

## Scientific Computing at INFN (and beyond)



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  - b) The National Recovery and Resilience Plan (NRRP).
  - c) Health-related initiatives.
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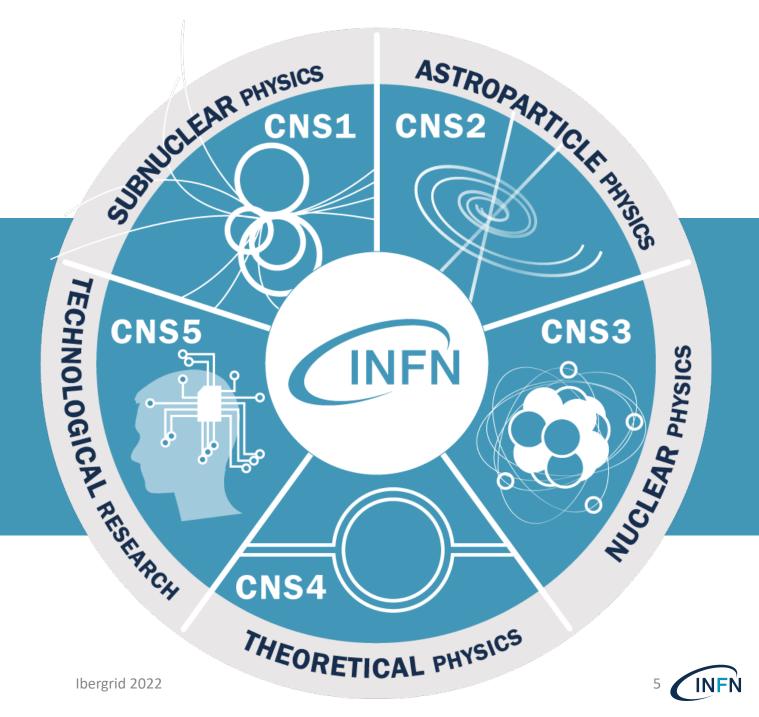
#### About myself

- Director of Technology at the Italian National Institute for Nuclear Physics (INFN) with some 30 years of experience in distributed computing for science.
  - Based in Bologna at CNAF, the INFN National Center for Data Processing and Computing Technology Research.
  - Coordinator of the INFN-wide computing & storage infrastructure.
  - Member of the INFN Computing management board.
  - <a href="https://www.linkedin.com/in/davidesalomoni/">https://www.linkedin.com/in/davidesalomoni/</a>, email: <a href="mailto:davide@infn.it">davide@infn.it</a>
- Adjunct Professor at the University of Bologna for the PhD program in "Data Science and Computation" and for the MD in Bioinformatics for the courses "Infrastructures for Big Data Processing" and "Biomedical Data Bases".
  - <u>https://www.unibo.it/sitoweb/d.salomoni/en</u>



### INFN and Computing

#### The **5 research lines** and the INFN National Scientific Committees



### The INFN Facilities

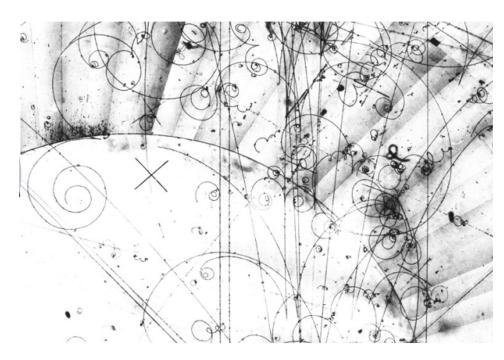




#### A brief history of computing @ INFN

CNAF (*"Centro Nazionale Analisi Fotogrammi"*) was founded, dedicated to what was at the time the most technologically challenging analysis method: bubble chambers images

**1962** 





The launch: the first director of CNAF Massimo Masetti (on the left) speaking with Luigi Gui (in the center) at the CNAF inaugural ceremony





The number of films to be analyzed increased to 100k's per year, introducing the need for more automation in the analyses.

"Computers" appeared at CNAF: IBM7094 and later IBM 360/44



IBM 7094 operator's console showing additional index register displays in a distinctive extra box on top. Note "Multiple Tag Mode" light in the top center.

