The GPU-based cluster @IBiSCo-ReCaS-Bari for containerized scientific applications

Gioacchino Vino[1], M. Antonacci[1], G. Donvito[1], A. Italiano[1], M. Perniola[2]

[1] INFN Bari

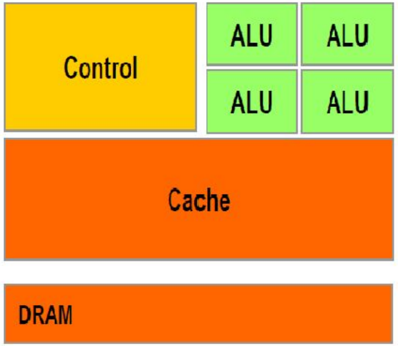
[2] Bari University

Workshop-IBiSCo / Napoli / 18-19 Apr 2024

Why GPU?

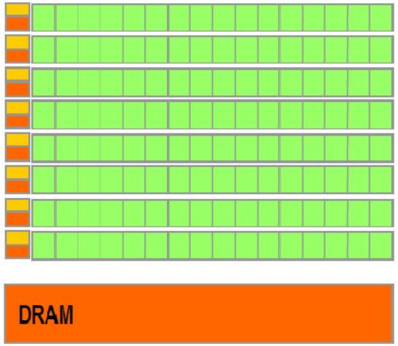
Control Processing Unit (CPU):

- Designed to handle complex tasks
- Low-level parallelism (<100 cores)



Graphical Processing Unit (GPU):

- Massively parallel hardware architecture (> 5000 cores)
- High performance of floating point arithmetic

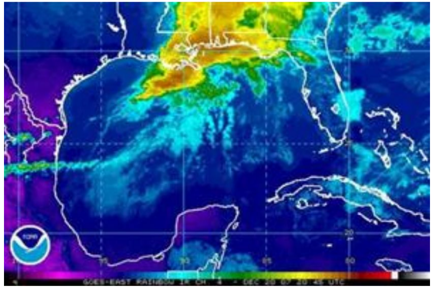


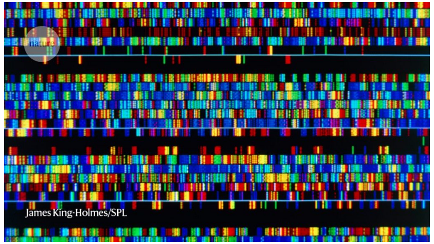
Make them suited for scientific workloads require a huge amount of floating point operations

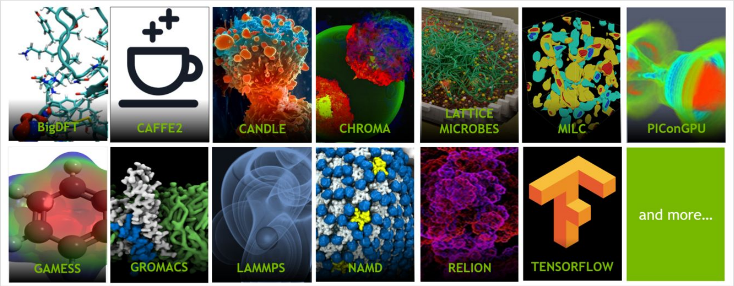
Why GPU?

GPU main applications:

- Machine Learning (Deep Learning) algorithms
- Image processing applications
- Whole-genome sequencing
- Simulations of physical models
- Almost all problems that involve many floating point operations.







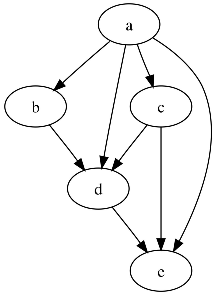
What we have: ReCaS GPU Cluster

Hardware Facility:

- Nodes: 10
- GPUs: 38 (V100 and A100 Nvidia GPU)
- Cores: 1755
- RAM: 13.7 TB
- Local Storage: 55 TB (SSD/HDD)
- Parallel File System: ReCaS storage based on IBM GPFS (12PB)
- Bandwidth between nodes: 10 Gbps

What we provide: GPU Cluster Services

- **Ready-to-use services:**
  - Interactive remote GPU-based IDE services:
    - Jupyter(Hub/Lab)
      - “web service for interactive computing across all programming languages”
    - Rstudio
      - “An integrated development environment for R”
  - Job Scheduler and Orchestration:
    - Support to GPU-based workflows represented as Directed Acyclic Graphs (DAG)

