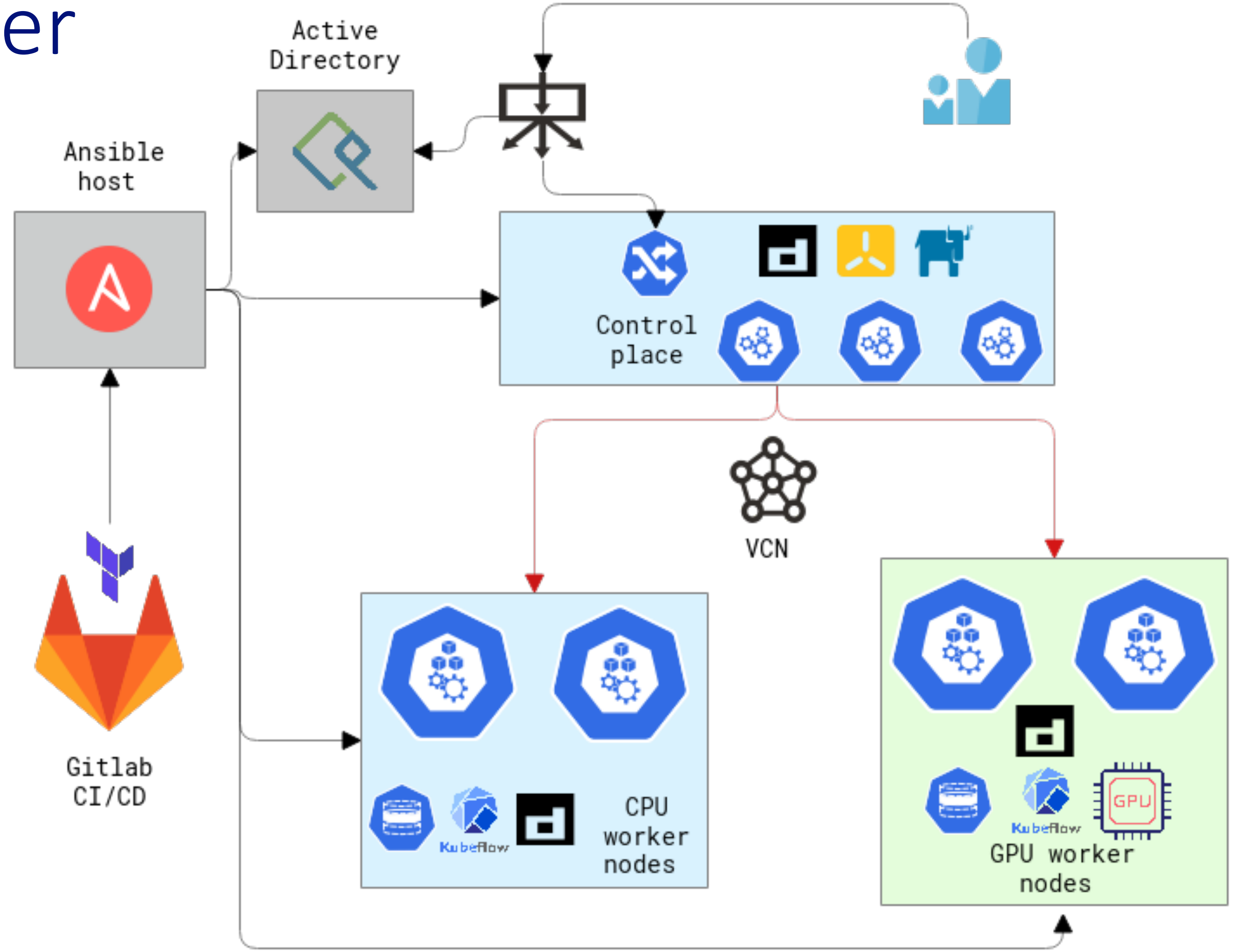
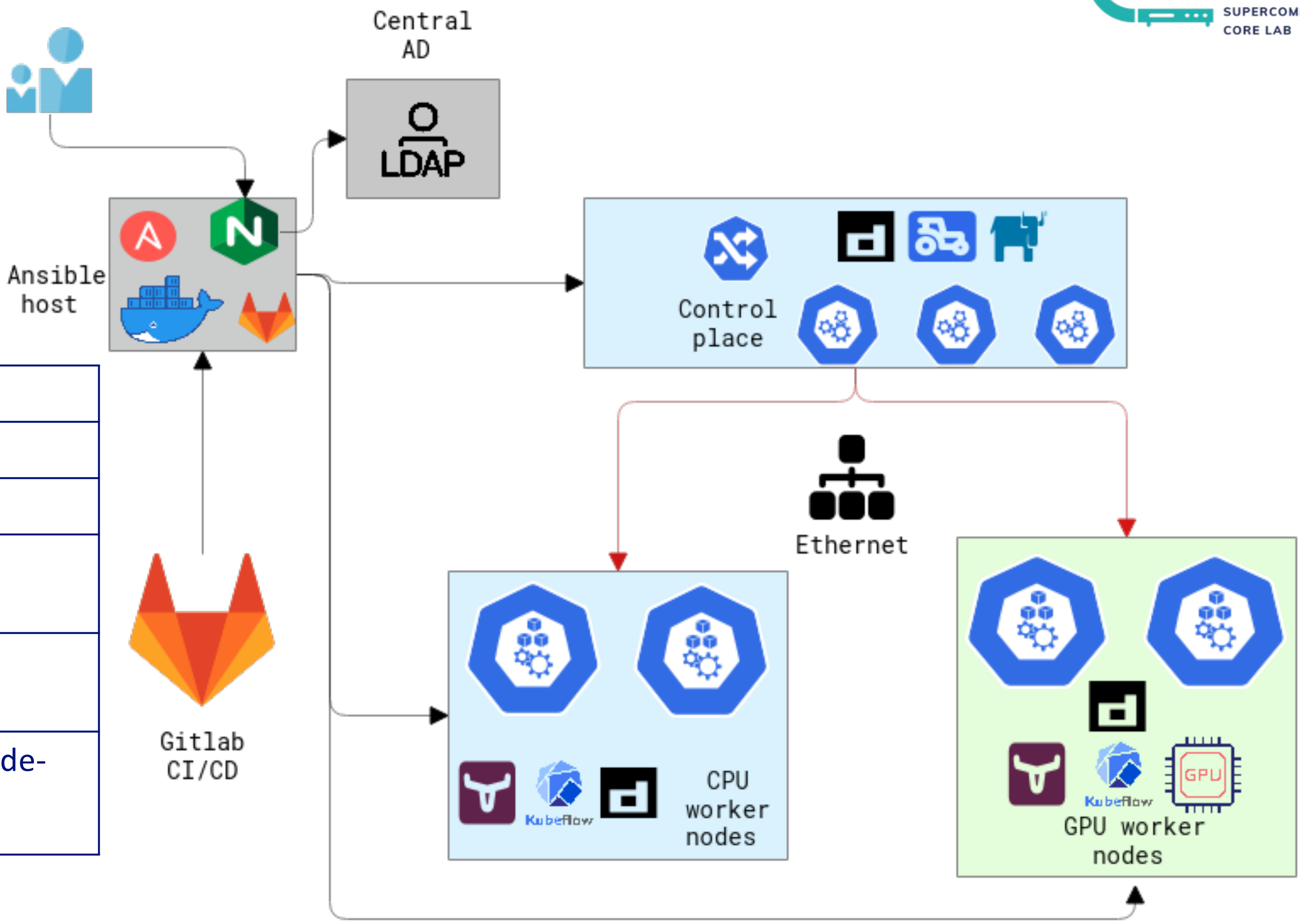
Cluster Infrastructure