~ 200 kflops

IBM System/360 Model 44



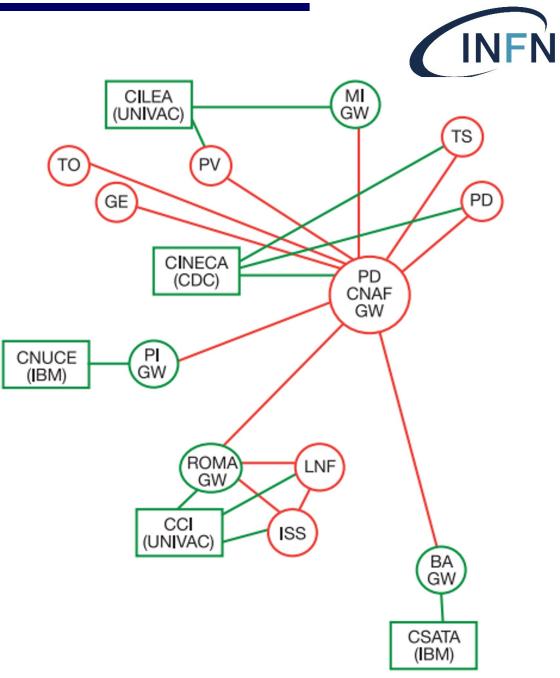
System/360 Model 44 front panel
Manufacturer
International Business Machines
Corporation (IBM)
Product
System/360
family
Release date
August 16, 1965
Discontinued
September 23, 1973

Memory 32–256 KB Core

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Computers became more and more popular among physicists; due to the distributed nature of INFN, they were installed in different structures and mostly handled independently. From the need to allow intercommunication, the <u>INFNet project</u> was started, using dial-up connections. <u>CNAF</u>, with its technology-related mission, became the central node of this effort. In the early 80s, a connection was built to CERN (via CERNet), first for direct access and later to FNAL. At the end of the 80s, INFNet was topping 64 kbit/s.



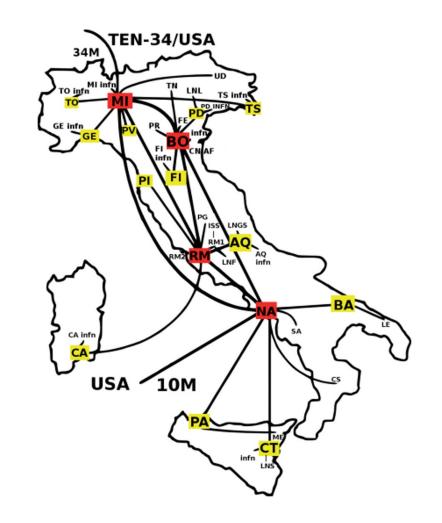




Remote access to computers was quickly becoming a need in other scientific domains; GARR was pioneering 2 Mbps connections by 1998, starting with a CERN-CNAF link and later with connections to CINECA, Rome and Milan. This is the infrastructure that handled LEP, TeVatron, SLC computing.

Over time, that became the backbone of research networking in Italy, which reached 34 Mbps by 1995. Still today, research networking is handled in Italy by GARR.

By that time, we were in the planning of the "LHC" era, and it was clear that Computing would have been a major effort for HEP and for INFN specifically. CNAF was again having a central role for INFN Computing.



Davide Salomoni

 1001
 60s
 1995

 Ten main international centers were selected to host the

Worldwide LHC Computing Grid (WLCG):

The

- In Italy, this was the Tier-1 at CNAF (red in the picture)
- 9 additional "Tier-2" centers were added, at LNL, LNF, Turin, Milan, Pisa, Rome, Naples, Bari, Catania (yellow in the picture)

The

70s-

- Then came the GRID, the Cloud, ...
- All these centers are still operational, even if their size has increased ~100x since then, and their interconnectivity now reaches multiples of 100 Gbps, thanks to the GARR-X network.
- Collectively, our distributed infrastructure currently offers about 140,000 CPU cores, 120PB of enterprise-level disk space, 100PB of tape storage.



