Simplifying HPC and ML Application Deployment across the Computing Continuum

Jack Brassil
Dept. of Computer Science
Princeton University

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Goal – Support mix of HPC and AI/ML workloads across platforms

- Diverse population of computational scientists needing Python horizontal and vertical scaling
- AI/ML research and training needs growing rapidly in Humanities and Social Sciences
- Some degree of cluster hardware divergence today (e.g., dedicated campus system for LLM research)
- Need to rationalize different software frameworks in use across campus; hard to train, hard to support, expensive
- Investigating *RAY* to provide a "single" (primary) framework to support on the widest range of target platforms

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(CC* Integration-Small: Unifying and Accelerating Campus Computational Science with Ray)

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Goal – Easily run workloads across the computing continuum

1. Public compute clouds
2. DoE Leadership Class Systems
3. NSF Shared SuperComputing Centers
4. NSF Computer & Networking Testbeds (FABRIC, CloudLab)
5. Regional AI Hubs
6. Conventional campus HPC clusters
7. Dedicated AI GPU clusters (Princeton Language & Intelligence)
8. Desktops & departmental clusters
9. IoT (e.g., Jetson, Raspberry Pi ?)

What is RAY?

- Python open-source distributed computing framework
- Easy to use, simple multi-programming abstractions, and integrated scheduling and cluster management
- Integrations with common data science and scientific computing tools
- Focus on support for simulation, training, and model serving for RL applications
- Supported by founders from UC Berkeley RISELab at Anyscale, Inc.

RAY

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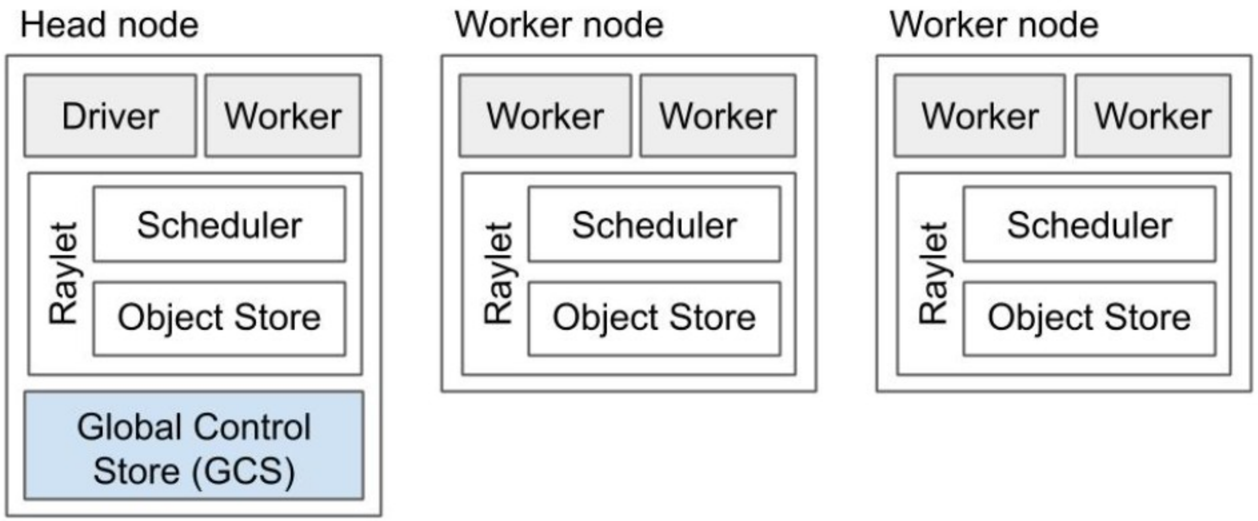
What is RAY?

Programming Model highlights:

- A *task* represents the execution of a remote function on a stateless worker. A future representing the result of the task is returned immediately. Futures can be retrieved using ray.get()
- An *actor* represents a stateful computation. Each actor (Class) exposes methods that can be invoked remotely and returns a future.
- *Dynamic task graph* computation – the execution of both remote functions and actor methods is automatically triggered when their inputs become available.

What is RAY?



The major components in a cluster: a Global Control Store (GCS), a distributed scheduler, and a distributed object store. Each component is horizontally scalable and fault-tolerant.