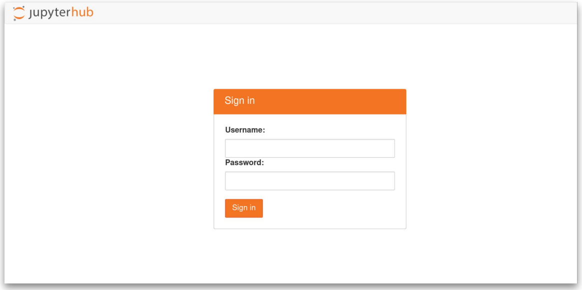


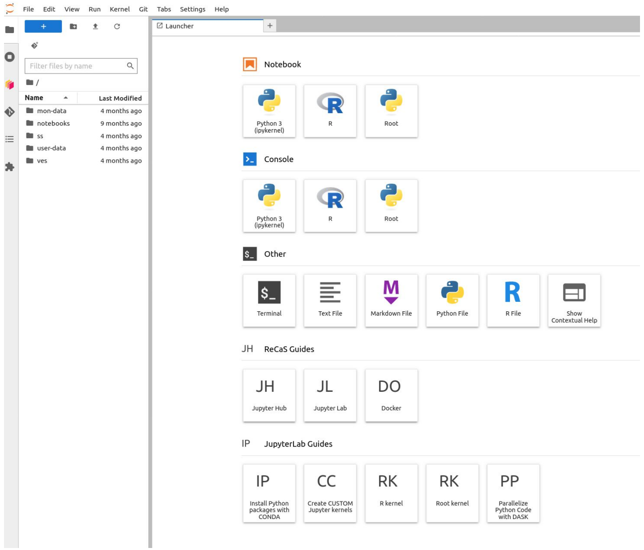
- **User-defined services**
  - Support and Knowledge sharing

What we provide: GPU Cluster Services

JupyterHub

- Centralized authentication system combining IAM and LDAP
- Use computing resources (CPUs and GPUs) on demand without set them aside for a given user
- JupyterLab 4.0
- Jupyter extensions
- Python3, R and Root kernels available
- Use conda environments with Jupyter kernels
- Dask and Dask Jupyter extensions
- Execute notebook in batch with papermill
- Service and technologies guides in the Jupyter Launcher

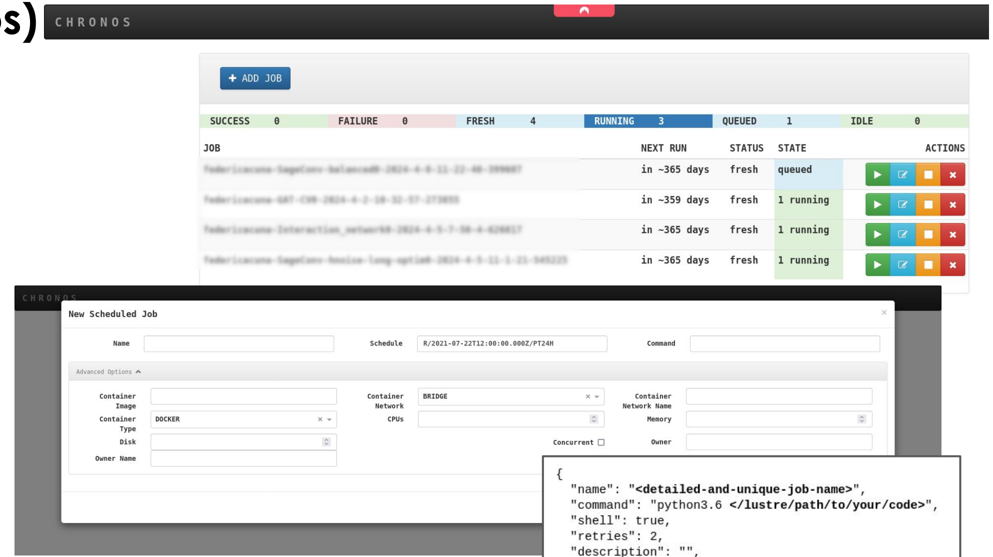




What we provide: GPU Cluster Services

Job Scheduler and Orchestration (Chronos)

- Provides an intuitive and simple User Interface (UI) where to check job status
- New jobs can be submitted using UI or via command line using a JSON file describing the job
- Manages heterogeneous requests:
  - 2 GPU / 4 CPU / 20 GB RAM
  - 100 CPU / 8GB RAM
- A Python client has been implemented to simplify the submission of general purpose applications and Jupyter Notebooks (papermill)




```
{
  "name": "<detailed-and-unique-job-name>",
  "command": "python3.6 </lustre/path/to/your/code>",
  "shell": true,
  "retries": 2,
  "description": "",
  "cpus": 4,
  "disk": 10,
  "mem": 8192,
  "gpus": 1,
  "environmentVariables": [],
  "arguments": [],
  "runAsUser": "<your-username>",
  "owner": "<your-username>",
  "ownerName": "<your-username>",
  "container": {
     "type": "mesos",
     "image": "<your-container-image>",
     "volumes": [{"containerPath":
"/lustre/path/to/your/home-directory", "hostPath":
"/lustre/path/to/your/home-directory", "mode": "RW"}]
  },
  "schedule": "R1//PT10S"
}
```