1962

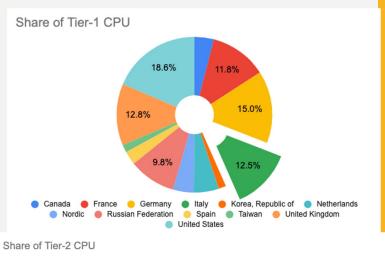
1988-

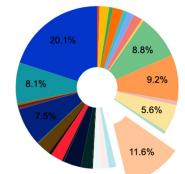
2000-

2005

#### WHERE ARE WE TODAY?

- INFN Distributed Computing federation delivers the LHC experiments O(7-20)% of their computing budgets
- "non LHC" (VIRGO, Astro, Nuclear, ...) is ~ 10-20% of the total
- Sites are of top quality among their peers, and have worked uninterruptedly for the last ~15 years
- In many cases, the infrastructures are close to those deployed in 2005 or slightly after
  - They could be bigger (CNAF uses ~1 MW, more recent centers are leaning towards ~10 MW)
  - They could be "greener"
    - Free cooling, direct cooling, ...
  - They could use more recent technologies, hardware and software
    - Go towards a national cloud, implement a datalake model for storage, ...

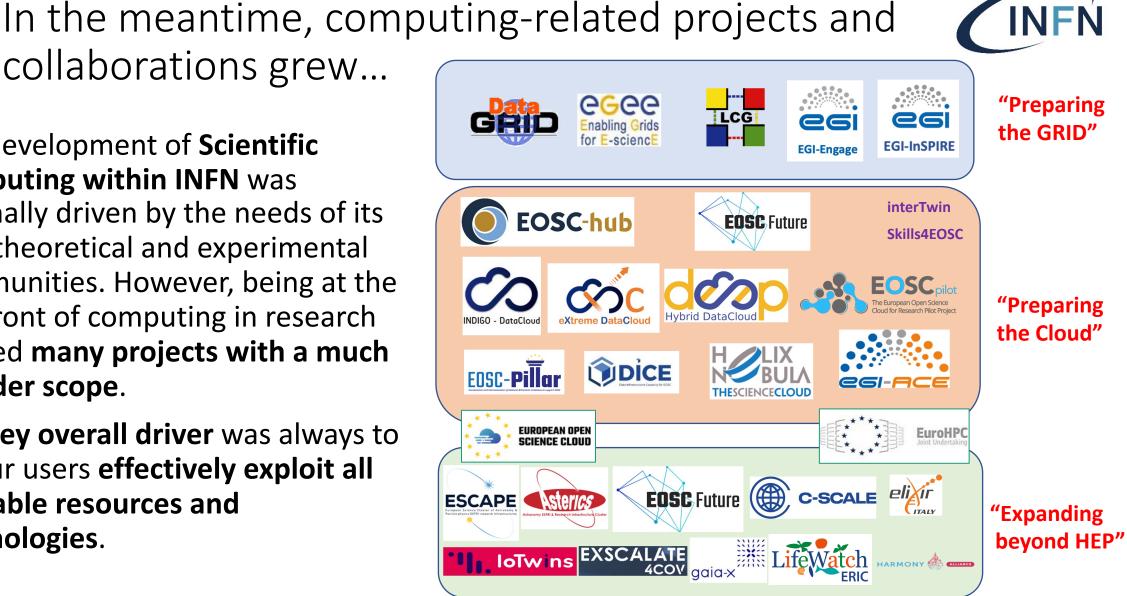






#### collaborations grew... eeee

- The development of **Scientific Computing within INFN** was originally driven by the needs of its own theoretical and experimental communities. However, being at the forefront of computing in research seeded many projects with a much broader scope.
- The key overall driver was always to let our users effectively exploit all available resources and technologies.





# Computing challenges (as we see them)

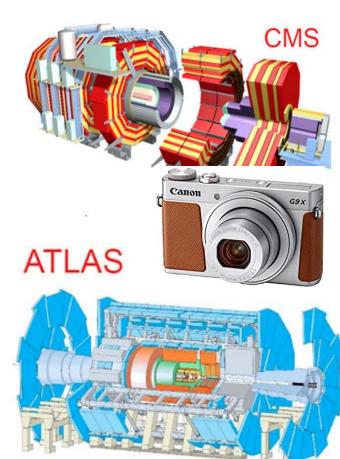
## The overall framework of computing challenges



- The next generation of High-Energy Physics (HEP) and of many other experiments presents **unprecedented needs for computing**, apparently close to "impossible".
- They are not far away: for instance, the "High-Luminosity LHC" experiments at CERN are only a few years ahead.
- In general, we see **two competing trends**:
  - "Moore's law is a term used to refer to the observation made by Gordon Moore in 1965 that the number of transistors in a dense integrated circuit (IC) <u>doubles about every two years</u>" – there are similar "laws" for storage, networks etc → if you wait long enough, every computing need will become economically affordable.
  - Experiment + physics complexity: every generation of experiments will collect more data, core complex events, more detailed snapshots.
- Who wins? Usually, we refer to "flat budget" as the situation where the needs increase with the same "slope" of technology → this leads to a theoretical constant amount of money per year.
  - This is sort of accepted by the Funding Agencies ...