Simple Ray programming example

```python
import numpy as np
N = 4000




def f(x):
    arr = np.random.randn(N, N)
    inv_arr = np.linalg.inv(arr)
    return x

futures = [f(i) for i in range(96)]
print(ray.get(futures))
```

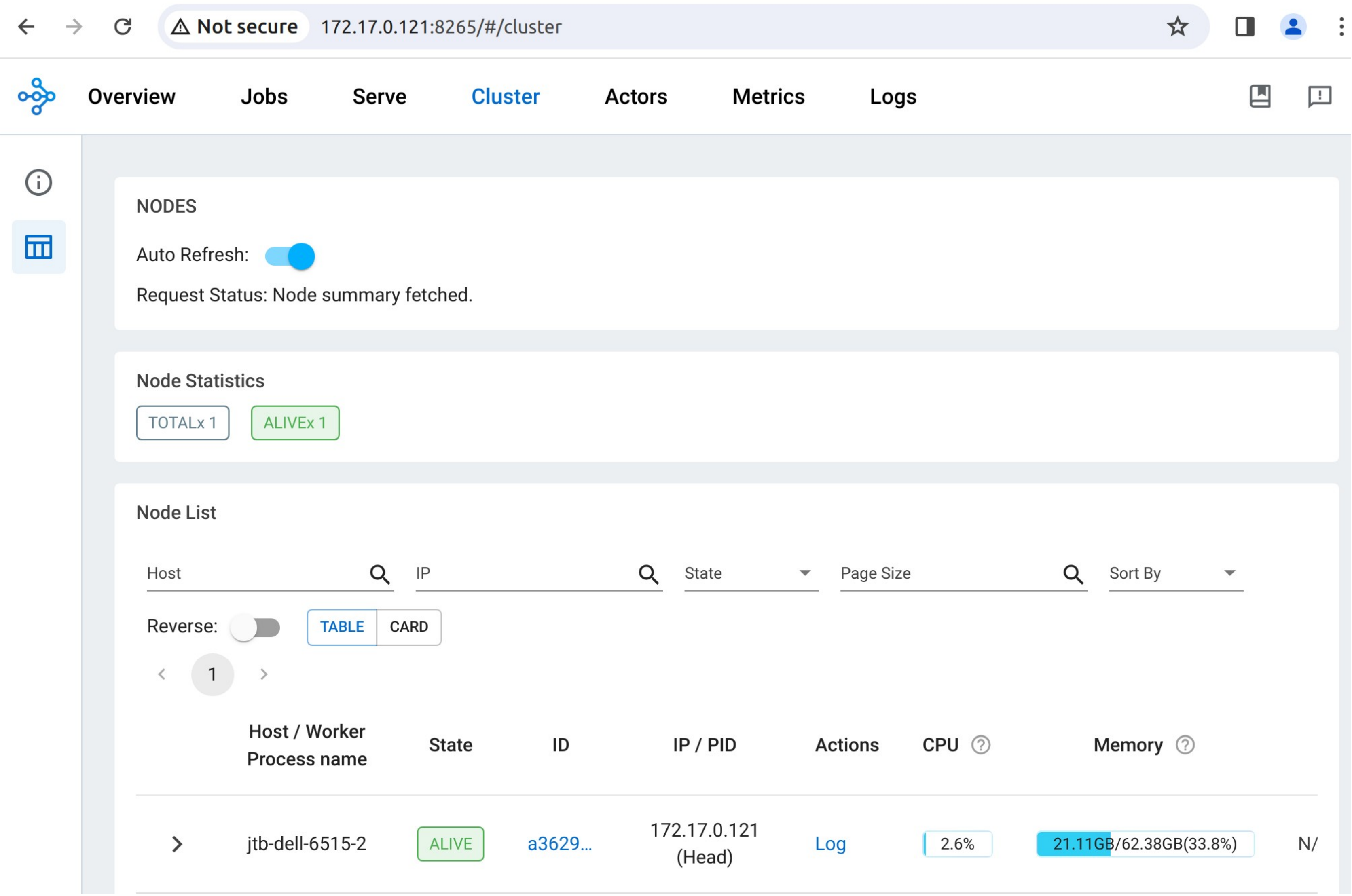
```python
import numpy as np, ray
N = 4000
ray.init()

@ray.remote
def f(x):
    arr = np.random.randn(N, N)
    inv_arr = np.linalg.inv(arr)
    return x

futures = [f.remote(i) for i in range(96)]
print(ray.get(futures))
```

