The new GPU-based cluster @ReCaS-Bari

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INFN Bari

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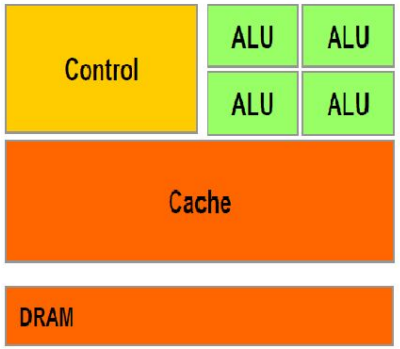
Progetti di rafforzamento del capitale umano destinato alle Infrastrutture di ricerca beneficiarie dell'Avviso D.D. del 28 febbraio 2018, n. 424

Why GPU?

Control Processing Unit (CPU):

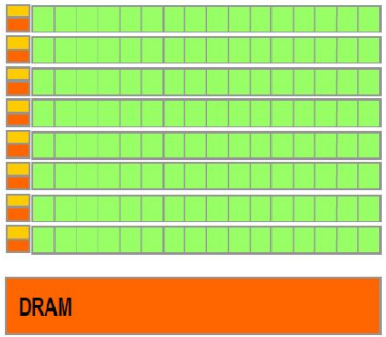
- Designed to handle complex tasks
- Low-level parallelism (<100 cores)



Graphical Processing Unit (GPU):

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

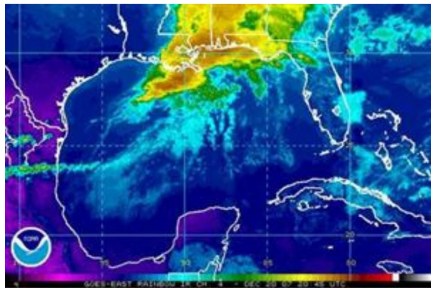
Make them suited for scientific workloads require a huge amount of floating point operations

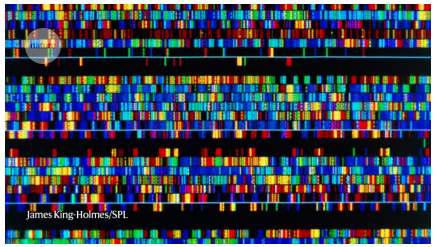


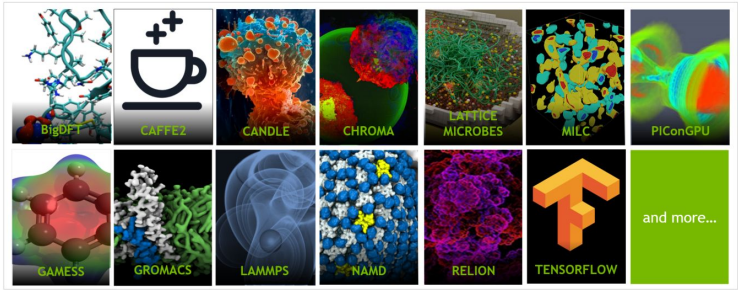
Why GPU?

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 users want

- Access to overall ReCaS-Bari storage
- Use the whole GPU cluster computing power
- Use GPUs efficiently without acquire new knowledge
- Build GPU custom applications in few minutes
- Use GPUs without worry about managing to underlying hardware and software
- Use the same code for 1 CPU or for all GPUs in the cluster

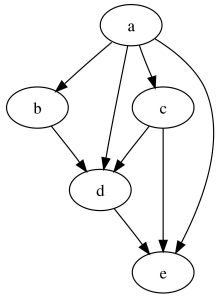
What we have: ReCaS GPU Cluster

Hardware Facility:

- Nodes: 10
- GPUs: 18 (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 (3800TB)
- Bandwidth between nodes: 10 Gbps

What we offer: ReCaS GPU Cluster Services

- **Ready-to-use services:**
  - Interactive remote GPU-based IDE services:
    - Jupyter Notebook
      - "web service for interactive computing across all programming languages"
    - Rstudio
      - "An integrated development environment for R"
  - Job Scheduler:
    - Support to GPU-based workflows represented as Directed Acyclic Graphs (DAG)
- **User-defined services**