## A back-of-the-envelope estimate of storage needs

- We can use a simplified model for "a detector":
  - It "takes a picture" of a collision event every 25 ns (@ 40 MHz)
  - It has ~ O(100) Million acquisition channels (10x for the detectors to come)
  - Assuming 1 channel = 1 byte, the raw data rate would be →
- 40e6 ev/s \* 100e6 byte/ev = 4 PB/s
  - 4 PB/s in 5 years would amount to 120 ZB (ZettaBytes)
- A "storage problem" is automatic, given the need to investigate rare events with a high precision.



JFN

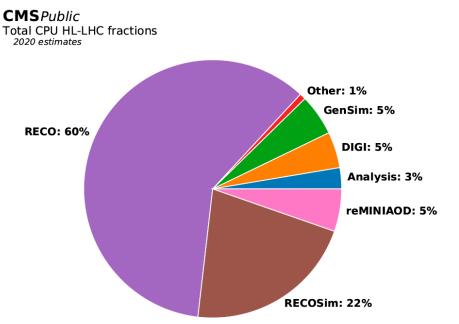
#### How about CPUs?

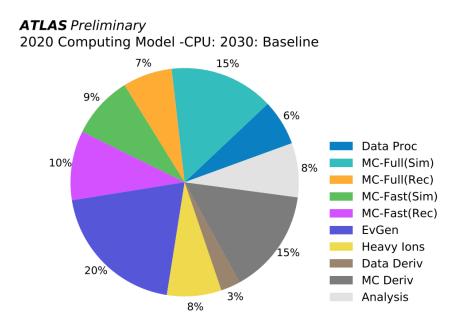


- Besides storage needs, it turns out that CPU power is also a problem.
- Where do we spend CPU time in current HEP experiments?
- Broad brush list:
  - Interpretation of RAW detector signals into physics objects ("Reconstruction")
  - Statistical studies of the reconstructed events ("Analysis")
  - Simulation of the physics processes ("Generators"), the detector response ("Simulation"), the electronics ("Digitization)"

## Where do we spend CPU time?

- Different experiments have different shares in the CPU utilization, but in general simulation (from partons to electronic signals) and reconstruction (from electronic signals to "physics objects" like jets, leptons, etc.) are the most time-consuming activities.
- As a rule of thumb, # of simulated events > # of collected events



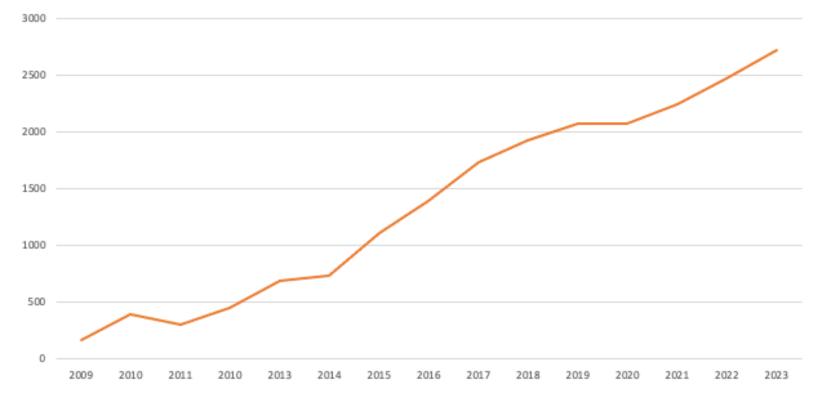


## How did computing for LHC (experiments at CERN) evolve?



#### CMS CPU (kHS06)

- Pre-LHC to Run 1 (CMS CPU) – 2x
- Another 10x was 2005-2009
- All with
  - The same sites
  - The same infrastructure



### Storage and CPU drive the trigger rate



- In an ideal world, all the 40 MHz 25 ns snapshots (i.e., events) would be saved and analyzed, leading to the 120 ZB in 5 years computed above.
- In practice, a much lower rate can be saved for \$\$ reasons; years of studies have defined the "minimum" possible rate that still preserves physics capabilities, at least for the most important physics channels.
- In the end, it is a tension between what you can afford and what you would like to collect; LHC history (CMS-ATLAS) shows that:
  - Run-1 (2010-2012) : 100-500 Hz (out of the 40 MHz)
  - Run-2 (2015-2018) : ~ 1 kHz
  - Run-3 (2022-2024) : 1-2 kHz
  - Run-4 (2027+, see later) : > 5 kHz