What's under ReCaS GPU Cluster

Apache Mesos:

- Abstracts all cluster resources in a single virtual entity
- Multi-users / High Availability / Manages many nodes

Marathon:

- Runs long running services on top of Apache Mesos
- High Availability / Load balancing

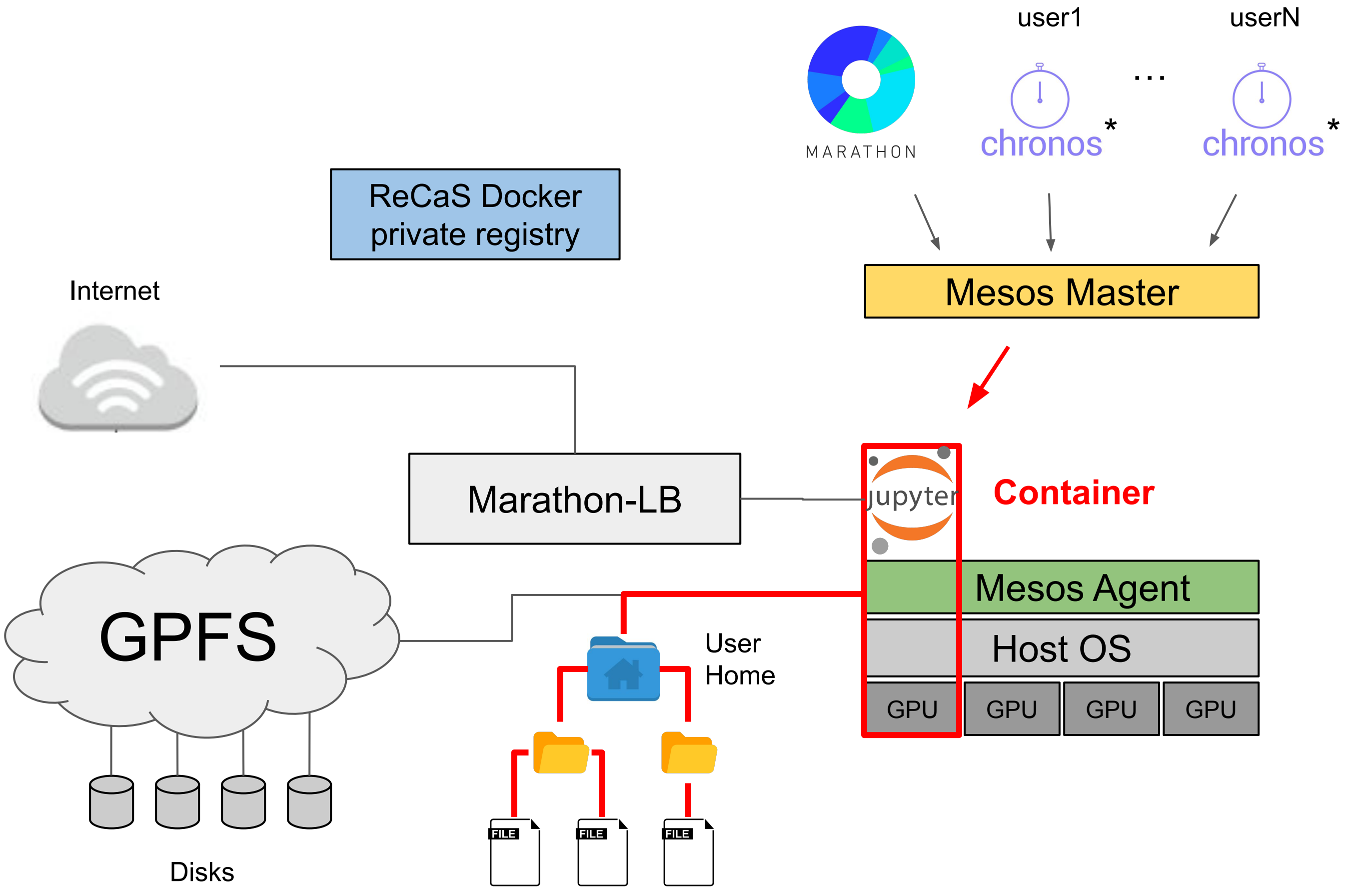
Chronos:

- Job scheduler for Apache Mesos
- Supports depending and periodic jobs

Docker

- Contains software, code, libraries and dependencies
- Isolates applications from the machine where it is executed
- Official images are available (Nvidia, TensorFlow, ...)

