IBiSco
Infrastructure for BIg data and Scientific COmputing

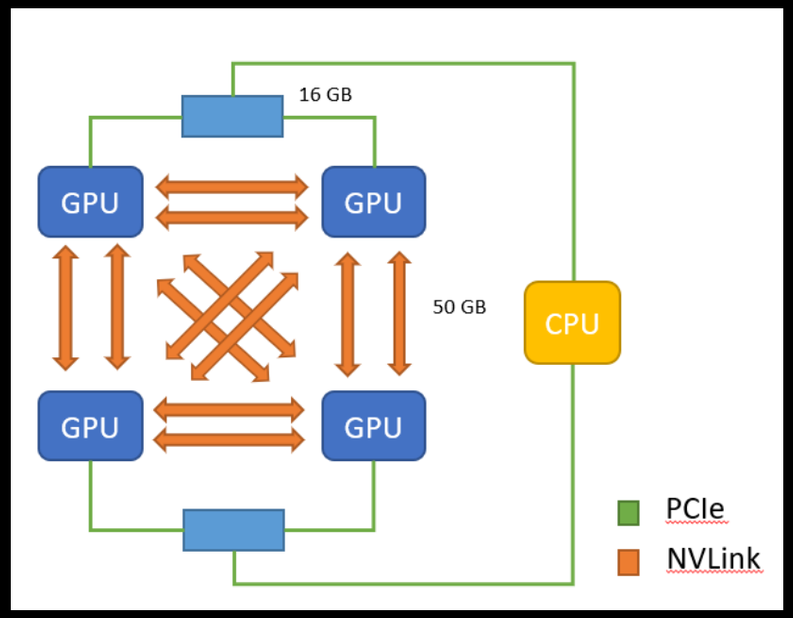
Computational resources @ CNR

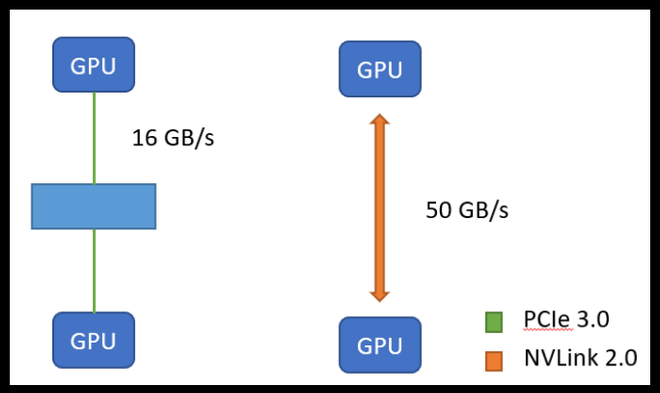
Giovanni Cantele - April 18, 2024

Computational resources

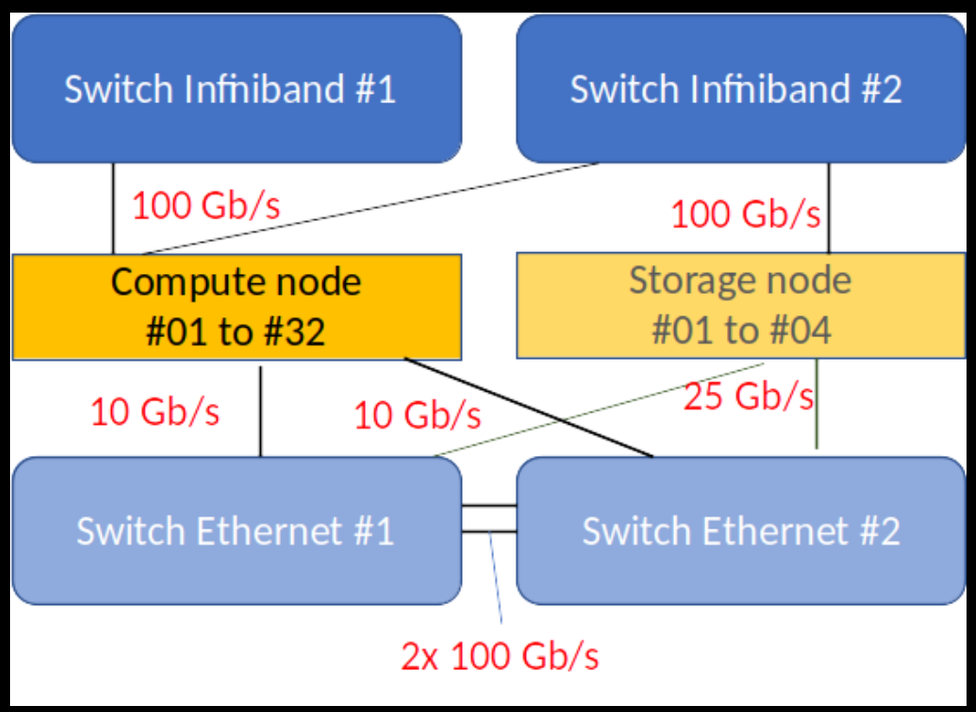
- 32 computing nodes + 2 switches
- 4 racks
- each computing node equipped with
  - **4 x GPU NVIDIA V100 (32 Gb memory each)**
  - 2 InfiniBand ports at 100 Gb/s
  - 2 x CPU Intel Gen 2 Xeon Gold (24 physical cores each)
  - 1408 GB RAM
- 4 storage nodes (16 HHD SAS, 16 TB each + 8 SSD SATA, 1.9 TB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