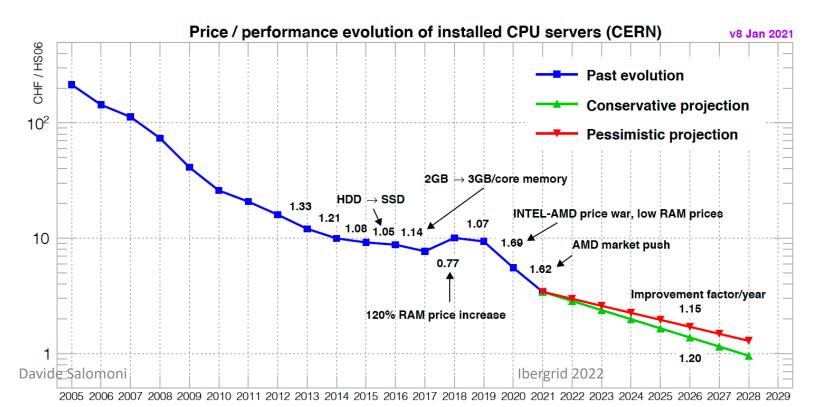
#### What is then the limiting factor?

- Apart from some limits on the electronics (*"I cannot dispatch more than X consecutive triggers"*), **the real limit** on the numbers and type of events collected by HEP and other experiments is **Computing**, and on its turn the **amount of money** one can dedicate to that.
- This can also be seen as a reversed process: I know what I can spend on computing → I know how many events I can collect → I know what type of physics I can do.
- Therefore, any R&D, new idea or solution which allows to reduce the costs of Computing is very visible and increases the physics potential of the experiments. <u>Ultimately, this is the reason why</u> <u>INFN is very interested in computing technologies and in related</u> <u>innovative solutions</u>.

#### How is technology going?



- In the glory days of 2000-2010, we were able to get year over year a +40% of performance for the same price ( $\sqrt{2} \approx 1.41$ ) on the type of technology we were interested in (linux boxes with x86 CPUs)
  - This made the CPU increase shown on a previous slide "harmless":  $(\sqrt{2})^{10}$  (2005-2015) = 32x
  - What about more recent times?

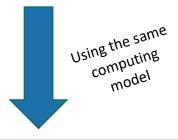


2005-2010: -60%/y 2010-2015: -20%/y 2015-2020: -10%y 2020-2022: some recovery seen, extrapolations are currently at -15/-20%/y

## Extrapolations for High-Luminosity LHC

- A 20% yearly increase in performance from 2021 to ~2028 gives us a speed-up factor from technology advancements of (1.2)<sup>7</sup> ~3.6x.
- Back-of-the-envelope linear estimates foresee increased needs for computing at High-Luminosity LHC of ~75x (box on the right).
- Therefore, we miss a factor 20x!
- How can we cope with this?
  - Get 20x more money from the Funding Agencies (<u>unrealistic</u>, the ballpark figure would be >> 1 BEur/y)
  - Find ways to reduce the needs...

1 LHC Experiment ~2020: ~200.000 CPU Cores; ~200 PB disk; ~350 PB tape

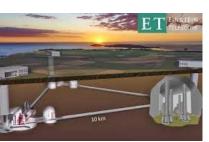


1HL-LHC Experiment ~2028: ~15M CPU Cores; ~15 EB disk; ~26 EB tape

#### What about other scientific domains?

- **DUNE**: ProtoDUNE in 2019 collected 3 GB/s (same as CMS at the same time); real DUNE expected 80x at the end of the 2020s.
- SKA: up to 2 PB/day (CMS ~3), to be collected and processed at "complex" locations.
- **Genomics**: a single genome ~100 GB. Any population study (>1M people) over 100 PB.
- **CTA**: ~ 10 PB/y in 2025+.
- **Virgo**: ~10% of a LHC experiment.
- ET aiming at being ~10% of a HL-LHC experiment.