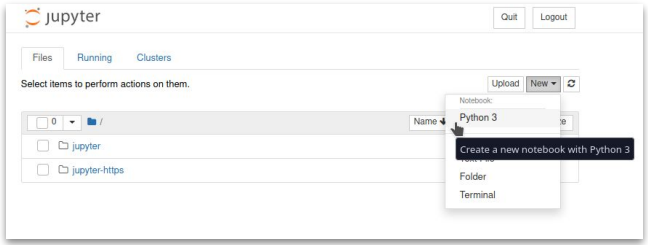


What we offer: ReCaS GPU Cluster Services

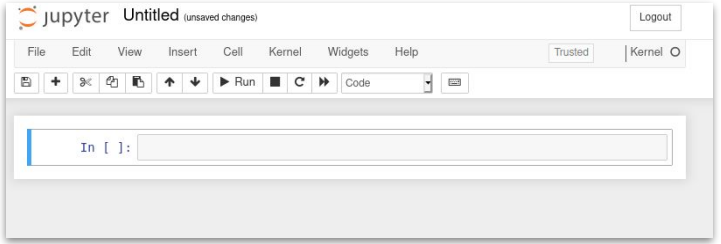
Jupyter Notebook remote IDE

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

- Users can immediately create a new Python3 script



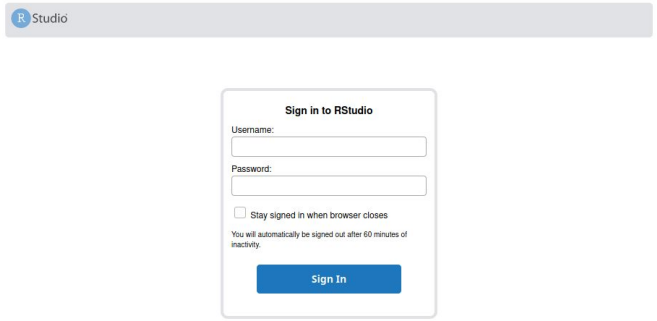
- The Jupyter IDE (Integrated Development Environment) will be available and users can already write code and execute it



- Python modules can be installed directly within the code

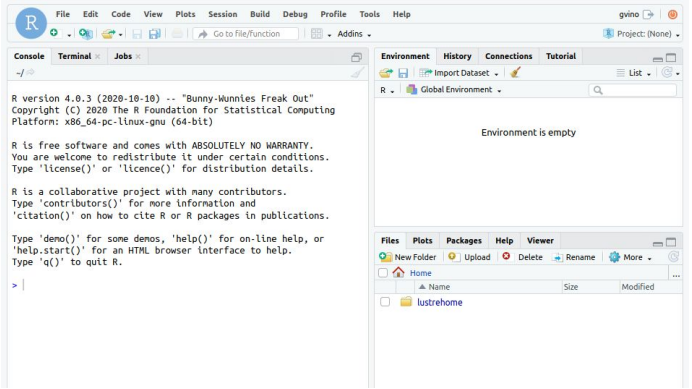
What we offer: ReCaS GPU Cluster Services