Computational resources



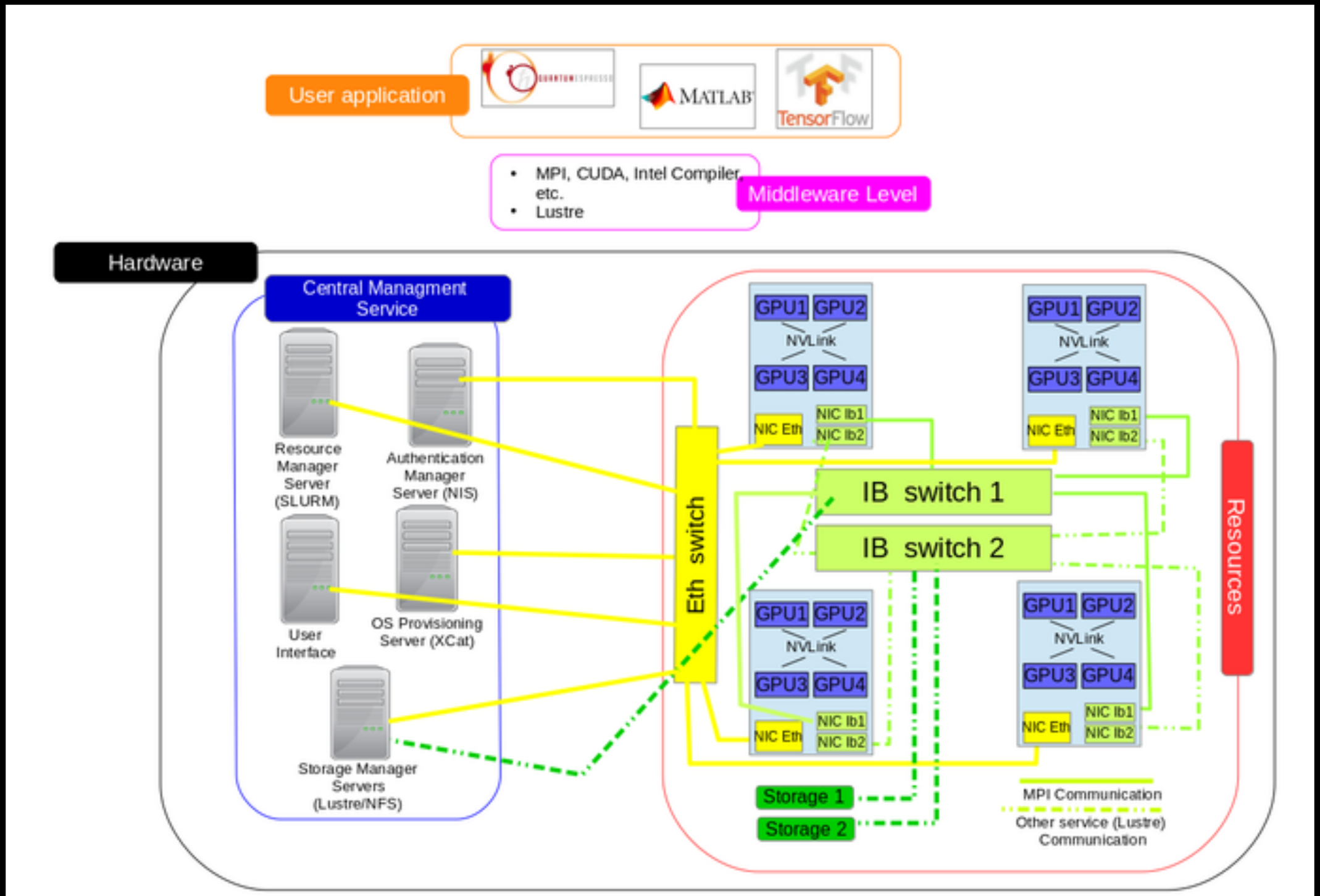


- available communication channels PCIe 3.0 and NVLink 2.0 for respectively GPU-CPU and GPU-GPU communication
- maximum throughput: 16 GB/s for PCI3 and 25GB/s x 2 = 50 GB/s (bidirectional communication) for NVLink



