

# Uninuvola: the computing portal of the Perugia University



UNIVERSITÀ DEGLI STUDI  
DI PERUGIA

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# Introduction



# Aim of the project

**Aim:** creation of a federated computing infrastructure prototype empowered with **software-defined networking capabilities**.

Design an infrastructure updated to the **European standards**.

It is a **potentially heterogeneous collection** of hardware.

All the expertise will be channelled to a new **Common Lab** project.





# The Uninuvola team



To cover all the possible scenarios we collected expertise from all over the university.

## Members

L. Fanò, M. Femminella, V. Poggioni, M. Battistoni, L. Angeloni, G. Costante, M.N. Faginas Lago, A. Lombardi, L. Pacifici, M. Mariotti, M. Di Mambro, G. Vitillaro, M. Pezzella.



# Infrastructure



# The physical nodes

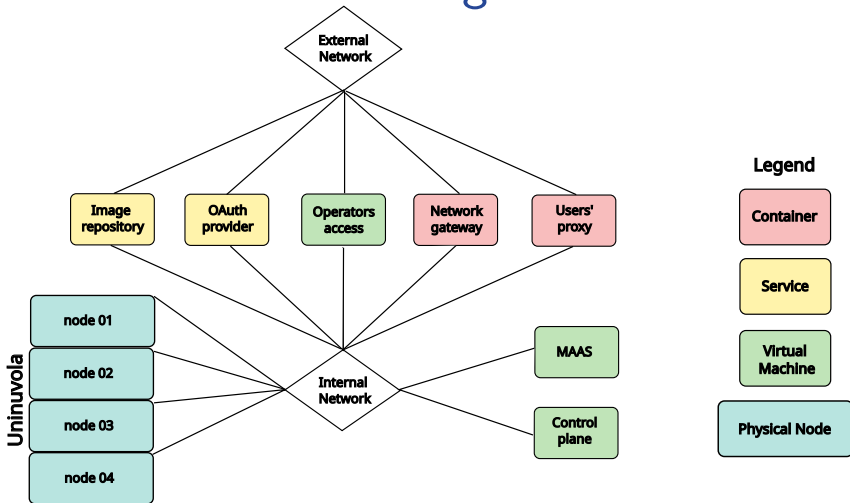
4 Dell Power Edge R940 nVME servers:

- 2 Intel Xeon Gold CPU
- 512 GB ECC DDR5 RAM
- 16 TB storage
- Management switch (1 Gbit/s)
- Communication switch (10 Gbit/s)





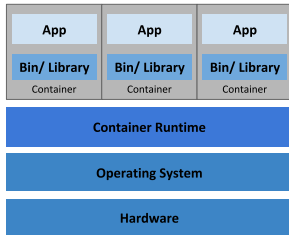
# Logical infrastructure





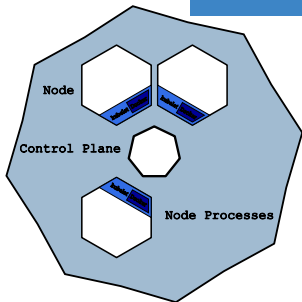


# Kubernetes



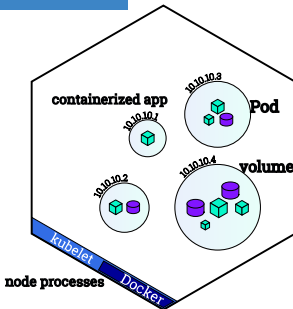
## Containers:

- Environmental consistency
- Cloud and OS distribution portability



Kubernetes Cluster

<https://kubernetes.io/>

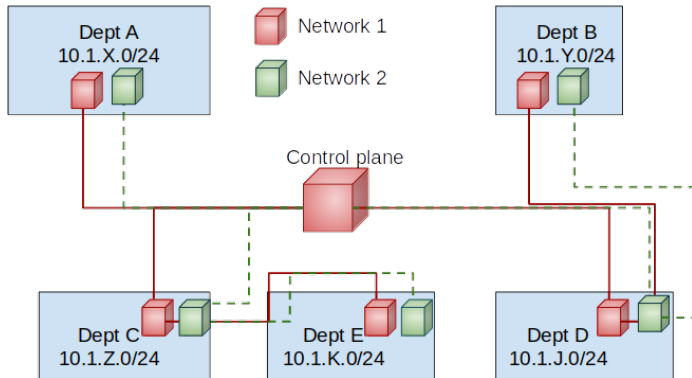


## Kubernetes:

- Automated management
- Declarative approach

# Network solution

A good network solution is essential for reliable, efficient and secure infrastructure.