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

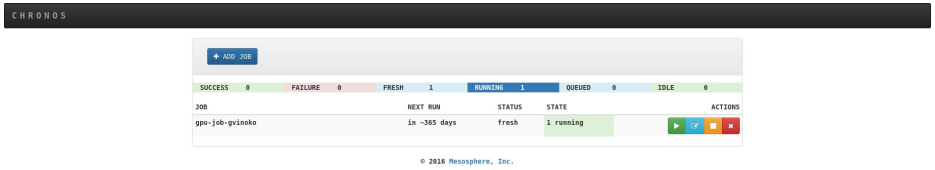


- R modules can be installed directly within the code

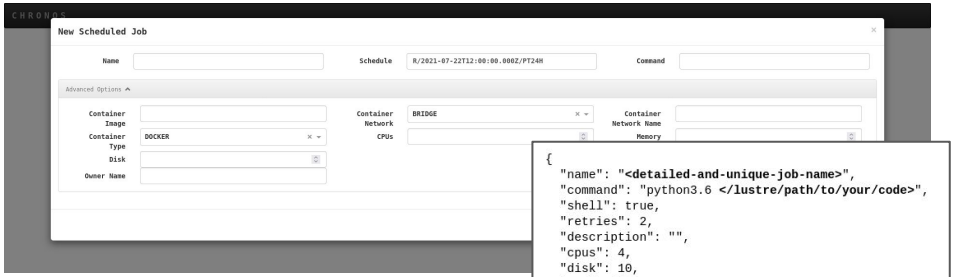
What we offer: ReCaS GPU Cluster Services

Job Scheduler (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




```
{
  "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"
}
```

- Manages heterogeneous requests:
  - 2 GPU / 4 CPU / 20 GB RAM
  - 100 CPU / 8GB RAM

What's under ReCaS GPU Cluster

Apache Mesos:

- Abstracts all cluster resources in a single virtual entity
- Multi-users
- High Availability
- Manages a lot number of nodes

Marathon:

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

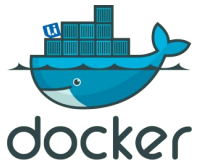
Chronos:

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

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, ...)

