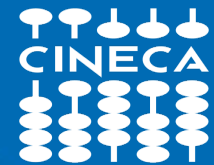

SCAI
SuperComputing Application & Innovation
CINECA

Sanzio Bassini – April 2021



CINECA a private not for profit consortium of public righth



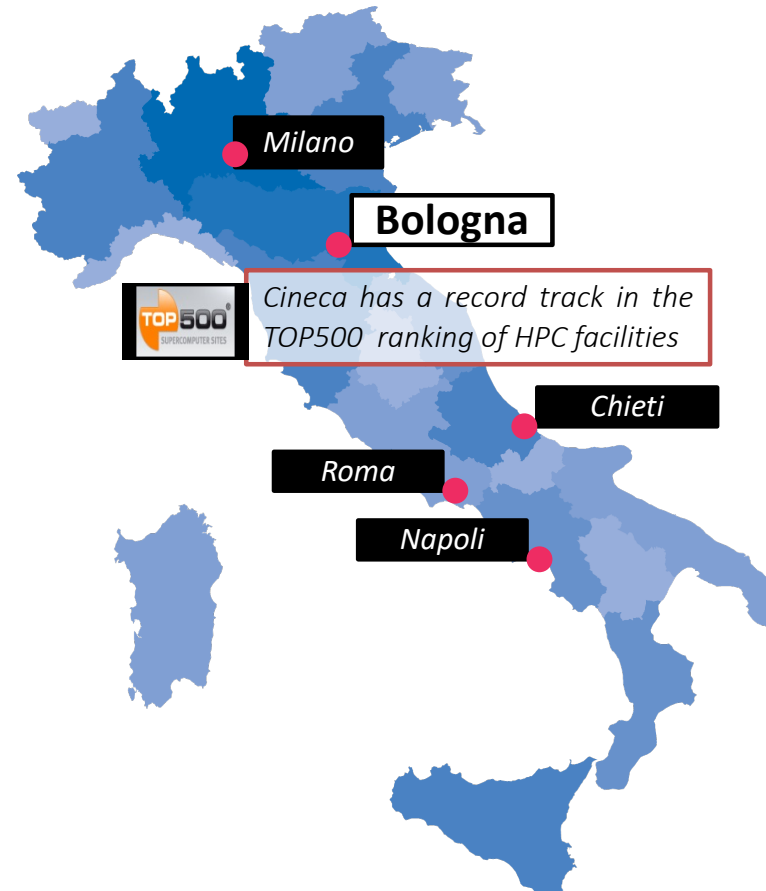
CINECA is a **Consortium of Universities**, founded in 1969 by (MIUR) to support scientific research
CINECA is a not-for-profit organization

Members:

- MUR & MIS
- 67 Italian Public Universities
- 9 Institutions,...

In-house provider:

- ❖ Supervised by MIUR
- ❖ No private capital
- ❖ 80% of activities towards Consortium members
- ❖ 20% Technology Transfer
- ❖ Annual Budget: ~ 100M€
- ❖ Employees: ~ 800



CINECA European position



- PRACE Tier0 Hosting Member
 - EuroHPC Pre-exascale Hosting Entity
 - EUROfusion HPC Service provider
 - Core partner of the Fenix action for the federation of HPC system
 - Project coordinator HPC-Europa for HPC Transnational Access
 - Eni Applications dev-ops and HPC System and Production mgmt
- 10** billions of computing hours over last 3 years
- 500** Students per year on our Courses and schools
- 4000** active users
- 2000** active projects



EuroHPC
Joint Undertaking



Tier-0
Flagship systems

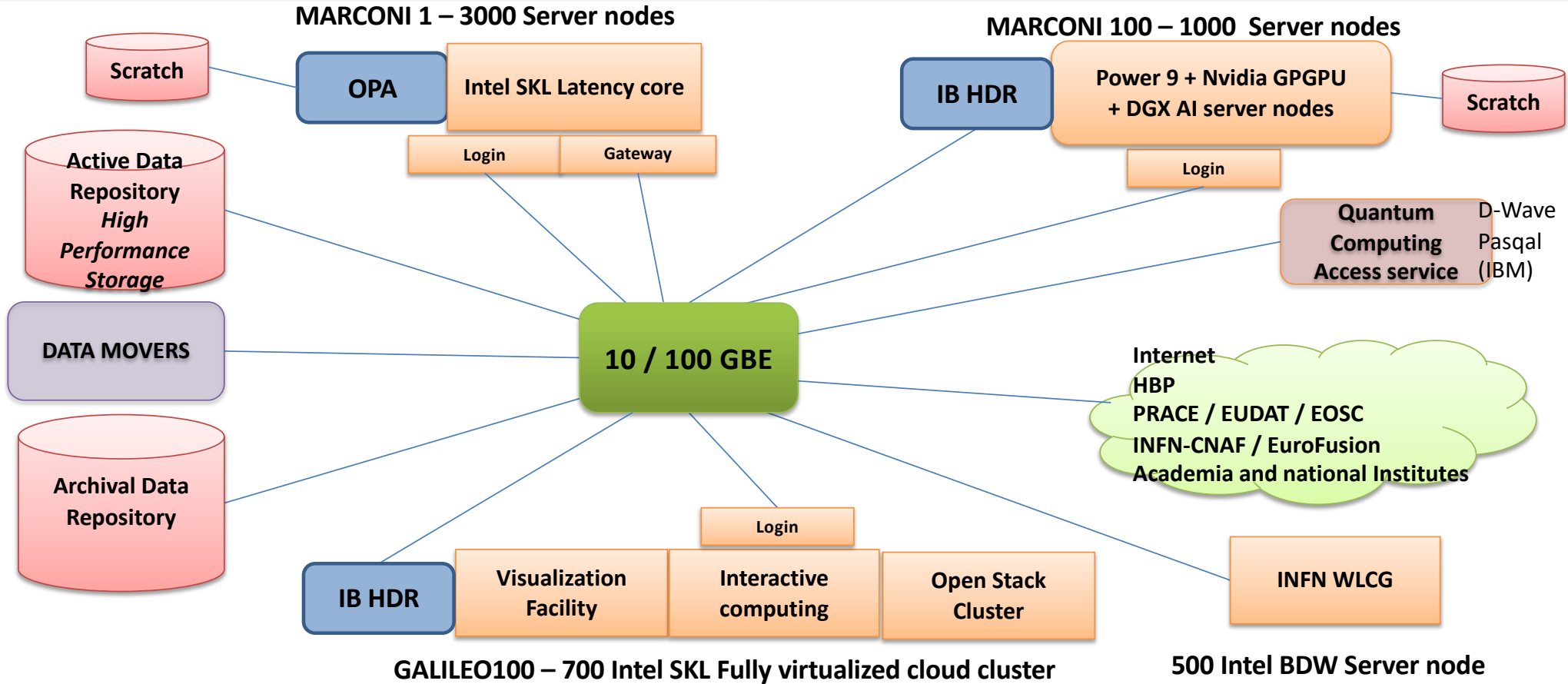
Tier-1
Supercomputing
systems

CINECA

Cloud + Data Repositories/Analysis

HPC Infrastructure

HPC architecture infrastructure (2Q2021)