- 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

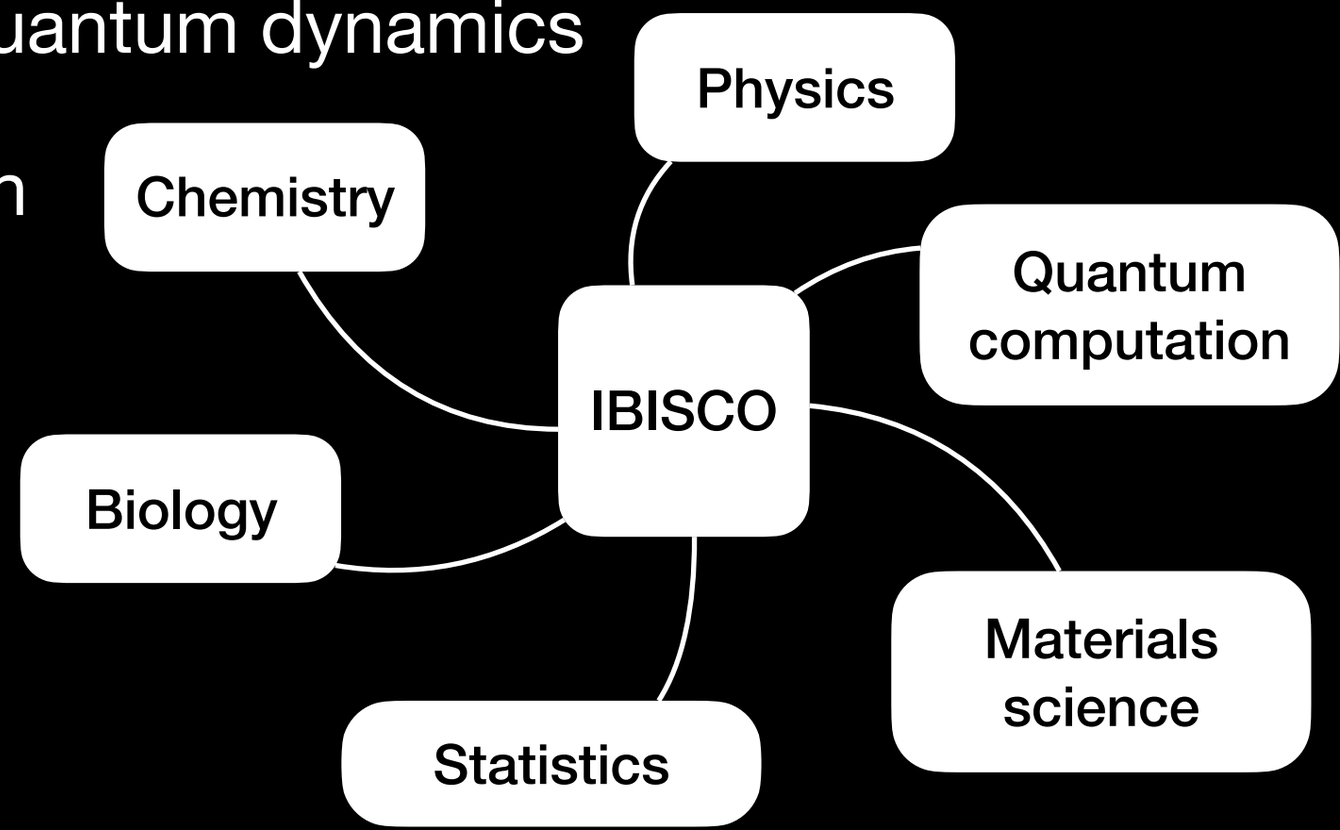
- the whole infrastructure originates from a combined effort of CNR, University of Naples “Federico II”, INFN

Acknowledgments

- CNR
  - CNR-SPIN and CNR-ISASI Institutes
  - Dr. Melania Paturzo, Dr. Oliviero Talamo
- UNINA
  - prof. G. Russo
  - prof. P. Lucignano
  - prof. G. Pepe
- INFN
  - Dr. Gianpaolo Carlino
  - Dr. A. Doria
- 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 basi 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