

IBiSco

Infrastructure for Blg data and Scientific COmputing

Computational resources @ CNR

Giovanni Cantele - April 18, 2024



The banner features logos for the European Union (UNIONE EUROPEA), the Italian National Council of Research (Consiglio Nazionale delle Ricerche), the Ministry of University and Research (Ministero dell'Università e della Ricerca), the National Operational Program (PON) for Research and Innovation, and the Institute of Applied Sciences and Intelligent Systems (IASIS).

UNIONE EUROPEA
Fondo Sociale Europeo
Fondo Europeo di Sviluppo Regionale

Consiglio Nazionale delle Ricerche

Codice progetto: PIR01_00011

Nome del beneficiario e titolo del progetto CONSIGLIO NAZIONALE DELLE RICERCHE
Progetto I.Bi.S.Co.
Infrastruttura per Blg data e Scientific COmputing

Obiettivo principale dell'operazione
Realizzazione di una infrastruttura di calcolo distribuita ad alte prestazioni per il calcolo scientifico

Asse - Azione
ASSE II - Azione II.1

Ministero dell'Università e della Ricerca

PON
RICERCA E INNOVAZIONE
2014-2020

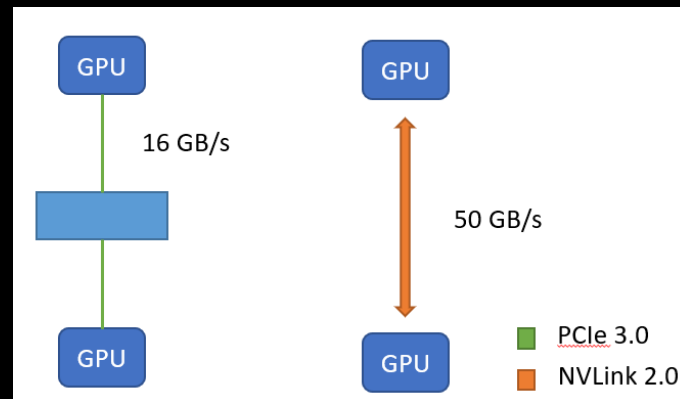
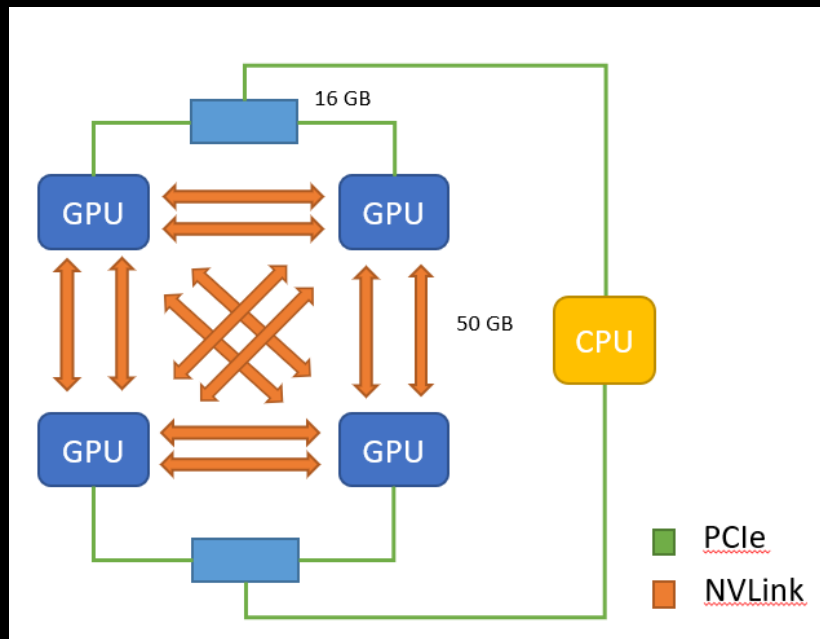
Institute of Applied Sciences and Intelligent Systems
IASIS

Computational resources

- 32 computing nodes + 2 switches
- 4 racks
- each computing node equipped with
 - **4 x GPU NVIDIA V100 (32 Gb memory each)**
 - 2 InfiniBand ports at 100 Gb/s
 - 2 x CPU Intel Gen 2 Xeon Gold (24 physical cores each)
 - 1408 GB RAM
- 4 storage nodes (16 HDD SAS, 16 TB each + 8 SSD SATA, 1.9 TB each)