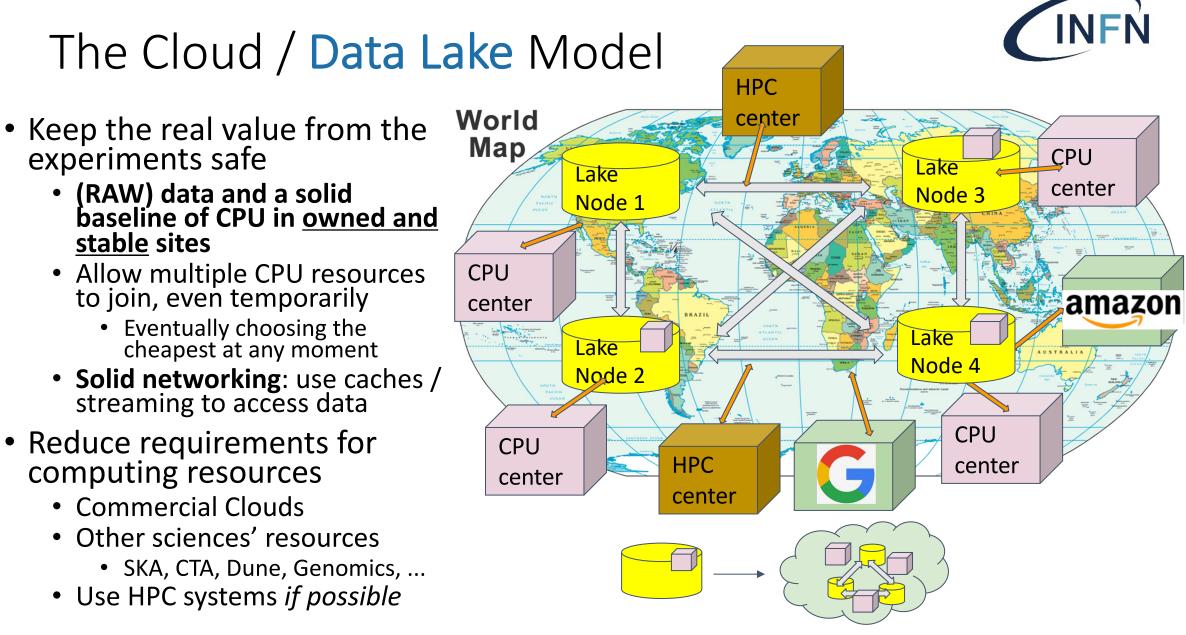




## How can we cope with these levels of requests?

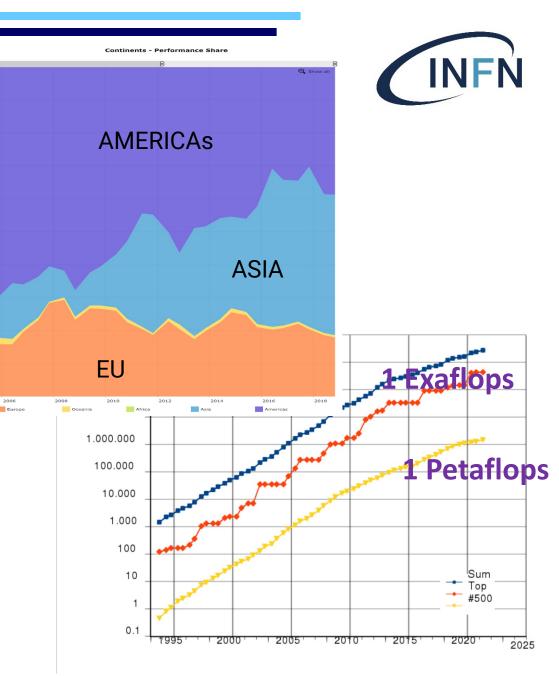


- We need some strategies to reduce *at least* the increase from 20x to ~1x. We can for instance consider:
  - **1.** Infrastructural changes
  - 2. Technological changes
  - 3. Physics / Science #1: change the analysis model.
  - 4. Physics / Science #2: reduce the scientific reach (for example increasing trigger thresholds).
    - Not even considered here ... it is the "desperation move" if we fail with everything else.
  - 5. Something unexpected...
- Let's discuss a bit about 1 and 2.