How ReCaS GPU Cluster works

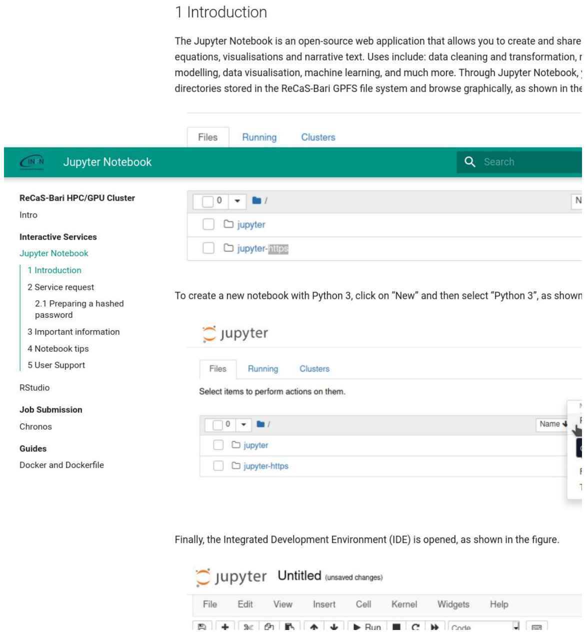


What we learned

- +50 users
- Applications:
    - Artificial Intelligence
    - Whole-genome sequencing
    - Image processing
- Average speed-up (vs CPUs) x5
- Most of the users requested support in the building of their custom docker container images
- Most of users are not well trained to use parallel programming paradigm

What we do: Share knowledge

- User programming skills are not enough to take advantage from the provided computation resources
- There is a **gap** between the goal and the user programming skill
- **Guides** and **video tutorials** to support users at the beginning
- Provide support in docker container image building
- Provide support in writing efficient code



What we plan: Future Developments

- **Kubernetes** will replace Apache Mesos since it overcomes some known limitations
- Chronos will be replaced with a more complex workflow scheduler, like **Apache Airflow**
- Adding distributed computing tools to the service portfolio like **Apache Spark**
- Integrate the cluster with **INFN-DataCloud PaaS**
- Investigate the use of **Infiniband** to speed-up the internode connections

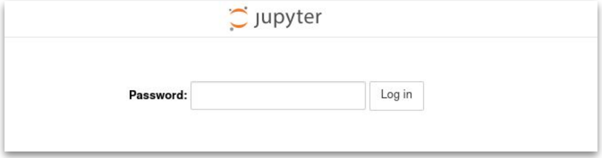
THANKS
FOR YOUR
ATTENTION

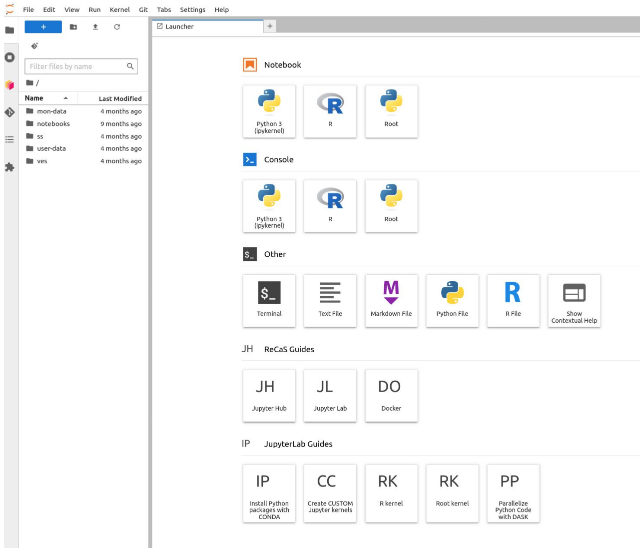
BACKUP

What we provide: GPU Cluster Services

JupyterLab

- Provided when user need to use a whole GPU
- Users have access to their home directory in the ReCaS distributed storage (GPFS)
- Users can immediately create a new Python3 script
- The Jupyter IDE (Integrated Development Environment) will be available and users can already write code and execute it
- Python modules can be installed directly within the code or using built-in terminal (pip or conda)