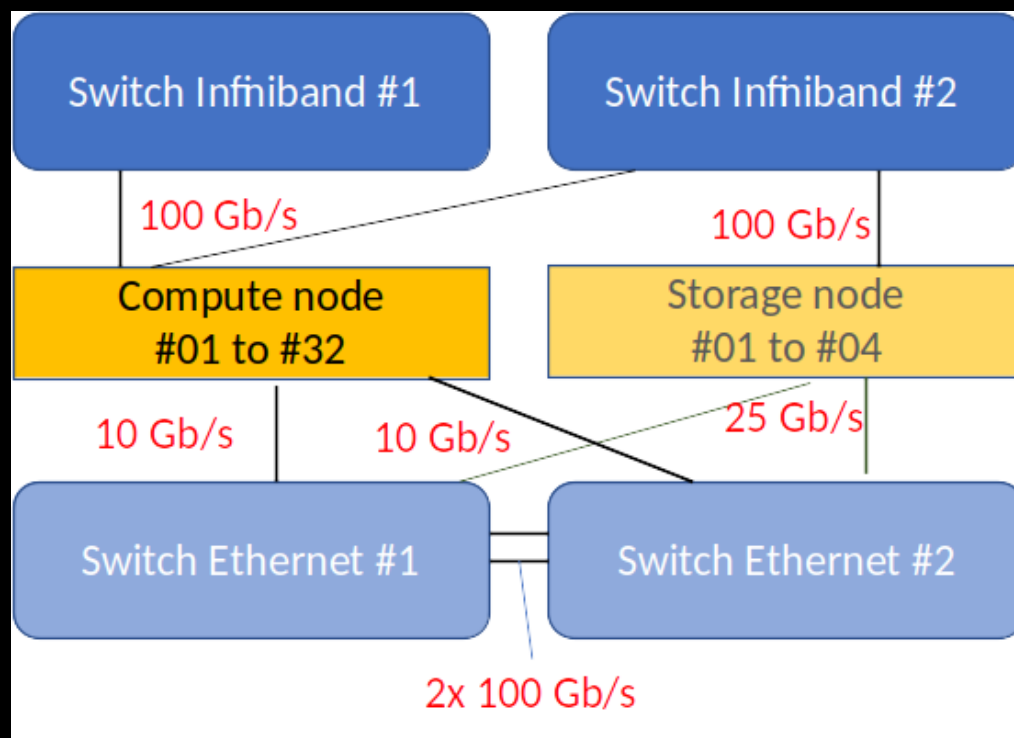


Computational resources



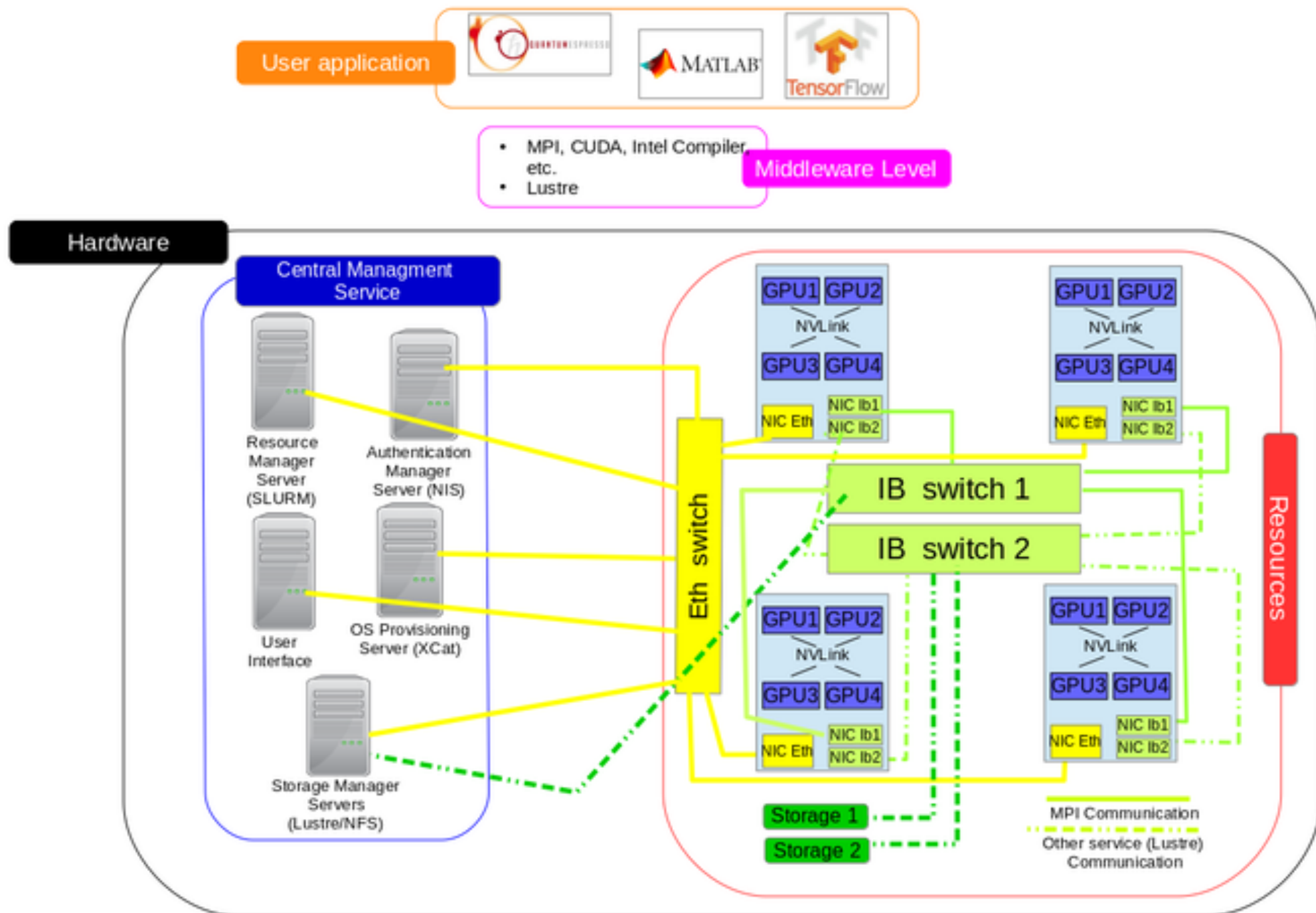
available communication channels PCIe 3.0 and NVLink 2.0 for respectively GPU-CPU and GPU-GPU communication

maximum throughput: 16 GB/s for PCIe 3.0 and $25\text{GB/s} \times 2 = 50\text{ GB/s}$ (bidirectional communication) for NVLink



hybrid InfiniBand-Ethernet network to allow different kinds of tasks to accommodate into the most efficient communication protocol

Computational resources



Computational resources

- 📌 Total CNR investment: ~ 800 kEuro
 - 21 computing nodes
 - 2 IB switches
 - 4 storage servers
 - several control units / monitors

- 📌 the whole infrastructure originates from a combined effort of CNR, University of Naples “Federico II”, INFN

Acknowledgments

CNR

- CNR-SPIN and CNR-ISASI Institutes
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UNINA