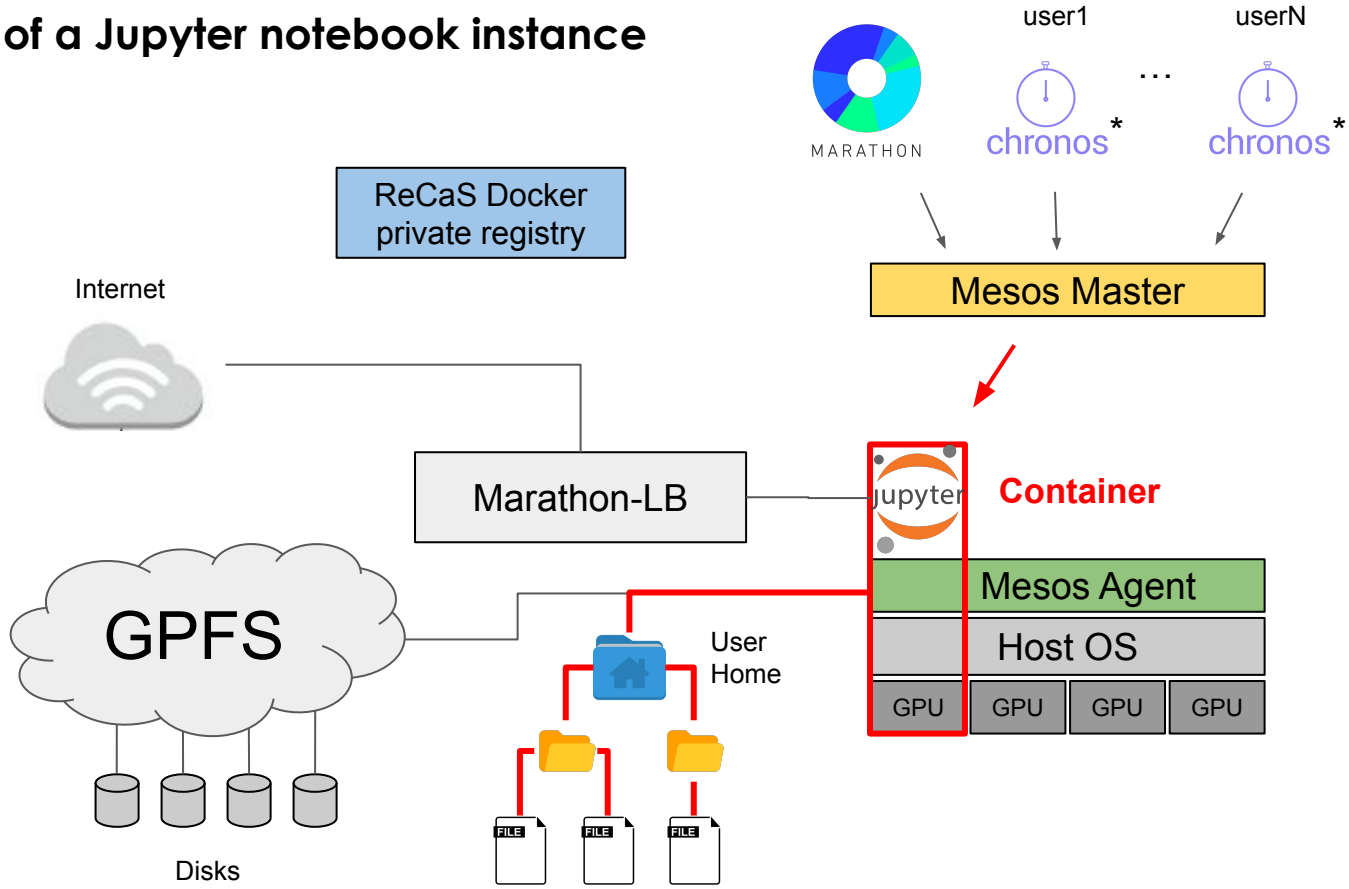


ReCaS GPU Cluster policies on Docker containers:

- Mandatory for security purpose
- Jupyter Notebook and RStudio containers have been developed in-house because the majority of the supported use cases needs them
- Not all users' containers can be developed in-house
- Users can build own Docker image for their specific use-case using a dedicated machine with GPU in ReCaS-Bari
- ReCaS GPU Cluster Docker Registry