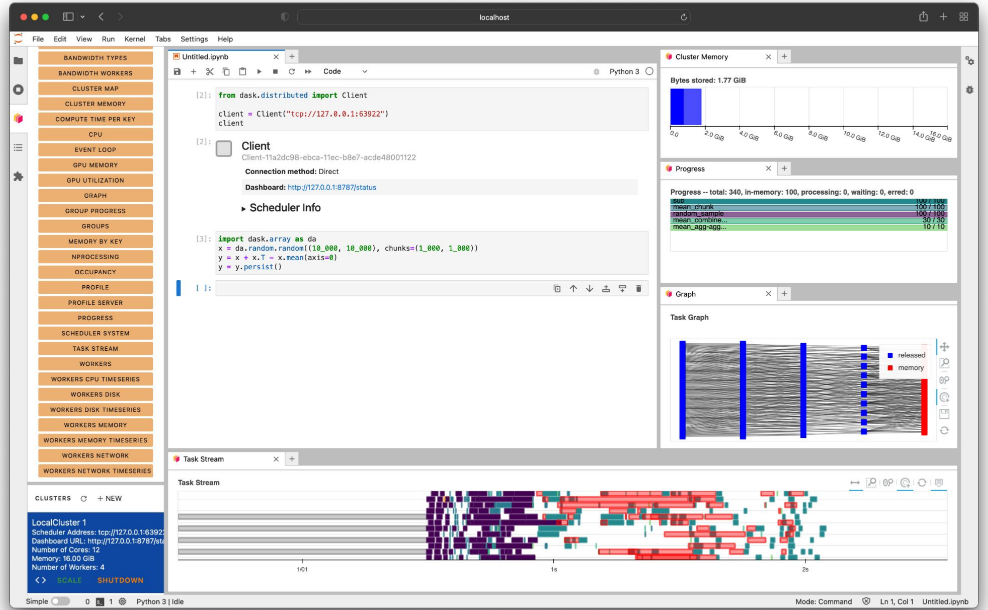




What we provide: GPU Cluster Services

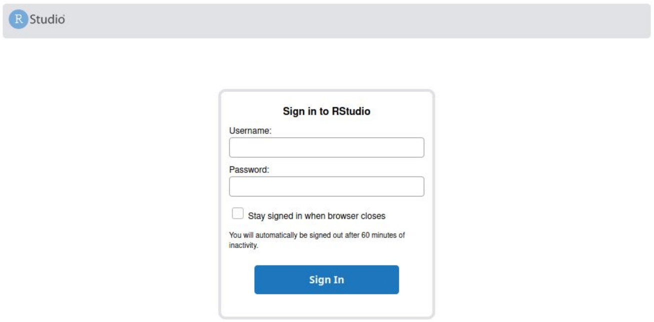
JupyterLab: Dask and Dask Jupyter extension

- Scale the Python libraries (like NumPy, pandas, and scikit-learn) on multiple cores and GPUs, using the same code
- Parallelize any Python code with Dask Futures
- Real-time resource usage Monitoring



What we provide: GPU Cluster Services

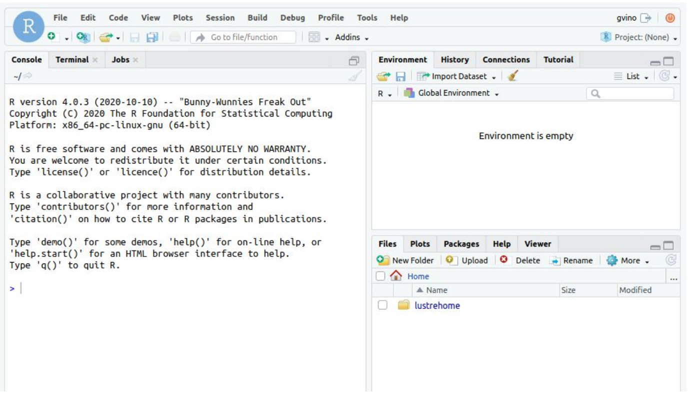
RStudio remote IDE



- After authentication, users have access to their home directory in the ReCaS distributed storage (GPFS)

- The Rstudio IDE (Integrated Development Environment) will be available and users can already write code and execute it

- R modules can be installed directly within the code



What’s under ReCaS GPU Cluster

Docker container:

- Contains software, code, libraries and dependencies
- Isolates applications from the machine where it is executed
- Official images are available (Nvidia, TensorFlow, ...)

ReCaS GPU Cluster policies on Docker containers:

- Mandatory for security purpose
- Jupyter and RStudio containers have been developed in-house
- Not all users’ containers can be developed in-house
- Users can build their own Docker image for their specific use-case using a dedicated machine with GPU in ReCaS-Bari
- ReCaS GPU Cluster Docker Registry is available