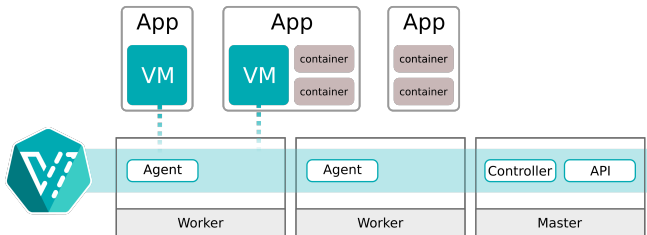


**OVN** is implemented through *kube-OVN*.

<https://www.kube-ovn.io/>

# Kubevirt

Kubevirt provides new features for the virtualisation functionalities to Kubernetes.



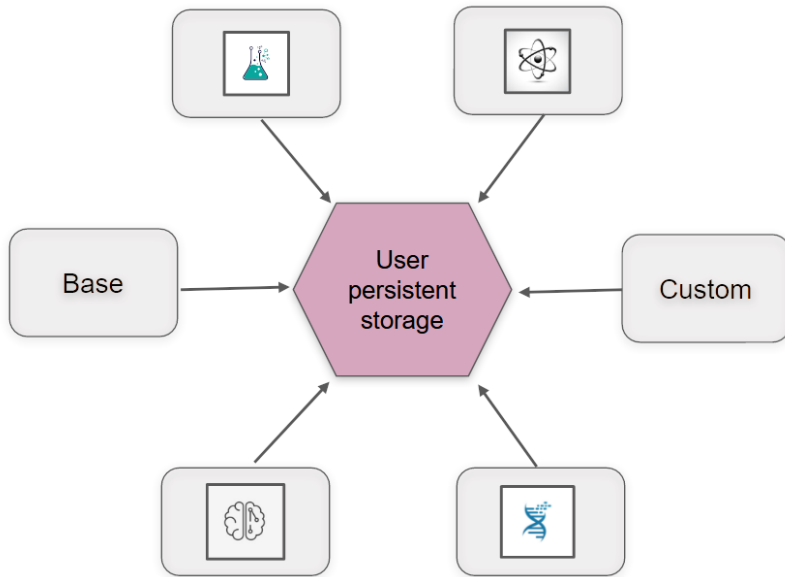
A KubeVirt VM is a Pod running a KVM instance in a container.

KubeVirt allows unique VM states and tracks and schedule Pods across nodes when migrating it.

<https://kubevirt.io/>

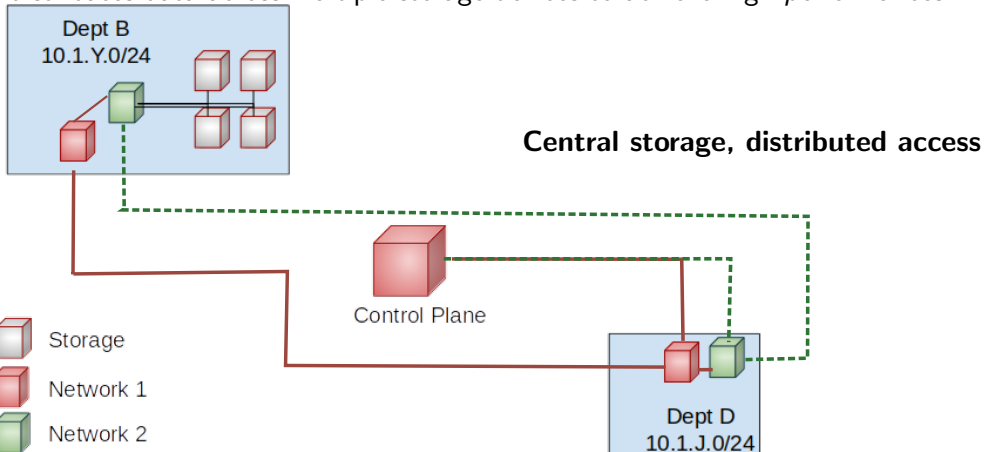


# Storage



# Storage

**CEPH** distributes data across multiple storage devices to achieve high *performances*.



<https://ceph.io/>



# JupyterHub on top of Kubernetes

JupyterHub has been chosen as computing environment manager.