#### Supercomputing (HPC)

- The world is full of Supercomputers. Why ?
  - Real scientific use cases
    - Lattice QCD, Climate modeling, ...
  - Industrial showcase ("Country XY is technologically capable")
    - And hence not 100% utilized: opportunities for smart users. *Can we be one of them?*
- Many not trivial problems to solve:
  - Data access (access, bandwidth, ...)
  - Accelerator Technology (KNL, GPU, FPGA, TPU, ???, ...)
  - Submission of tasks (MPI vs Batch systems vs proprietary systems)
  - Node configurations (low RAM/Disk, ...)
  - Not-too-open environments (OS, ...)
- Some hints of global slowing down, but not for top systems where the "HPC war" is on
- 1 Petaflops = 10<sup>15</sup> floating point operations per second
- 1 Exaflops = 10<sup>18</sup> floating point operations per second



share 20

#### HPC integration @ INFN



- Experimentation with HPC systems (CINECA, mostly) started in 2019 for LHC-like workflows, with excellent results using 4 PRACE grants
  - Demonstration of the capability to execute LHC workflows on HPC systems
  - Demonstration of the capability to execute workflows on non-standard architectures (Power9)

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- Demonstration of the capability to circumvent HPC security via user-level tools  $\ensuremath{\textcircled{\odot}}$ 

Enabling CMS Experiment to the utilization of multiple hardware architectures -- a Power9 Testbed at CINECA T.Boccali<sup>1</sup>, A.Malta Rodrigues<sup>2</sup>, D.Spiga<sup>3</sup>, M.Mascheroni<sup>4</sup> for the CMS Collaboration <sup>1</sup>NFN Sezione di Pisa, <sup>2</sup> University of Nebraska-Lincoln, <sup>3</sup>INFN Sezione di Perugia, <sup>4</sup>University of California San Diego

Extension of the INFN Tier-1 on a HPC system

Tommaso Boccali<sup>1</sup>, Stefano Dal Pra<sup>2</sup>, Daniele Spiga<sup>3</sup>, Diego Ciangottini<sup>3</sup>, Stefano Zani<sup>2</sup>, Concezio Bozzi<sup>4</sup>, Alessandro De Salvo<sup>5</sup>, Andrea Valassi<sup>6</sup>, Francesco Noferini<sup>7</sup>, Luca dell'Agnello<sup>2</sup>, Federico Stagni<sup>6</sup>, Alessandra Doria<sup>8</sup>, Daniele Bonacorsi<sup>9</sup>

### First experiences with a portable analysis infrastructure for LHC at INFN

Diego Ciangot inflytola Malo Bochali<sup>2</sup>, Andrea Ceccanti<sup>3</sup>, Daniele Spiga<sup>1</sup>, Davide Salomoni<sup>3</sup>, Tommaso Tedeschi<sup>1</sup>, and Mirco Tracolli<sup>1</sup>

Integration of CINECA-PRACE into CMS Computing

First tests of Job Distribution on PowerPC

Daniele Spiga Marco Mascheroni Tommaso Boccali

Daniele Spiga Mirko Mariotti <u>Tommaso Boccali</u> (for the INFN team - see last page)

Diego Ciangottini



#### However, HPC => technological changes

- As we have seen, the unitary cost of our computing (the CPUs) *does not decrease fast enough*; this is true for OUR computing (Linux PCs with Intel x86 architecture), but not necessarily for ALL computing.
- GPGPUs and FPGAs and even more ASICs are better at metrics such as Operations/\$\$, while ARM and Power8/9 architectures are better at Operations/Joule.
  - ... but in most cases using fruitfully at least the first category needs a complete rewriting of the code – which costs a lot!

| Table 6. SLOCCount measured lines of source code for ATLAS and CMS. |                      |                    |                         |  |  |  |
|---|----------------------|--------------------|-------------------------|--|--|--|
| Experiment  | Source Lines of code | Development effort | Total estimated cost to |  |  |  |
| Туре  | (SLOC)               | (person-years)     | develop                 |  |  |  |
| ATLAS   | 5.5M                 | 1630               | 220 M\$                 |  |  |  |
| CMS   | 4.8M                 | 1490               | 200 M\$                 |  |  |  |

As a reference:

- the Linux Kernel is: 15M SLOC, 4800 FTEy, 650M\$ (3x CMS)
- Geant4 is: 1.2M SLOC, 330 FTEy, 45 M\$ (1/4x CMS)