Parallelizing 96 4000x4000 matrix inversions

Ray dashboard



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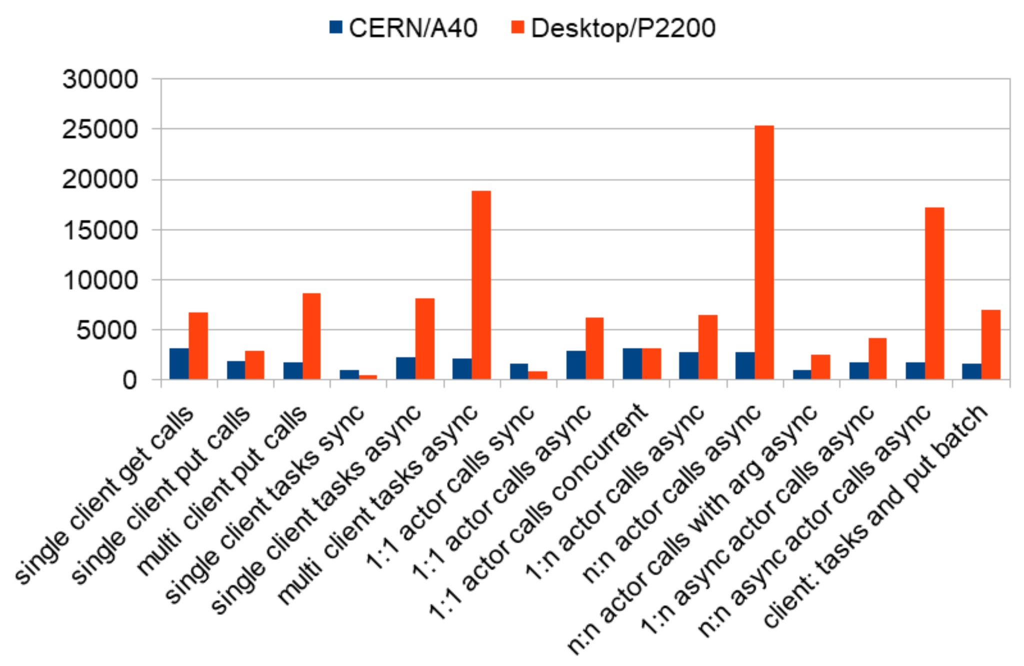
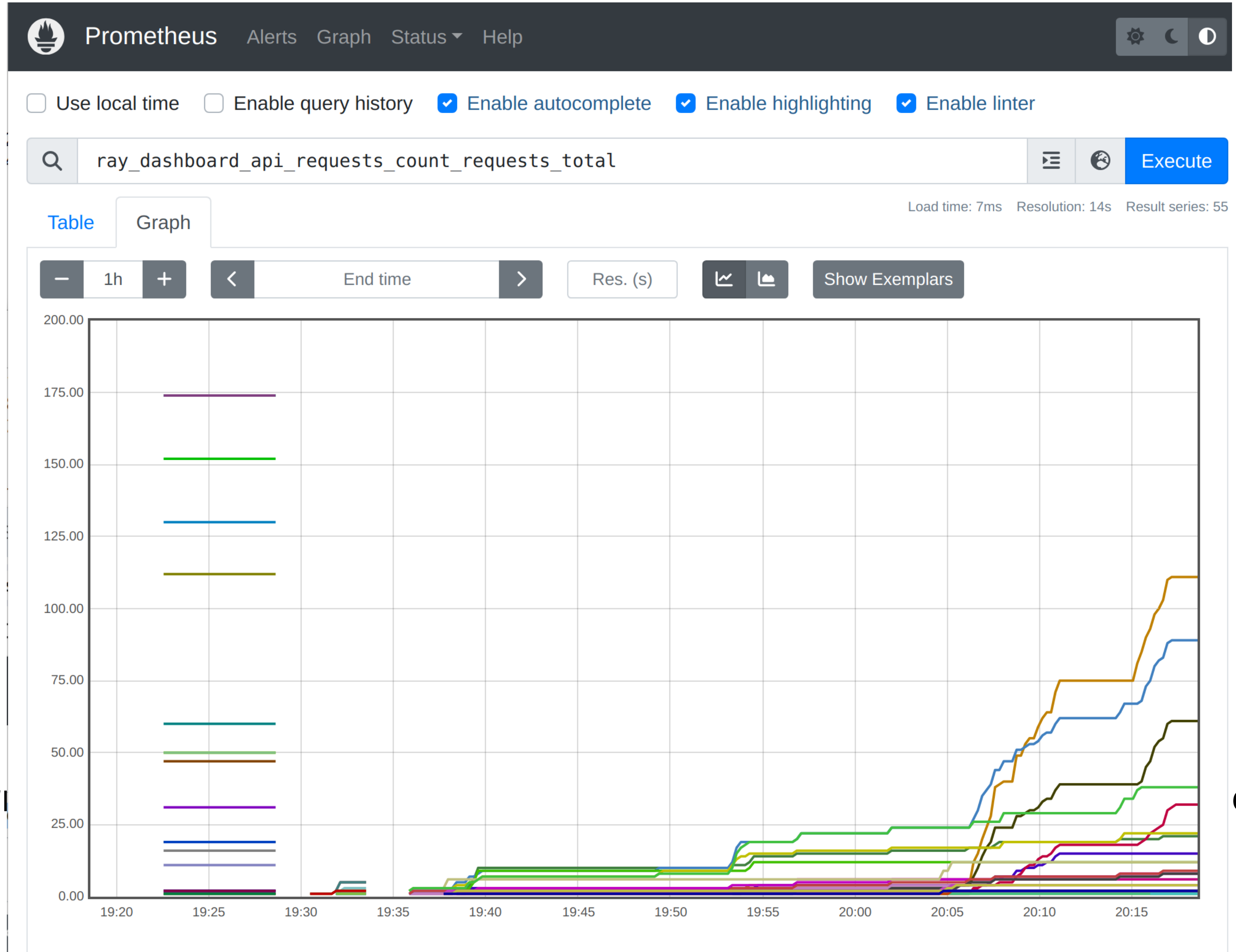
Ray microbenchmarks