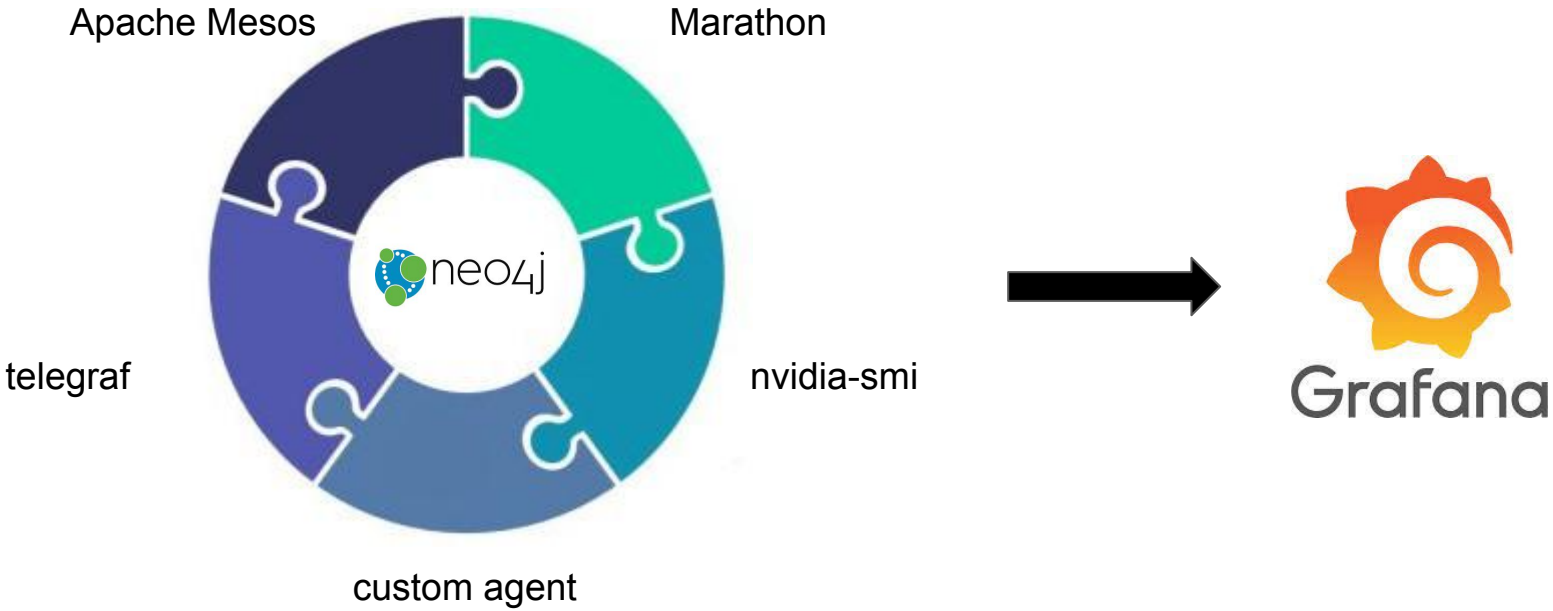
How ReCaS GPU Cluster works

Deployment of a Jupyter notebook instance



What's under ReCaS GPU Cluster

Monitoring



Use case: Multi-charm reconstruction with ML in ALICE 3

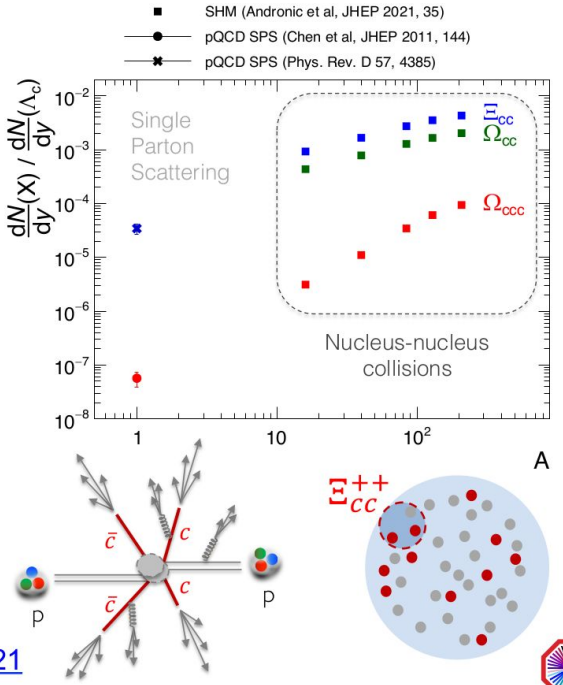
Motivation and challenges

Working Team:

- Domenico Elia
- Annalisa Mastroserio
- Domenico Colella
- Gioacchino Vino
- David Chinellato (CERN)

Multi-charm baryons: from low to high density QCD

- Charm production in general: almost exclusive to hard scatterings due to large mass (~1275 MeV/c^2)
- Formation of Ξ_{cc}^{++}, Ω_{cc}^{+}, Ω_{ccc}^{++}: extremely unlikely in single parton scattering (unlike e.g. J/ψ)
- Multi-parton interactions and multi-charm: multiple charm quarks combine into hadrons
- In nuclear collisions:
  - High density of charm quarks leads to much larger multi-charm population
  - Described by SHM (g_c) and coalescence
  - Enormous dynamic effect!



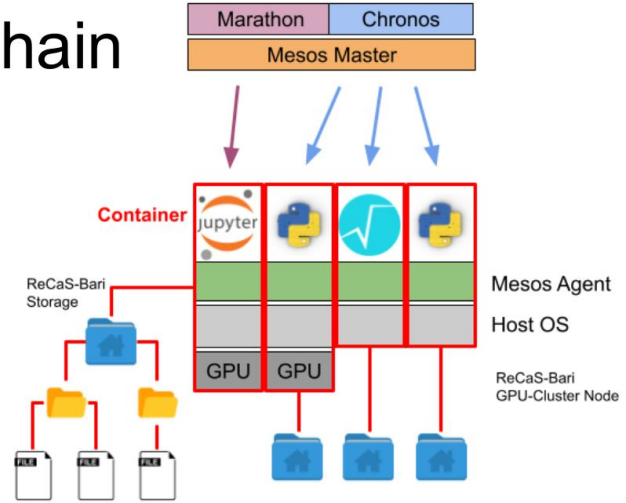
D. D. Chinellato, ALICE 3 workshop 18-19.10.2021