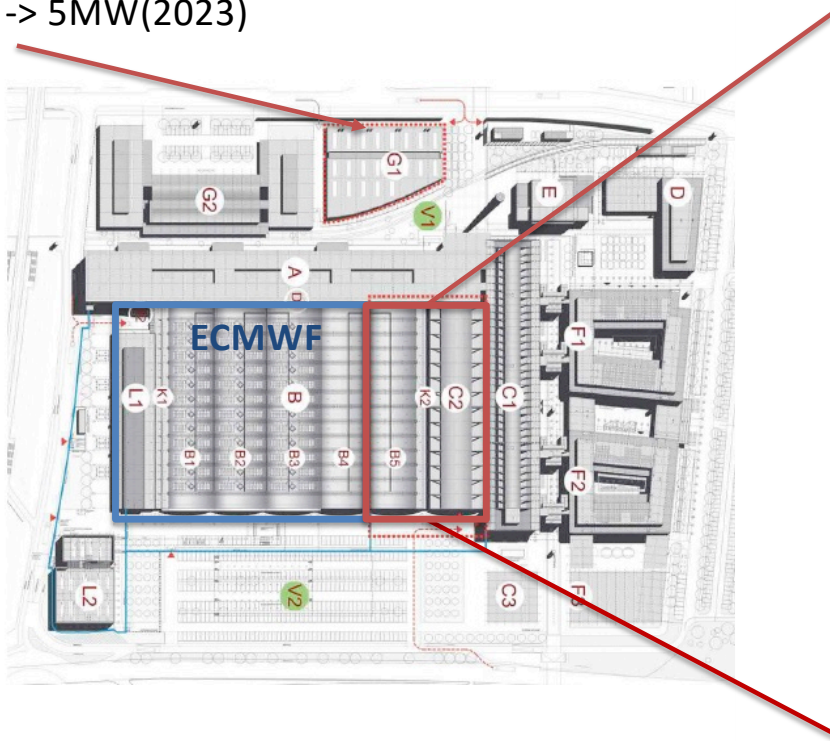




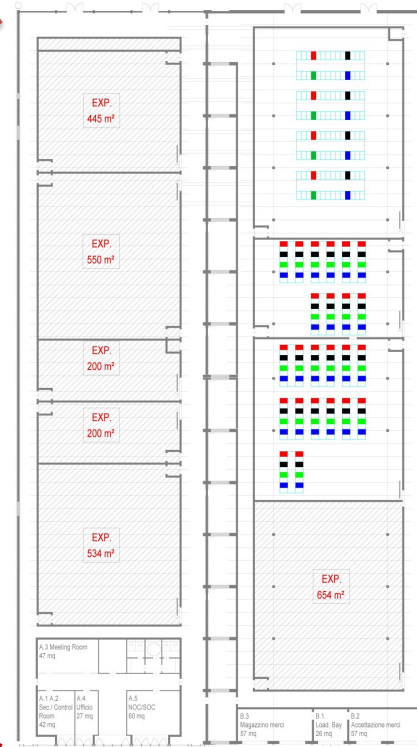
A modern energy efficient new data center designed for hosting a full exascale system



Cooling equipment
3MW (2020) -> 5MW(2023)



PUE < 1.1

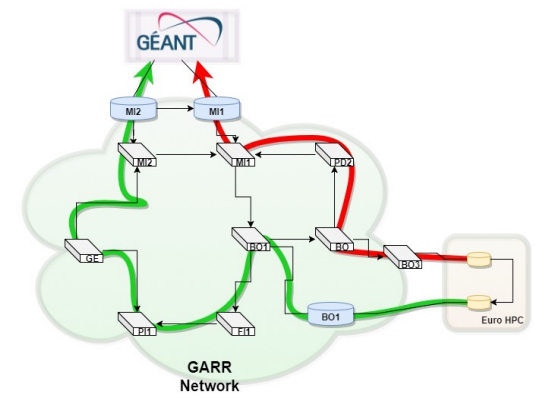


DATA ROOM STAGE 1: 1600 sqm
DATA ROOM STAGE 2: 2600 sqm
ANCILLARY SPACES: 900 sqm

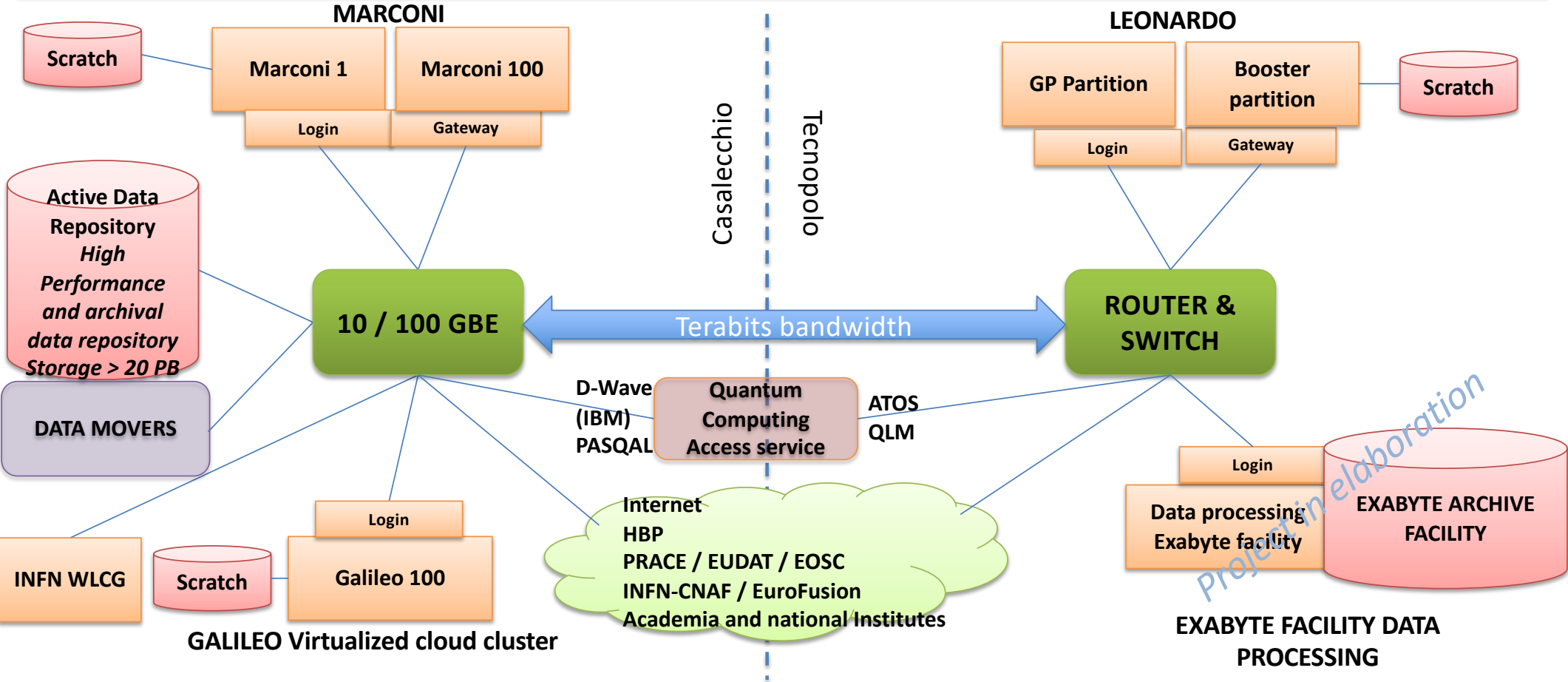
Computer Rooms
10MW (2020) -> 20MW (2023)