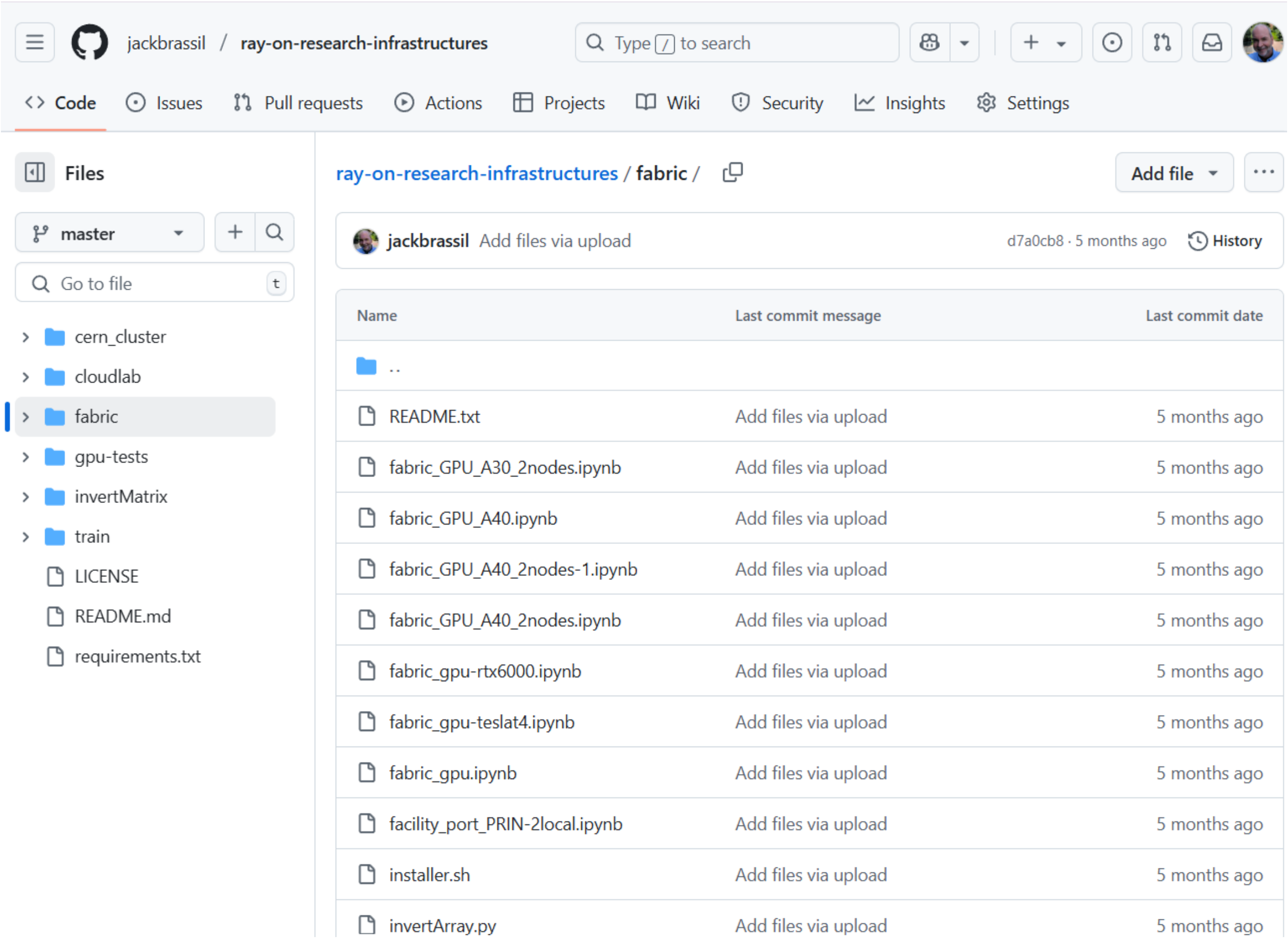
Permits quick performance comparison of different execution environments