Cloud cluster

Provision	Terraform
Manage	Ansible
OS	CentOS 8
K8s Distro	k3s
Container Runtime	containerd
Storage class	NFS



On-Prem cluster



Provision	None
Manage	Ansible
OS	Rocky Linux 9.2
K8s Distro	RKE2
Container Runtime	containerd
Storage class	Longhorn on node-local storage

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Lessons Learnt

- Master in HA
- K3s vs RKE2 (mysql vs etcd)
- DiskPressure – `CrashLoopBackOff`
- Multi-node cluster is important for PoC
- NVIDIA GPU operator vs Device plugin
- Node feature discovery add-on
- Appropriate Container Network Interface (Ethernet + IB + …..)

Lessons Learnt

- Identity management in a container
  - Per user image vs injecting credentials via Configmaps
- The `kubectl` CLI use in Jupyter session – restricted to namespace
- Customize base images form Kubeflow
  - https://www.kubeflow.org/docs/components/notebooks/container-images/
- The Kubeflow UI is useful, until there is a problem. `kubectl` access is needed to investigate what went wrong. That's a user support ticket for HPC centers.
- The `kubectl describe` output and `kubectl logs` are not always helpful
- For high throughput workflows (with SPMD), `restartPolicy=OnFailure` provides resiliency

Thank you

Questions and contact:
mohsin.shaikh@kaust.edu.sa