8MW hot water DLC
Compute nodes

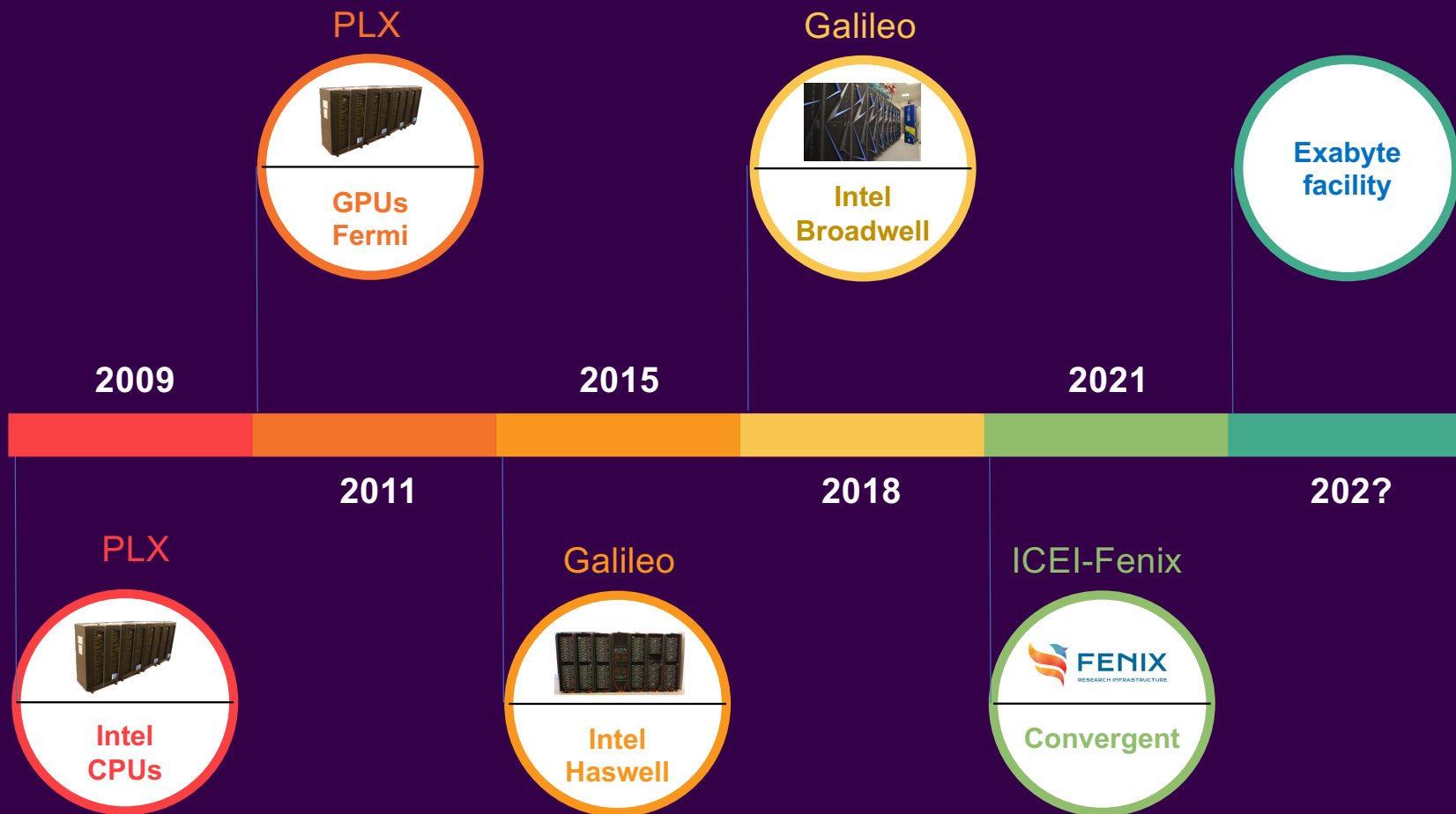
2MW AIR Cooled
Storage + Ancillary



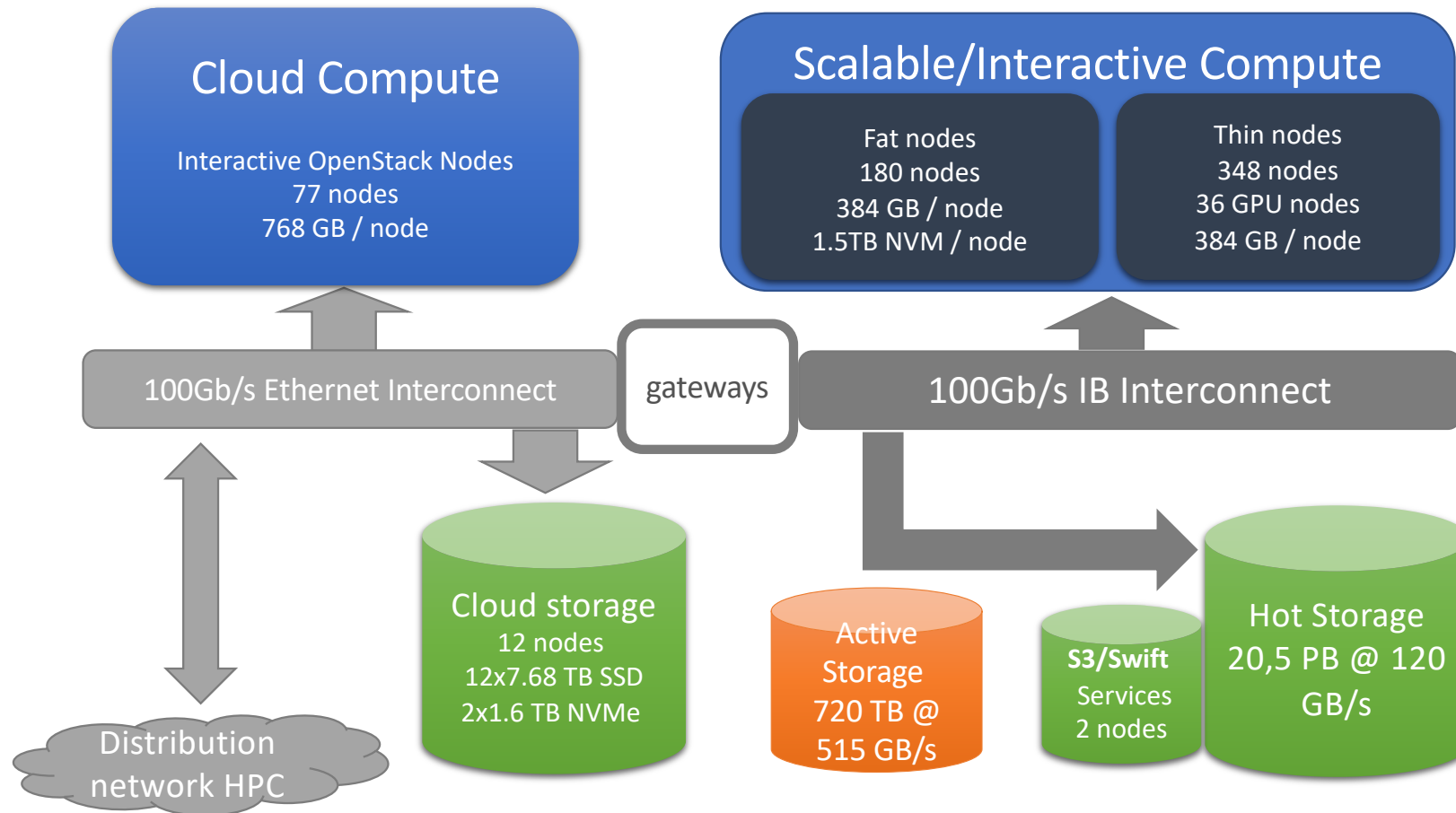
Project / Roadmap of the new infrastructural architecture



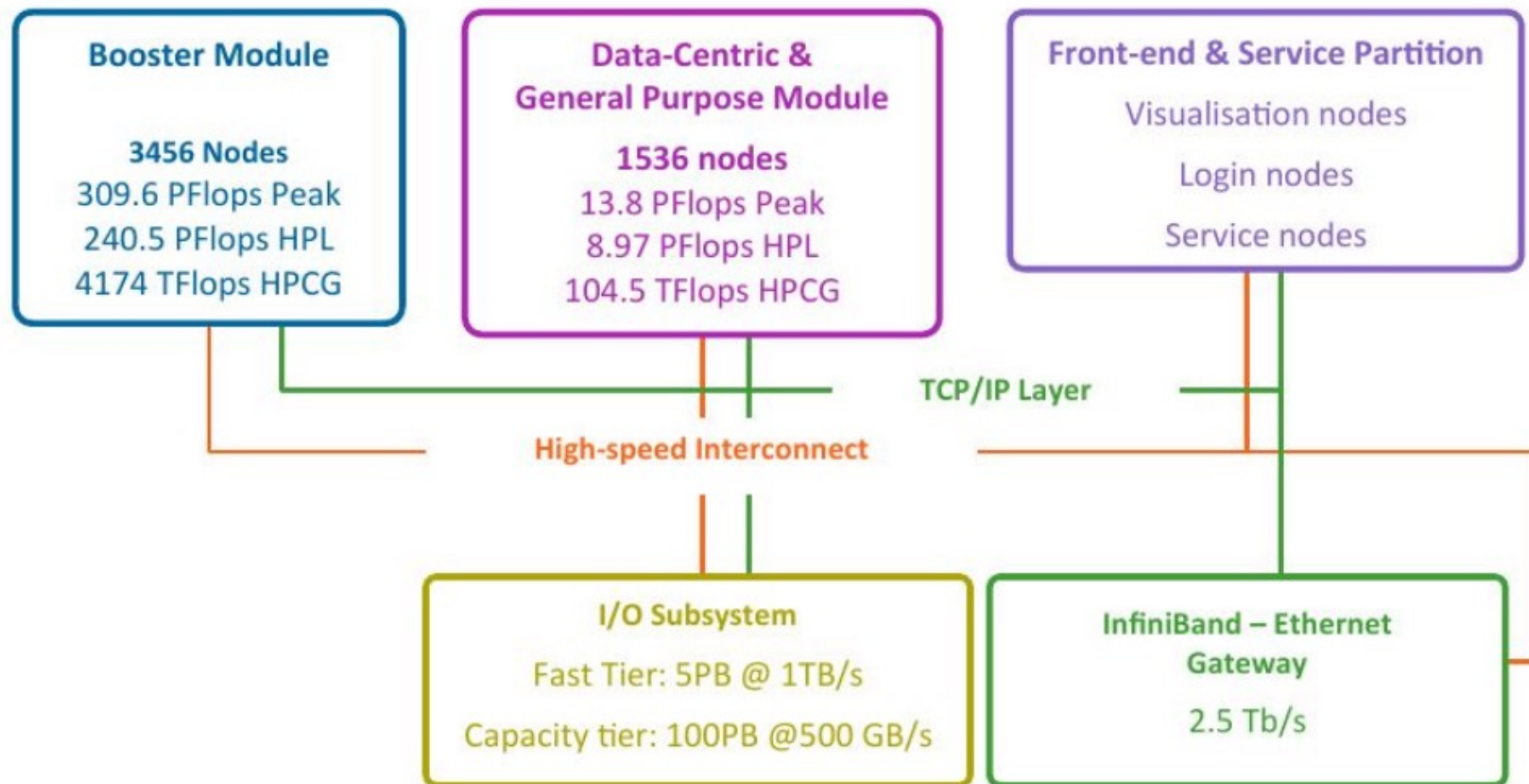




ICEI-Fenix Infrastructure (Galileo100)