Ray Integrations (Visualization)



Per[...] [...]ents

RAY on NSF Research Infrastructures



- CloudLab and FABRIC testbeds as illustrative cluster settings
- Advantages include access to small clusters, diverse GPUs, ease of experimentation, experiment in wild, testing and deployment of RL apps, federated learning apps
- All necessary artifacts on Project github

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Case 1: NSF CloudLab

- Experiments with 5 bare metal GPU nodes at CloudLab Wisconsin

- Easy to instrument cluster for monitoring RAY, cluster management, task placement, Ray jobs API

- Methodology – run single, multiple, and mixed easy to understand jobs (e.g., large matrix inversions, training a Pytorch Lightning Image Classifier on MNIST data) various platforms)

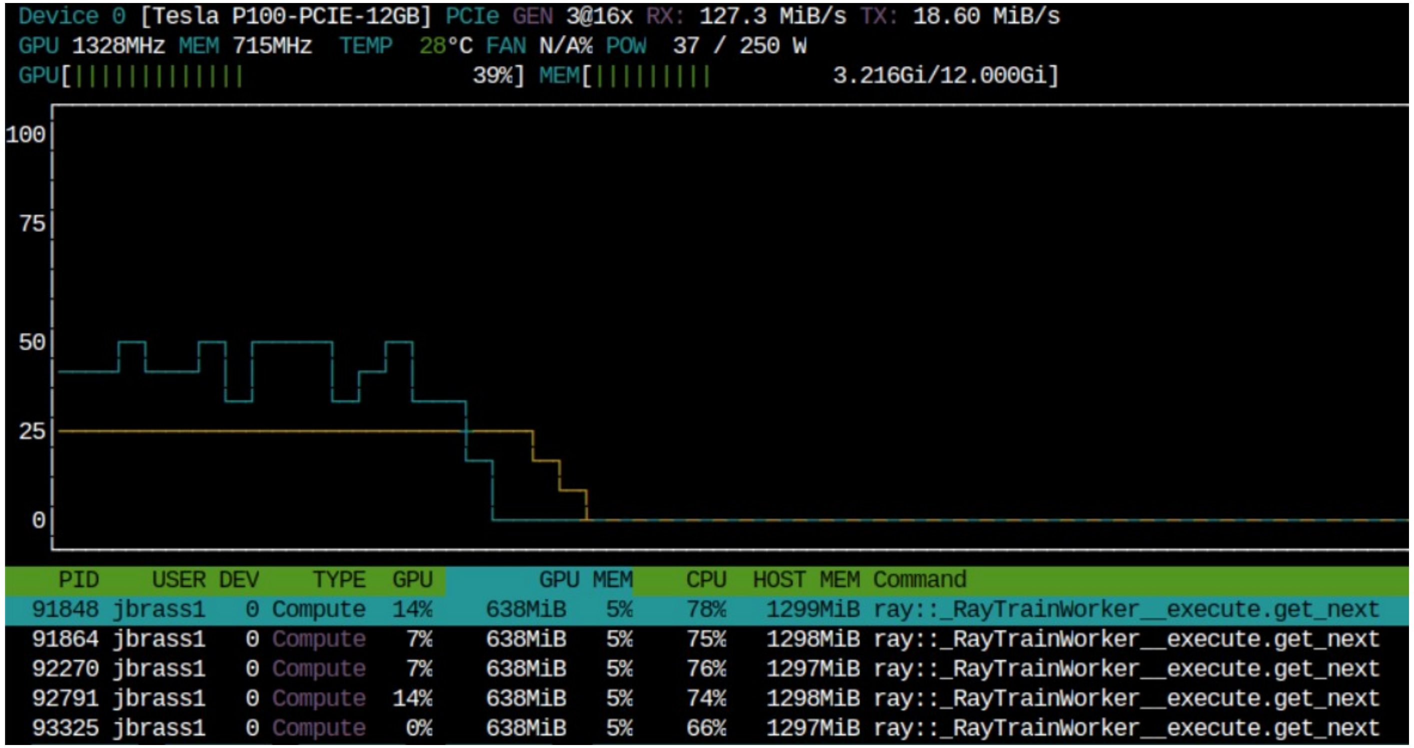
head: ray start --head --node-ip-address= '128.105.144.55:6379'