Use case: Multi-charm reconstruction with ML in ALICE 3

ML method and analysis chain

ML analysis chain (Gioacchino):

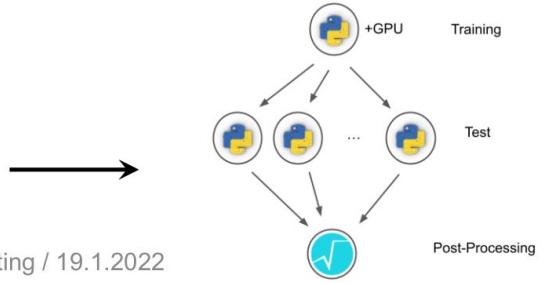
- fully developed from scratch
- ReCaS-Bari GPU-Cluster used:
  - ✓ nodes equipped with NVIDIA A100 or V100
  - ✓ cluster managed with Apache Mesos
  - ✓ services deployed with Mesos and Docker Containers



Each container has access to ReCaS-Bari Storage (3.8 PB)

Remote IDE (Jupyter Notebook and Rstudio) with access to GPU are available with Marathon (Development phase)

Analysis can be submitted as a set of dependent tasks (Directed Acyclic Graph) with Chronos (Production phase)



Use case: Multi-charm reconstruction with ML in ALICE 3

Preliminary results:

- better than standard, especially at low p_T
- up to a factor of 4-5x improvement for $p_T < 2$ GeV/c

Impact on future measurements:

- ML-based selection has potential to allow measurement of multi-charm down to 0 p_T
- included in the **ALICE 3 Letter of Intent** recently published

Work ongoing:

- still room to improve ML-based selection performance, in particular exploiting p_T-dedicated training

ALICE 3 LoI:
https://cds.cern.ch/record/2803563

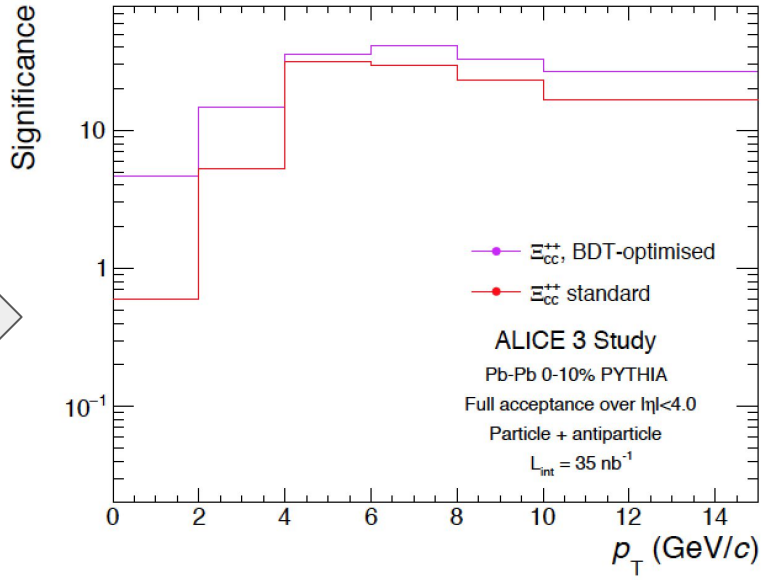


Figure 33: Ξ_{cc}^{++} significance in 0-10% central Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.52 TeV as a function of p_T with a 2.0 T magnetic field using standard selections and using machine learning.