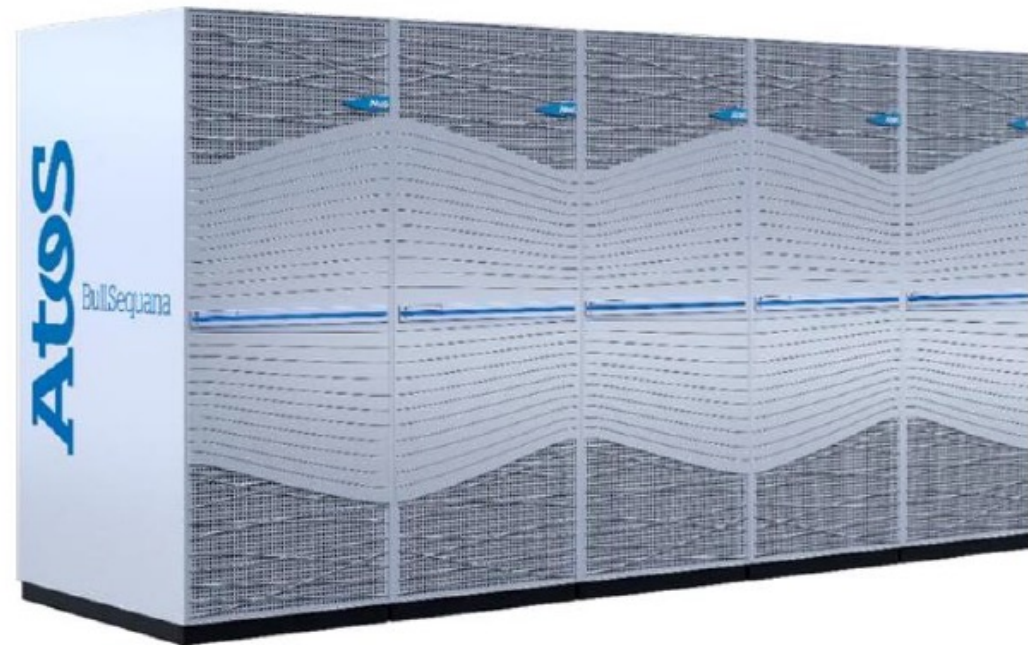


Leonardo in a nutshell



General specifications

- Based on **Atos XH2000** platform technology
- Computing racks **95% Direct Liquid Cooled**
- **Warm water**: Inlet temperature of 38 degrees
- NVIDIA Mellanox **HDR 200** interconnect
 - Dragonfly+ topology
 - 1.11:1 (intra-cell)
 - 0.8:1 globally
- **Bull Smart Energy management** suite
 - Bull Energy Optimizer
 - Bull Dynamic Power Optimizer



HPC Activities and services



Excellence in
Science
Open Access
Peer review
Italian
Supercomputing
Resource
Allocation &
PRACE



Research &
Development
Regional,
National and EU
funded projects



Added value
service and
support for
innovation



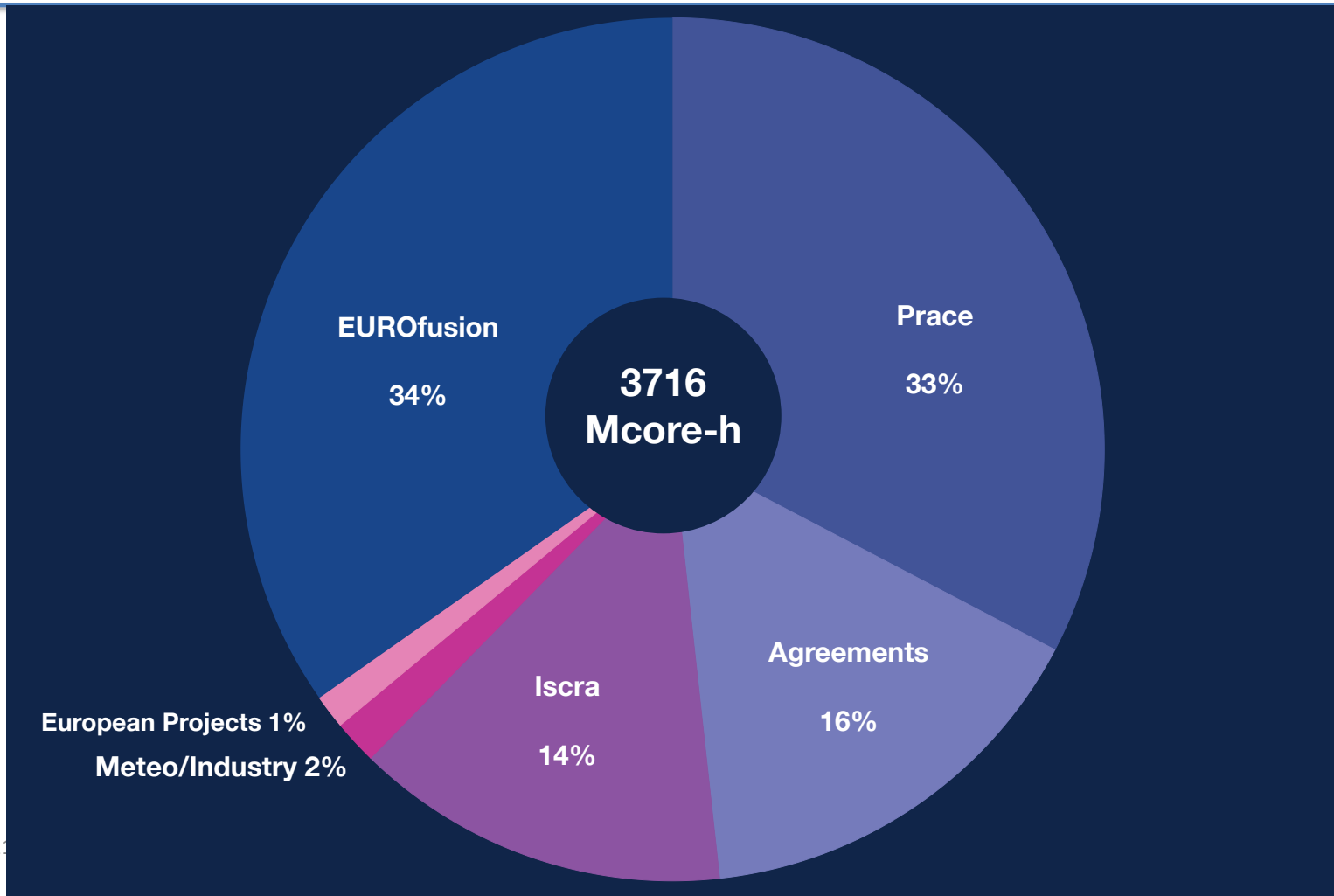
Excellence in Science

Thanks to Davide Coero Borga
(INAF)