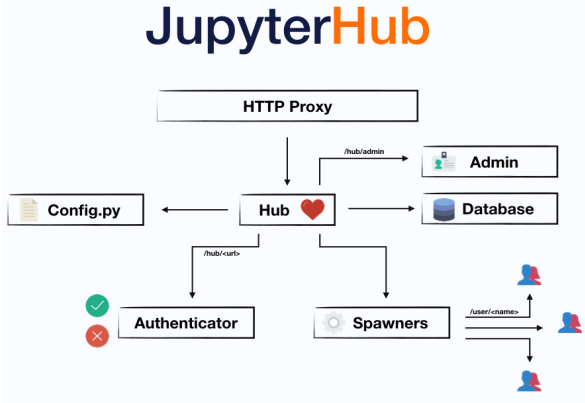
## Users:

- Built-in image and resource selector
- Notebooks and terminal interface

## Administrators:

- Easy to configure and maintain
- Quick implementations of add-ons

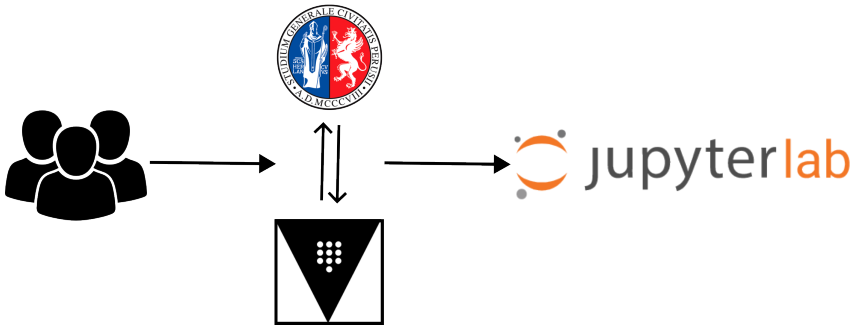
<https://jupyterhub.readthedocs.io/en/stable/>  
<https://z2jh.jupyter.org/en/stable/>





# Authenticator

HashiCorp Vault is used as **OAuth2 authenticator** back-end for the University LDAP.



<https://www.vaultproject.io/>



# Use cases





## Server Options

UniNuvola Base

Computational Chemistry

Machine Learning

Computational Physics

Quantum Computing

Other images

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Image

Other... ▾

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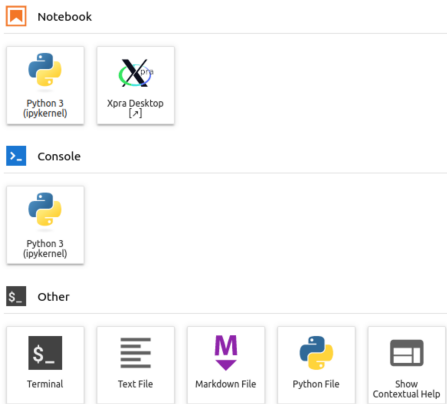
|

Start

# The opening page



# The Uninuvola base image



The Uninuvola base image is the minimal package from the official JupyterHub for Kubernetes.

**Xpra** is installed as remote desktop service.

**Rclone** guarantees the access to external cloud storage.

<https://github.com/Xpra-org/xpra>  
<https://rclone.org/>



# The chemistry image

## Molecular dynamics:

$$x(t + \Delta t) = x(t) + v(t)\Delta t + 0.5a(t)\Delta t^2$$

$$v(t + \Delta t) = \frac{a(t)+a(t+\Delta t)}{2} \Delta t$$

## Codes:

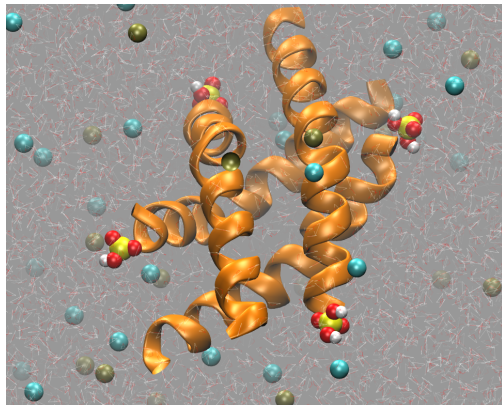
- NAMD3 - OpenMP and GPU native;
- Ambertools - Python library;
- DL\_POLY - MPI;
- VMD - GUI, analysis tool.