Use case: CNR/IREA Napoli (work in progress)

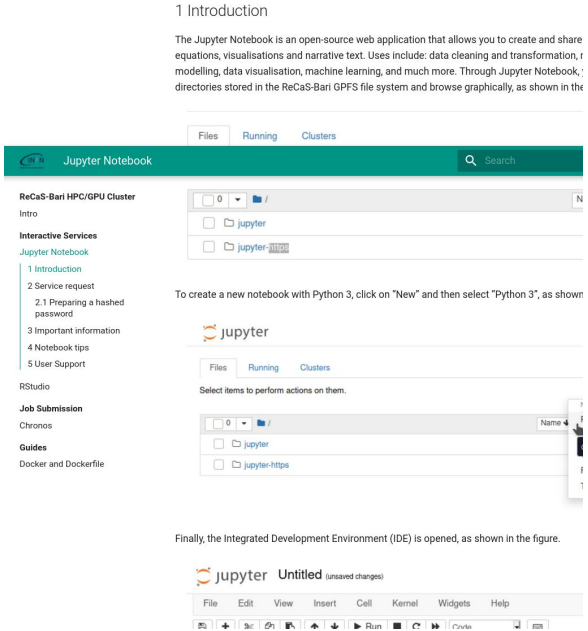
- Dedicated nodes in the cluster
- Multi-node HPC/GPU application
- Containers communicate each other to share partial results
- Marathon will be used to deploy containers
- Chronos will be used to submit jobs

What we learned

- 28 users
- Applications:
  - Artificial Intelligence
  - Whole-genome sequencing
  - Image processing
- Average speed-up (vs CPUs) x10
- Most of 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 want: Improve user learning curve

- There is no enough to provide performance tools:
  users should use them ….
  …efficiently
- There is a **gap** between the goal and the knowledge of users
- **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 want: Future Developments

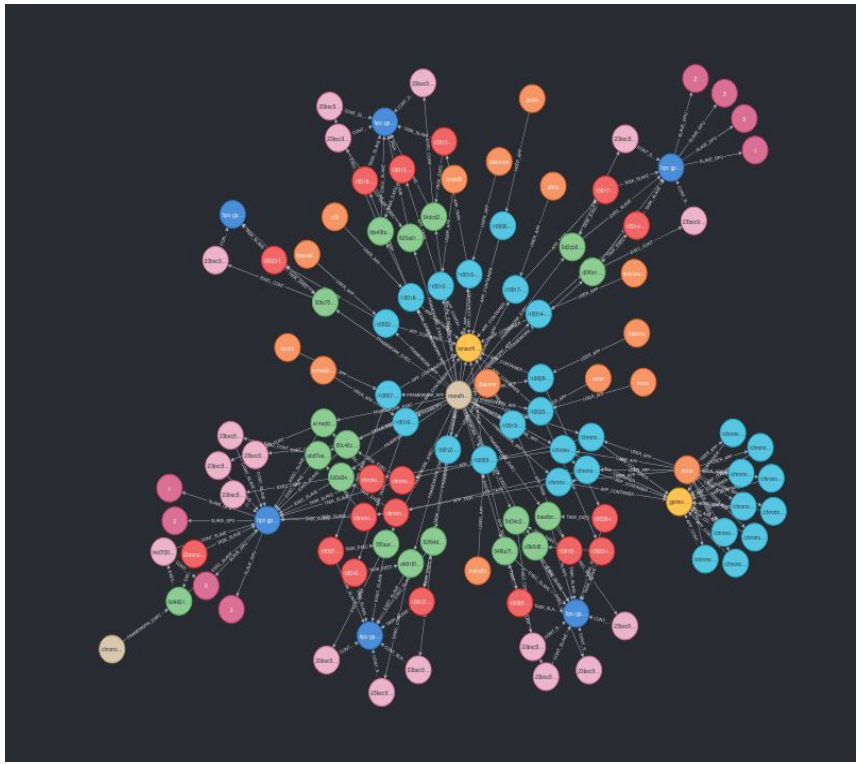
- **Kubernetes** will replace Apache Mesos since it overcomes some known limitations
- Chronos will be replaced with a more complex workflow scheduler, like **Apache Airflow**
- Adding distributed computing tools to the service portfolio like **Apache Spark** and **Dask**
- Integrate the cluster with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

THANKS

FOR YOUR

ATTENTION

BACKUP




influxdb


Grafana