Production 2020 in core hours

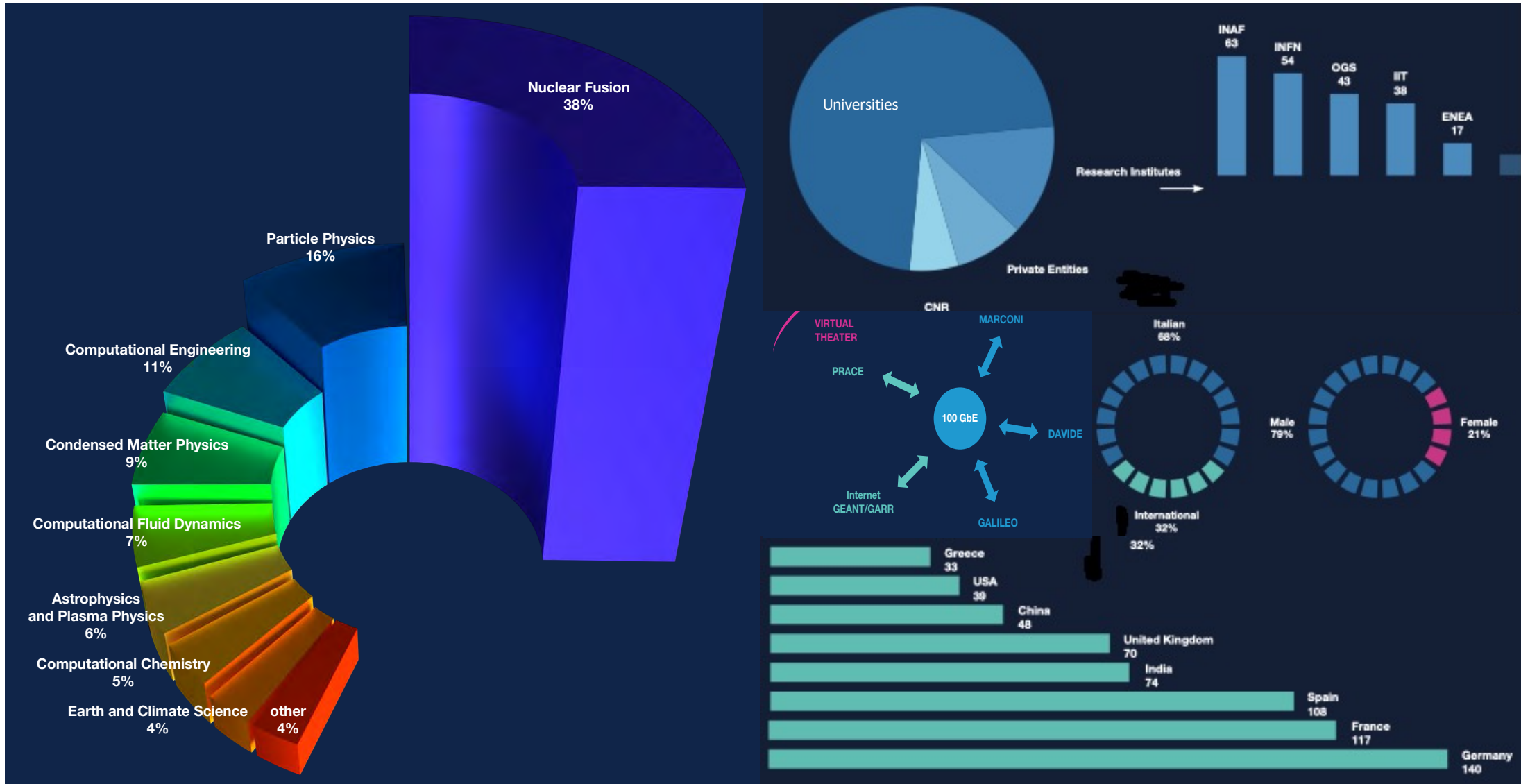
(core-h)	shared	reserved fixed	total used (fixed reserved)	total capacity	used %
Galileo	212'444'824	59'766'336	272'211'160	323'813'376	84%
Marconi A2	178'985'767	58'752'000	237'737'767	279'659'520	85%
Marconi A3	267'804'224	1'013'356'800	1'281'161'024	1'344'162'816	95%
Marconi100	101'252'867	14'807'040	116'059'907	181'386'240	64%
TOTAL	760'487'682	1'146'682'176	1'907'169'858	2'129'021'952	90%