<https://www.ks.uiuc.edu/Research/namd/>

D.A. Case et al, *J. Chem. Inf. Model.* 63, 6183, 2023

M. F. Guest, A. M. Elena & A. B. G. Chalk *Mol. Simulat.*, 47,194 2019

<https://www.ks.uiuc.edu/Research/vmd/>





# Machine learning image

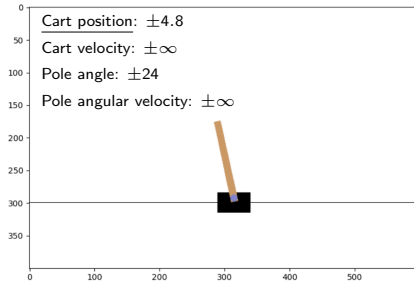
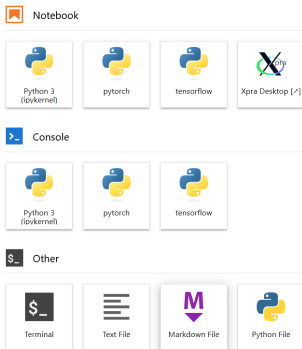
The image serves **Mathematics** and **Engineering** departments

Installed notebooks:

- Pytorch
- Tensorflow

Tests performed:

- Reinforcement learning
- Flower classification



<https://pytorch.org/>

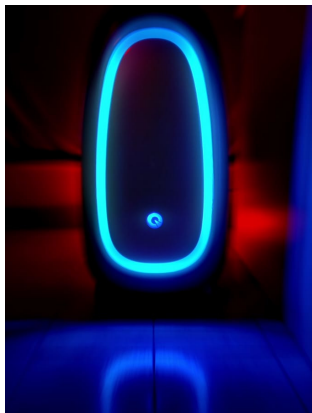
<https://www.tensorflow.org/>

[https://pytorch.org/tutorials/intermediate/reinforcement\\_q\\_learning.html](https://pytorch.org/tutorials/intermediate/reinforcement_q_learning.html)

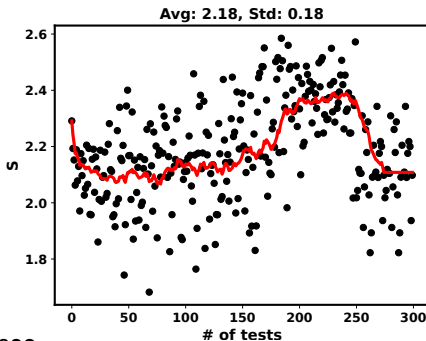
[https://www.tensorflow.org/hub/tutorials/image\\_feature\\_vector](https://www.tensorflow.org/hub/tutorials/image_feature_vector)



# Uninuvola and Quantum computers



The SpinQ Triangulum is a liquid NMR quantum computer with 3  $^{19}\text{F}$  nuclei as qubits.



## CHSH experiment

Alice and Bob have access to one half of an entangled two-qubit pair each randomly.

What is the best strategy for guessing correctly?

G. Feng et al., *arXiv:2202.02983*, 2022

<https://github.com/SpinQTech>

J. F. Clauser et al, *Phys. Rev. Lett.* 23, 880, 1969; Erratum *Phys. Rev. Lett.* 24, 549, 1970



# Ongoing steps and Outlooks



# Conclusions:

## Ongoing steps

- Definition of a queuing system (*kueue*).
- Creation of a **dashboard** for the virtual machines
- Extension to other research teams (e.g. **Genomics** and **Geology** )
- Fully distributed infrastructure over a 100Gb/s internal with multiple control planes
- **Uninuvola-GPU** addition of GPU nodes

## Outlooks

- All materials will be made available *via* publications and repositories.
- The fully functional prototype will be available in the **Summer 2024**.
- Bursting to a public cloud (*virtual kubernetes*)



# Acknowledgment

Thanks to all the Uninuvola's members for the project, and the PNRR for the foundings!

I would like to thank the ISGC 2024 organisers for giving us this opportunity!

&

you for your attention!

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