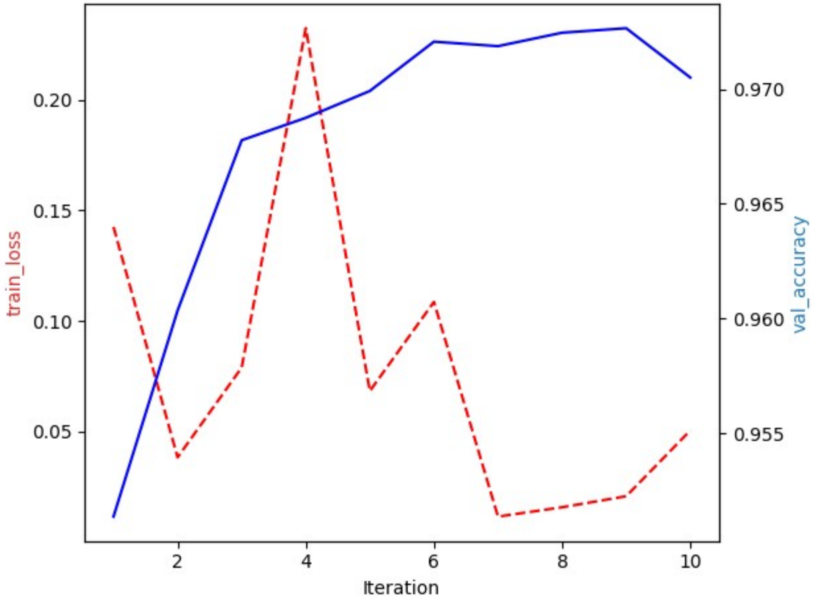
workers: ray start --address='128.105.144.55:6379' --node-ip-address= 128.105.144.[44,45,57,59]

RAY_ADDRESS='http://127.0.0.1:8265' ray job submit
--working-dir . -- python ./invertMatrix.py &

CloudLab – Example

- Simple Pytorch image classifier training
- GPU fully busy at < 10 simultaneous jobs
- Online and offline monitoring (nvtop, btop, TensorBoard)