Production per access method



Production per discipline

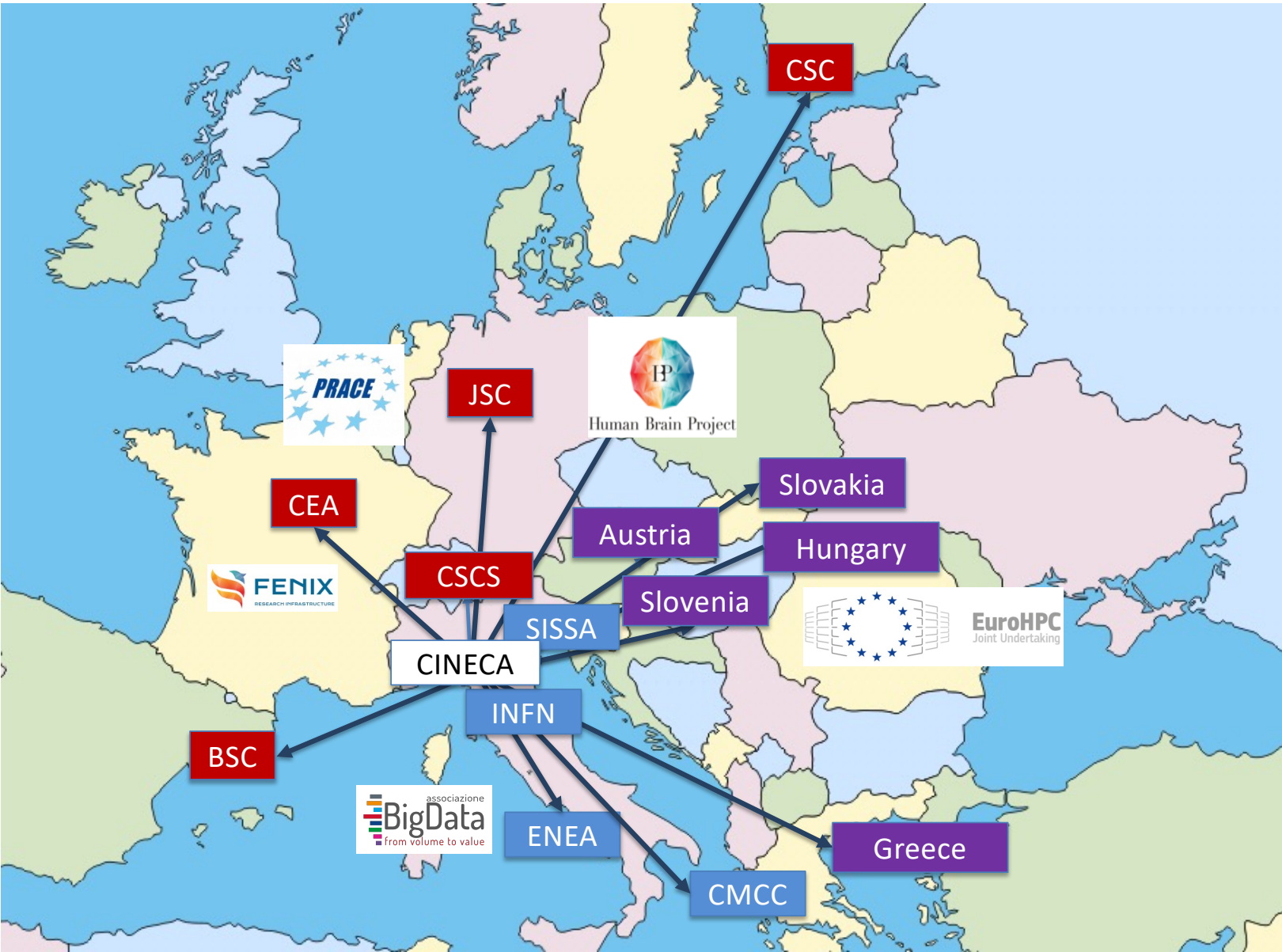
3600 User



Research and Development



THE EUROPEAN HPC NETWORK
FOCUSED ON THE BOLOGNA HUB



CINECA, BSC, CEA, JUELICH,
CSCS, CSC



Human Brain Project



CINECA, BSC, CEA, JUELICH,
CSCS



EuroHPC
Joint Undertaking

LEONARDO CONSORTIUM:
ITALIA, AUSTRIA, SLOVENIA,
SLOVAKIA, UNGHERIA, GRECIA



CINECA, INFN, ENEA,
CMCC, SISSA

Partecipazione in Horizon 2020 current active projects



HPC infrastructure



Digital infrastructure



HPC Center of Excellence



Environment



Big Data / AI / ML



Life Science



Multimedia / Cultural Heritage



Energy efficiency

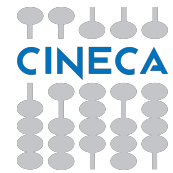


EUPEX

SC for Covid



H2020 - new projects in 2020



Type of Action	Acronym	Title
Approved and Funded		
EuroHPC-CSA	CASTIEL	Coordination and Support for National Competence Centres on a European Level
EuroHPC-RIA	EUROCC	Italian National Competence Centers in the framework of EuroHPC
EuroHPC-RIA	FF4EuroHPC	FF4EUROHPC: hpc innovation for european smes
EuroHPC-RIA	LIGATE	High throughput docking
EuroHPC-RIA	ACROSS	Bigdata, Artificial Intelligence Cross Stack Platform Towards Exascale
EuroHPC-RIA	EXAFOAM	Open FOAM
EuroHPC-RIA	ADMIRE	Adaptive multi-tier intelligent data manager for Exascale
H2020 RIA SC	E4CoV	Exscalate for coronavirus
H2020 RIA SC	ORCHESTRA	Connecting european cohorts to increase common and effective response to sars-cov-2 pandemic
H2020-RIA	EUHubs4Data	Bdva hpc innovation for european smes
H2020-RIA	DICE	EOSC-Storage service
H2020-RIA	GENOMED4ALL	Genomics and Personalized Medicine for all though Artificial Intelligence in Hematological Diseases
H2020-SC1 – Health	PanCareSurPass	PanCare studies of the scale-up and implementation of the digital Survivorship Passport
Hydrogen JU-RIA	e-SHyIPS	Ecosystemic knowledge in Standards for Hydrogen Implementation on Passenger Ship
EuroHPC-RIA	EUPEX	Pilot towards exascale
EuroHPC-RIA	HPCQS	Quantum computing simulators
Submitted		
EuroHPC-RIA	EPI SGA2	European microprocessor initiative
Destination Earth	DTO	Ocean2.EU Digital Twin of the Ocean

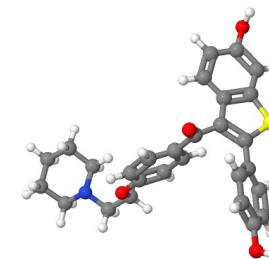
- Drug Discovery
- Corona virus biology
- X-ray crystallography and Cryo-EM
- High Performance Computing
- Structural biology and bioinformatics
- Genomics
- Structure based drug design
- Sequence and protein analysis
- Assay development biochemical and phenotypic
- Biochemical and phenotypic screening
- Protein production and characterisation
- In-vivo testing and animal models
- Chemical libraries and logistics
- Compound repurposing and regulatory affairs

Dompe farmaceutici spa	Italy
Politecnico di milano / Dipartimento di elettronica, informazione e bioingegneria	Italy
CINECA	Italy
Università degli studi di Milano	Italy
Katholieke universiteit leuven	Belgium
International institute of molecular and cell biology in warsaw	Poland

University Of Naples	Italy
University of Cagliari	Italy
SIB Swiss Institute of Bioinformatics	Switzerland
KTH ROYAL INSTITUTE OF ECHNOLOGY	Sweden
Associazione BigData	Italy
Istituto Nazionale Di Fisica Nucleare	Italy
Chelonia	Switzerland

Elettra Sincrotrone Trieste	Italy
Fraunhofer Institute for Molecular Biology and Applied Ecology	Germany
Istituto Nazionale per le malattie Infettive	Italy
Barcelona Supercomputing Center	Spain
Forschungszentrum Jülich GmbH	Germany

The project identified the osteoporosis drug **raloxifene** as possibly active against COVID-19. In June, the Exscalate4Cov consortium requested EMA access to clinical trials for the use of Raloxifene in COVID-19 patients.



Commission: Osteoporosis drug shows promise against coronavirus

Clinical trials are still needed to show if it would actually work for infected patients.

By SARAH WHEATON | 6/18/20, 6:00 PM CET | Updated 6/18/20, 7:09 PM CET

EU-backed researchers are requesting clinical trials to study the osteoporosis drug Raloxifene after virtual and laboratory tests suggest it could be active against the COVID-19 virus.

The research consortium, known as Exscalate4CoV, used supercomputers to virtually screen more than 400,000 molecules for potential efficacy against the coronavirus. Then they used laboratory and biological tests to look at 7,000 specimens that appeared promising. Of the 40 molecules that showed activity against the virus, Raloxifene seems to be the “most promising,” according to a



Coronavirus: Using European supercomputing, EU-funded research project announces promising results for potential treatment

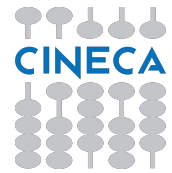
MENU | CERCA | la Repubblica | R+ | Rep: | PER ABBONARSI | ACCEDI

Coronavirus, il supercomputer italiano scopre terapia con 'raloxifene'



On 27/10/2020 AIFA gave the green light to the start of the clinical study of raloxifene in paucisymptomatic patients affected by the SARS-CoV-2 virus.

EXSCALATE4COV: the most relevant virtual screening simulation in the world for the fight against the pandemic underway was performed in Italy.



November 18, 2020 - Last weekend the Exscalate4Cov Consortium carried out the most complex supercomputing simulation dedicated to creating new knowledge on the Sars Cov 2 virus.

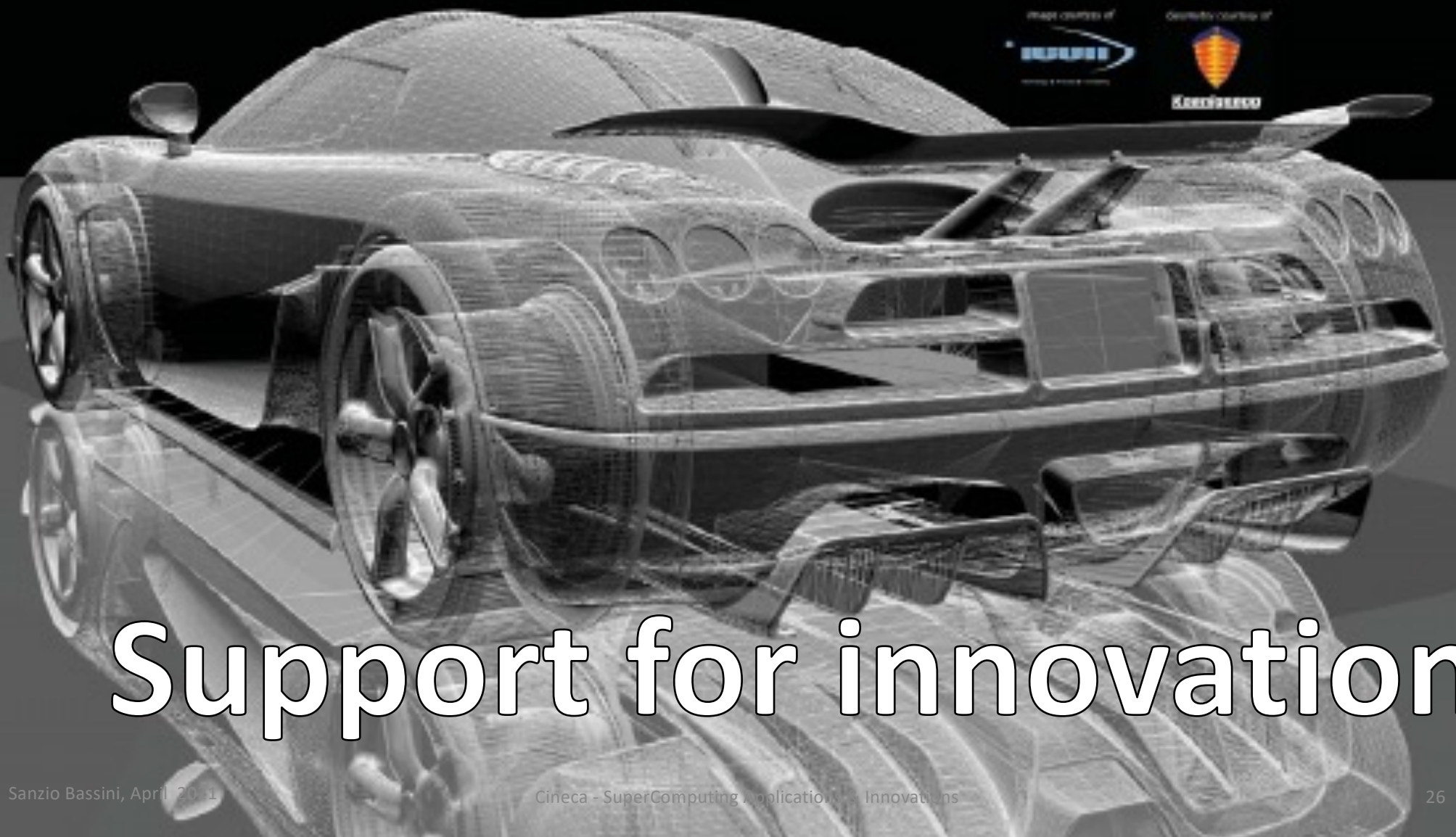
The aim was to simulate the behavior of the virus to identify the best therapeutic methods to neutralize it.