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- prof. G. Pepe

INFN

- Dr. Gianpaolo Carlino
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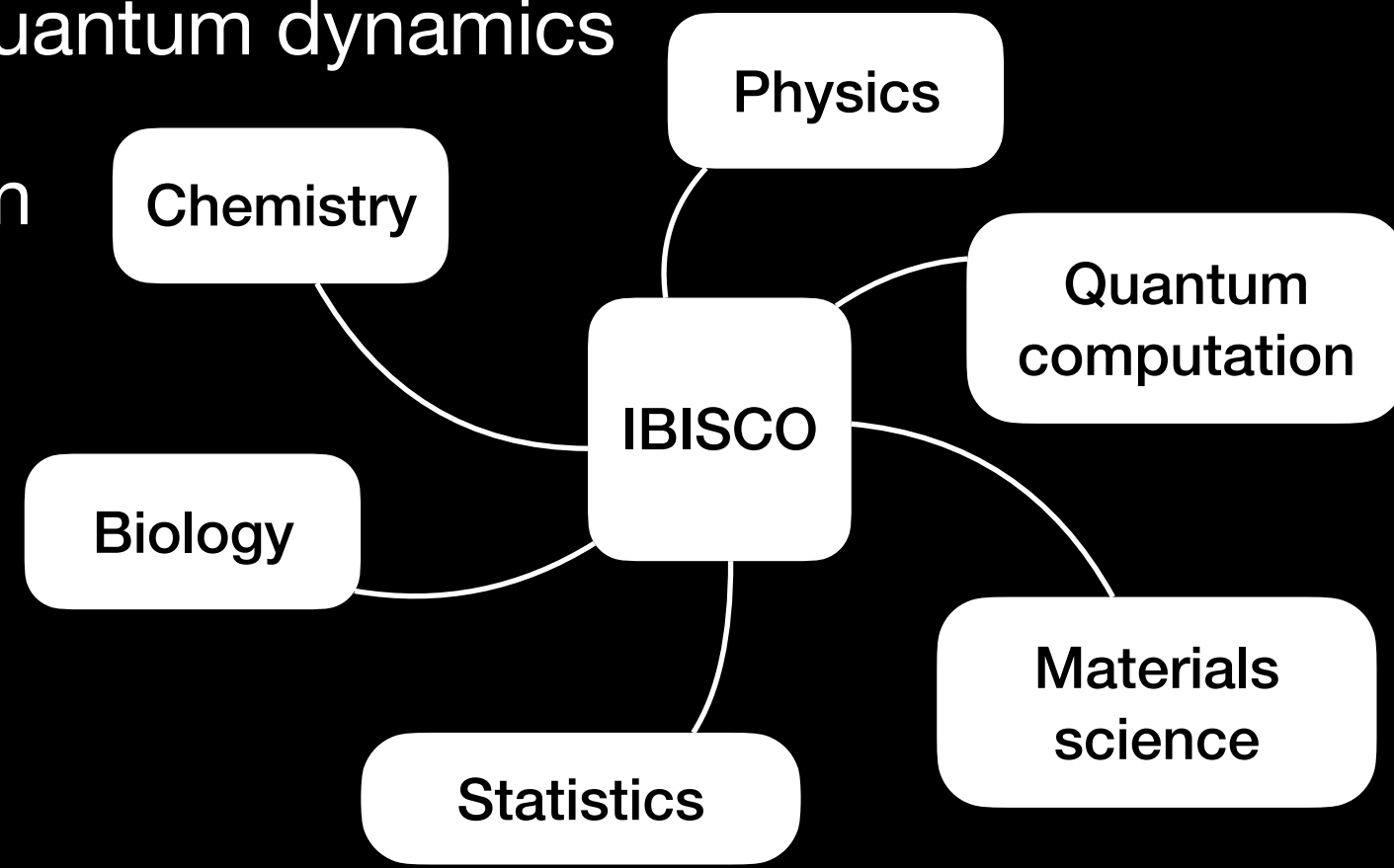
IBISCO team

- Dr. Luisa Carracciuolo
- Dr. Davide Bottalico

Research activities

📌 Multidisciplinary approach → hybrid architecture approach

- Bioinformatics
- Molecular chemistry and dynamics, quantum chemistry
- Quantum algorithms and quantum dynamics
- Material science and design
- Statistical mechanics
- ...



Research activities

📌 Multidisciplinary approach → hybrid architecture approach

● examples of computational tasks

■ run the same serial instance thousands of times (to compute averages, correlation functions, and so on)

■ diagonalize large matrices

■ Fast Fourier Transform for plane-wave basis set-based problems

■ compute matrix operators, operate with matrix operations

■ data or image analysis

■

Research activities

- Depending on the particular application, the HPC architecture is expected to fulfil user requests in terms of
 - number of computing cores and/or
 - RAM memory and/or
 - high speed/low latency inter-node communication and/or
 - high speed writing to and reading from disk
- graphical processing units are devised as accelerators to provide huge numbers of computing cores

Installed software

- 📌 Intel OneAPI (compiler suites, libraries)
- 📌 NVIDIA HPC SDK (compiler suites, libraries)
- 📌 OpenMPI
- 📌 Matlab
- 📌 several packages for scientific computing
- 📌 SLURM for job accounting and queues

Thank you for your attention

- more specific talks on research activities and computational-related aspects will be given in the next
- these should better bring out how a hybrid architecture might efficiently meet the needs of very complex and very different research tasks