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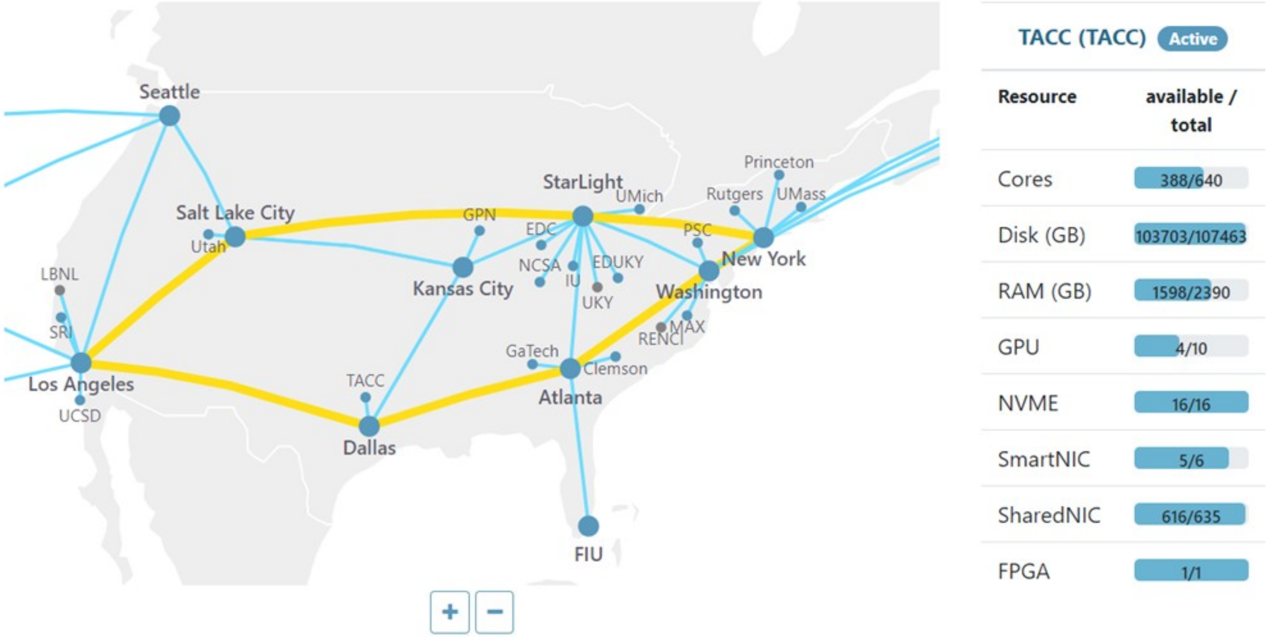
Case 2: NSF FABRIC Research Infrastructure

- Testbed connecting major instruments, compute clouds, and universities
- Permits collaborative sharing of on- and off-campus computing systems
- whatisfabric.net



Ray over FABRIC

- Step 1 - FABRIC Preliminaries. Build a global network topology

```
# Preliminaries (e.g., import FABlib libraries)

from ipaddress import ip_address,
IPv4Address, IPv6Address, IPv4Network, IPv6Network
from fabrictestbed_extensions.fablib.fablib
import FablibManager as fablib_manager
fablib = fablib_manager()

#Create FABRIC slice
slice_name = ’4node-2site’
node1_name = ’prin1’; node2_name = ’prin2’;
node3_name = ’ucsd3’; node4_name = ’ucsd4’;
net_name=’net1’
slice = fablib.new_slice(name=slice_name)

# Add network
net1 = slice.add_l2network(name=net_name,
subnet=IPv4Network("192.168.100.0/24")
```

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Ray over FABRIC

- Step 2 – Deploy VMs across FABRIC sites. Deploy contributed bare metal nodes across sites.

```
# Node1
node1 = slice.add_node(name=node1_name,
  site='PRIN', cores=4, ram=16, disk=32,
  image='default_ubuntu_22')
iface1 = node1.add_component(model='NIC_Basic',
  name='nic1').get_interfaces()[0]
iface1.set_mode('auto')
net1.add_interface(iface1)
.
.
.
# Node4
node4 = slice.add_node(name=node4_name,
site='UCSD', cores=4, ram=16, disk=32,
image='default_ubuntu_22')
iface4 = node4.add_component(model='NIC_Basic',
name='nic1').get_interfaces()[0]
iface4.set_mode('auto')
net1.add_interface(iface4)

# Create topology

slice.submit()
```

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Ray over FABRIC

- Step 3 – Deploy executables & tools

```
# Upload configuration files

result1 = node1.upload_file
 ('config_script.sh', 'config_script.sh')
        .
      .
        .
result4 = node4.upload_file
 ('config_script.sh', 'config_script.sh')

# Additional script arguments

script_args="net-tools wireshark"

# Run configurations

stdout, stderr = node1.execute(f'chmod +x
 config_script.sh && ./config_script.sh
 {script_args} >> config1.log')
      .
        .
        .
stdout, stderr = node4.execute(f'chmod +x
 config_script.sh && ./config_script.sh
 {script_args} >> config4.log')
```