Specifically, more than **70 billion molecules** were simulated **on 15 virus** interaction sites for a total of more than **1 trillion interactions evaluated in just 60 hours**, with the aim of identifying the best molecules ever that can be used against COVID. -19.

Thanks to the computer centers and the software optimized by the **Polytechnic of Milan and by CINECA** it was possible to reach the new goal of **5 million simulated molecules per second**.

For comparison, the Italian simulation is **more than 300 times larger and 500 times faster** than the one made in the in June at the Oak Ridge National Laboratory computer center. (<https://blogs.nvidia.com/blog/2020/05/26/covid-autodock-summit-ornl/>).

The execution was performed on **HPC5 field of Eni**, the most powerful HPC system in Europe, and on **Marconi100 of Cineca**, optimized thanks a workflow designed by **SAS to exploit SAS Viya** platform for artificial intelligence and advanced data modeling.



Support for innovation

Strong Ecosystem



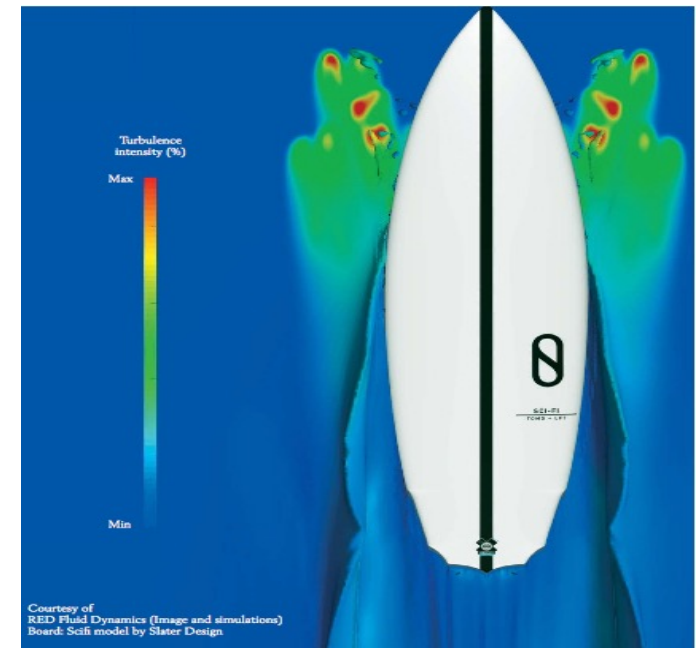
Big data & AI for manufacturing production

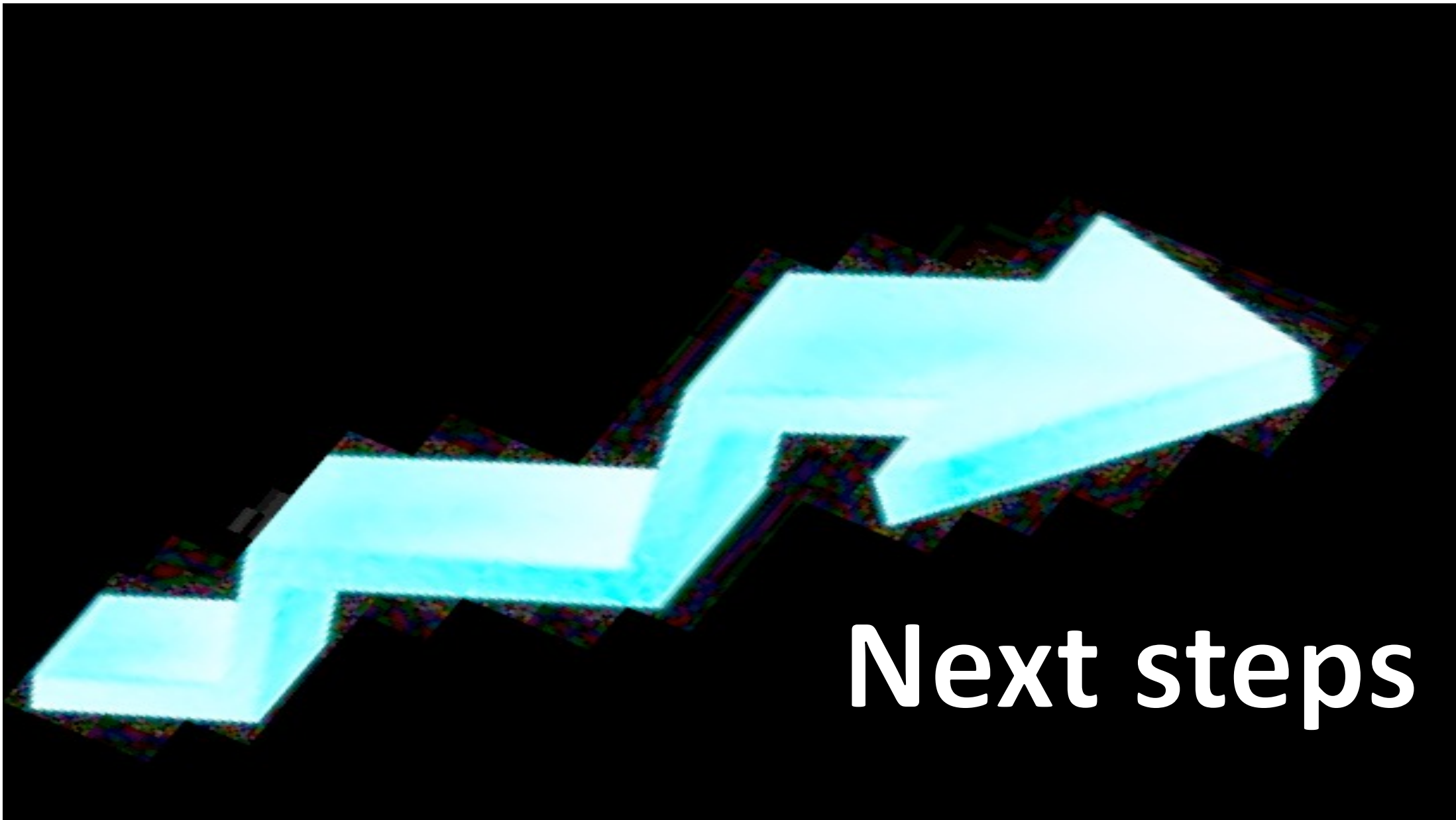
- Università Bologna, l'Università Cattolica del Sacro Cuore, Ferrara, Modena Reggio Emilia e Parma, CNR e INFN, Istituto Ortopedico Rizzoli, Bologna Business School, **CINECA** , Fondazione Golinelli.
- **45 companies**

Current collaborations with Industry and SME



Aero Sekur S.P.A.
Altran Italia S.P.A.
Amet S.R.L.
Ares Design Modena S.R.L.
Arpae - Agenzia Regionale per la Prevenzione, l'Ambiente e l'Energia dell'Emilia- Romagna
Arpap - Agenzia Regionale per la Prevenzione, l'Ambiente del Piemonte
Azienda Provinciale per i Servizi Sanitari – Provincia Autonoma di Trento
Azienda Sanitaria Locale Teramo
Azienda Usl Roma 3
Azimut Benetti S.P.A.
Chiesi Farmaceutici S.P.A.
Crestoptics S.P.A.
Dainese S.P.A.
Dompé Farmaceutici S.P.A.
Elica S.P.A.
Eni S.P.A
Ferrero Technical Services S.R.L.
Ferretti S.P.A.
Fondazione Res Ricerca e Salute
Industrie Salieri Italo S.P.A.
L'air Liquide S.A.
Neos S.R.L.
Nolangroup S.P.A.
Olsa S.P.A.
Philip Morris Manufacturing & Technology Bologna S.P.A.
Rai - Radiotelevisione Italiana S.P.A.
Remosa S.R.L.
Unipolsai Assicurazioni S.P.A.
Wam Industriale S.P.A.





Next steps

Scope: Create a focused system to support innovation for industries and SMEs



Ff4eurohpc connects business with cutting-edge technologies.

<https://www.Ff4eurohpc.Eu/>



European federation of data driven innovation hubs.

<https://euhubs4data.eu/>



EuroHPC National Competence Centre (NCC)

<https://www.eurocc-project.eu/>; <https://www.cineca.it/progetti/euro-cc-italian-competence-center>

<https://www.cineca.it/index.php/news/eurocc-centro-di-competenza-nazionale>



CASTIEL closely associated with EuroCC, combines the National Competence Centres (NCC)

formed in EuroCC <https://www.castiel-project.eu/>



A Competence Center for **Industry 4.0**

<https://bi-rex.it/en/>

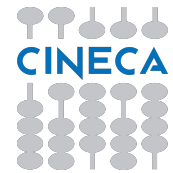


Industry 4.0 European Digital Innovation Hub



DIH ER²digit - Emilia-Romagna Ecosistema Regionale di innovazione Digitale

Scope: Health and life science
Portal Service & GDPR Compliance



Centralized repository for
human genomic data



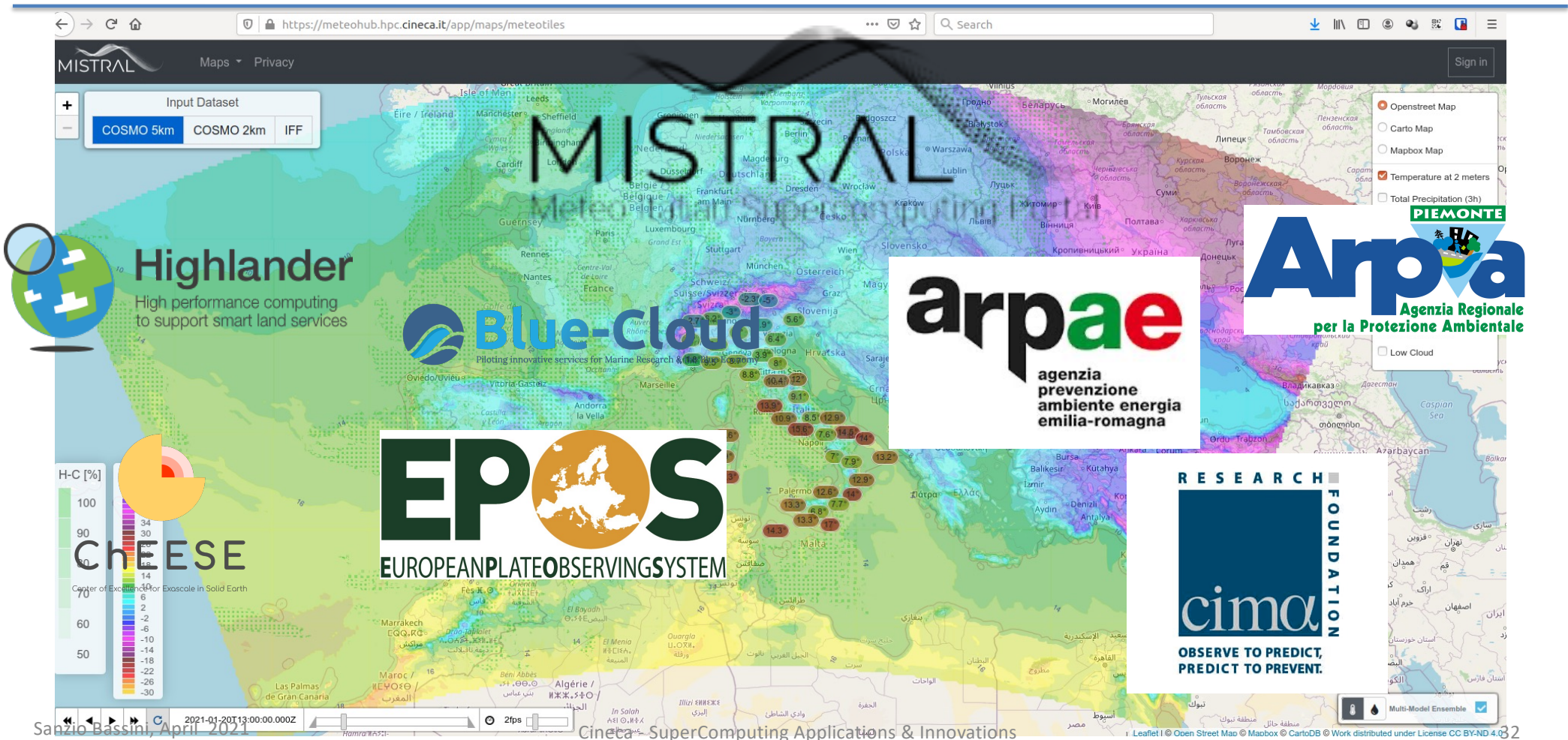
PanCareSurPass



Por Fesr RER Pilot
biobanking &
genomic data
processing

Scope: Weather / Climate / Environment

<https://www.mistralportal.it/opendata/>



Sanzio Bassini, April 2021

Cineca SuperComputing Applications & Innovations

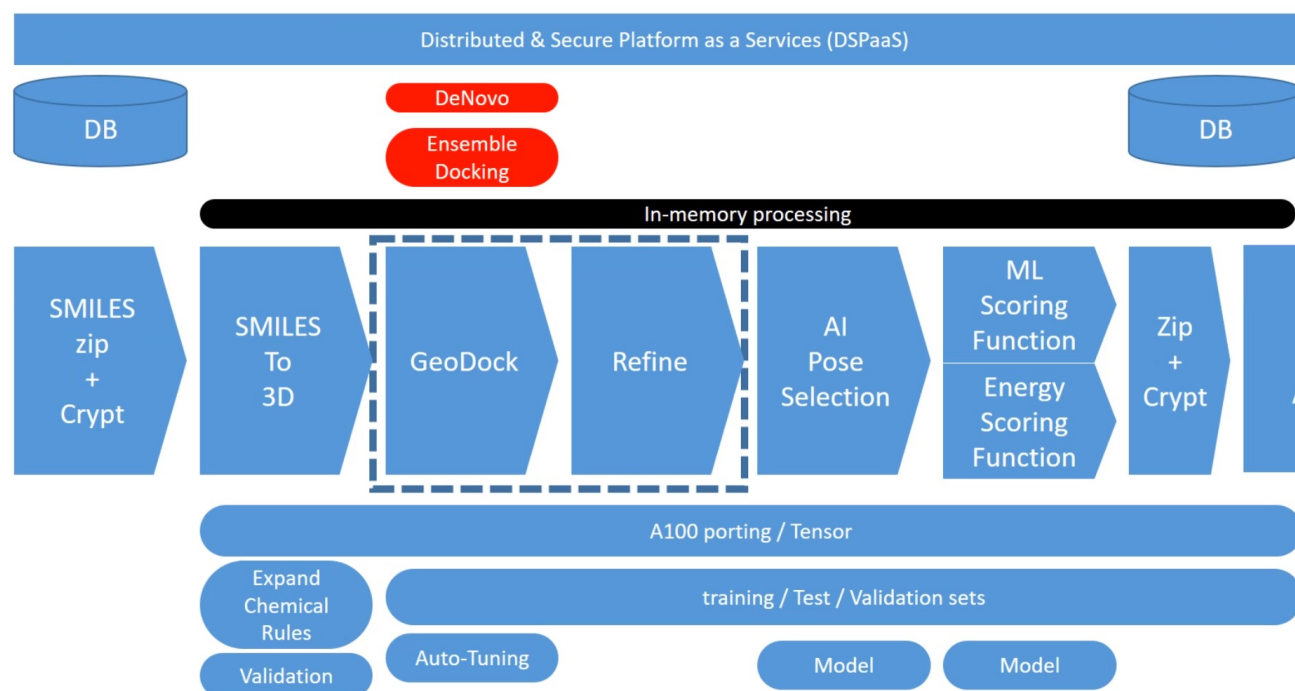
Leaflet | © Open Street Map © Mapbox © CartoDB © Work distributed under License CC BY-ND 4.0

Scope: Drug repurposing in partnership with Dompè Pharmaceutical



EXSCALATE
4COV

LiGen™ 4.0



LIGATE

EUPEX

Scope: quantum computing
<https://www.cineca.it/index.php/temi-caldi/quantum-computing>



QUANTUM COMPUTING

CINECA makes available to researchers of Italian universities and research centers that participate in the call IS CRA-C, resources on the most advanced and mature quantum computing technologies currently available, as well as access to quantum emulators installed on the Marconi100 system.

HPCQS

Agreement CINECA CERN INFN
Hosting a QC test bed system in
Collaboration with UNIPD & INFN
Access to QC physical system
Hosting ATOS QLM
QC Emulator running on M100:
Unipd, QSKIT, Pasqal, ...