Ray over FABRIC

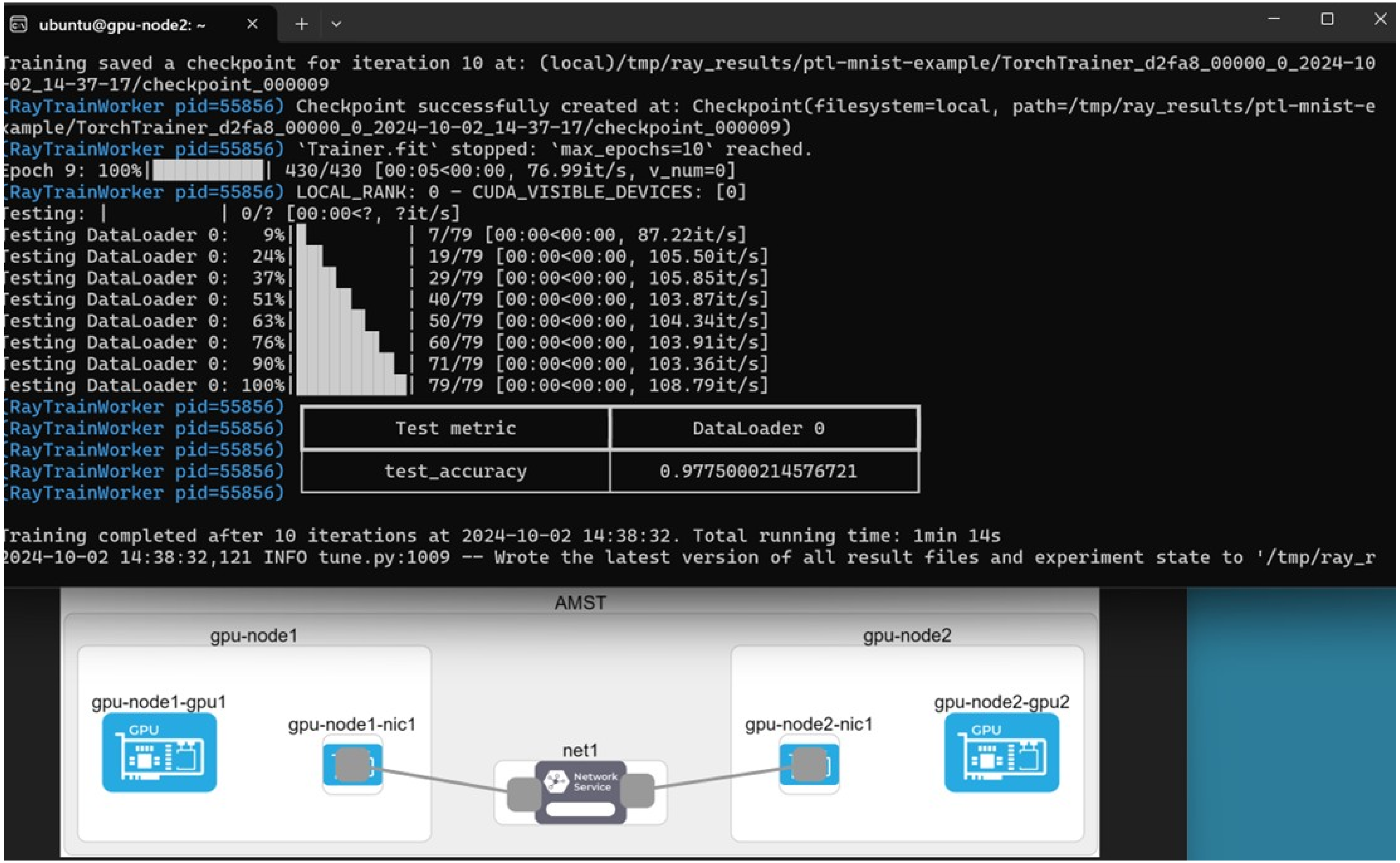
- Step 4 – Run Ray benchmarks

```
------------config_script.sh------------
#!/bin/bash
args=$@
sudo apt install -y $args

pip install -U "ray[default]"

if (worker_node):
  ray start
  --address='192.168.100.3:6379'
  --node-ip-address=192.168.100.3
ray microbenchmark
else:
  ray start --head
  --node-ip-address=192.168.100.3
  --metrics-export-port=8080
  --dashboard-host=192.168.100.3
```

Example: Using Ray on FABRIC testbed



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Open Challenges

- Characterizing RAY performance across multiple, diverse academic platforms.
- Understanding how RAY can streamline teaching distributed systems to a growing cohort of students spanning multiple disciplines.
- Create best practices for multiple job entry points for conventional SLURM clusters
- Optimize RAY performance on hybrid clouds, multiclouds, lower performance interconnects, edge systems

  Thanks!

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Conclusion

- Characterizing RAY performance across multiple, diverse academic platforms.
- Understanding how RAY can streamline teaching distributed systems to a growing cohort of students spanning multiple disciplines.
- Seeking to build and strengthen a RAY community across university Research Computing organizations!

Thanks!

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