#### And that's only the "core code" ...

- We rely on many externals (Geant4 is an external, ROOT is an external, Pythia is an external), which greatly inflate the total code size.
- This (in unreadable fonts) is the list of externals for a typical CMS release:

alpgen qd root cxxdefaults sockets catch2 gcc-ccompiler gcc-f77compiler mpfr cmsswdata codechecker csctrackfinderemulati cuda-stubs cuda-gcc-support cvs2git dablooms db6 dmtcp doxygen eigen fastjet-contrib fastjet-contrib fastjet-contrib archi gcc-analyzer-ccompiler gcc-analyzer-cxxcompi gcc-atomic gcc-checker-plugin gcb geant4-parfullcms geant4data py2-numpy openloops git glibc glimpse gmake gnuplot gosam gosamcontrib hdf5 igprof intel-license ittnotify lapack lcov libffi libxslt llvm md5 openblas ofast-flag openmpi professor py2-sympy py2-absl-py py2-appdirs py2-appdirs py2-attrs py2-attrs py2-attrs py2-attrs py2-avro py2-avro py2-backports cachetools py2-certifi py2-chardet py2-climate py2-colorama py2-contextlib2 py2-cryptography py2-cx-oracle py2-cython py2-dalooms py2-decorator py2-decorato flawfinder py2-fs py2-funcsigs py2-functools32 py2-future py2-gitby2-by2-gitby2-gitby2-gitby2-google-common py2-googlepackages py2-grpcio py2-h5py py2-h5py-cache py2-hep ml py2-histogrammar py2-html5lib py2-gitby2-hyperas py2-hyperopt py2-idna py2-ipaddress py2-ipykernel py2-ipykernel py2-ipython\_genutils py2-jedi py2-jionja2 py2-jionja2 py2-jionpickle py2-jionyter\_client py2-jupyter\_console py2-jupyter\_core py2-keras-application py2-keras-preprocessi py2-kiwisolver py2-lint py2-lizard py2-llvmlite py2-lxml py2-lz4 py2-markdown py2-markupsafe py2-matplotlib py2-mccabe py2-mock py2-more-itertools py2-mpld3 py2-mpmath py2-nbdonvert py2-nbdonver notebook py2-numba py2-numexpr py2-oamap py2-onnx py2-ordereddict py2-packaging py2-pandos py2-parsimonious py2-parso py2-pathlib2 py2-pbr py2-pexpect py2-pickleshare py2-pillow py2-pip py2-pluggy p py2-prometheus\_client py2-prompt\_toolkit py2-protobuf py2-prvlock py2-psutil py2-ptyprocess py2-py py2-pyasn1-modules py2-pybind11 py2-pybrain py2-pycodestyle py2-pycodestyle py2-pycodestyle py2-pydit py2-pygithub py2-pygiments py2-pygiments py2-pymongo py2pyopenssl py2-pyparsing py2-pysqlite py2-pytest py2-python-cjson py2-python-dateutil py2-python-ldap py2-pytaml py2-pyzmq py2-qtconsole py2-rep py2-repoze-lru py2-requests py2-root\_numpy py2-root\_pandas py2-rootpy py2-scikit-learn py2-scipy py2-seaborn py2-send2trash py2-setuptools py2-simplegeneric py2-singledispatch py2-six py2-soupsieve py2-sqlalchemy py2-stevedore py2-subprocess32 py2-terminado py2-terminado py2-testpath py2-theanets py2-theanets py2-theanets py2-theanets py2-soupsieve py2-sqlalchemy py2-stevedore py2-subprocess32 py2-tables py2-terminado py2-testpath py2-theanets py2-thea tornado py2-trgdm py2-trgitlets py2-typing py2-typing extensions py2-uncertainties py2-uproot-methods py2-urtualenv py2-virtualenv py2-virtualenv py2-virtualenv py2-webencodings py2-webencodings py2-webencodings py2-webencodings py2-uproot py2-xpoot py2-xp pydata pyminuit2 pygt python-paths python tools rootglew scons sloccount tcmalloc tcmalloc minimal tensopy2-virtualenvwrapperrflow tinyxml2 xtl blackhat boost boost header python bz2lib cascade headers ccache-ccxmpiler ccache-crxcompiler ccache-f77compiler zlib gmp photos\_headers pythia6\_headers openssl clhep clhepheader cppunit cuda curl libxml2 dcap root\_interface xz xerces-c vecgeom\_interface hepmc\_headers distcc-cccompiler distcc-f77compiler dpm expat fastjet fftyet fftw3 freetype gbl gdbm gsl giflib google-benchmark libjpeg-turbo hector heppdt madgraph5amcatnlo llvm-cxxcompiler jemalloc jimmy headers ktjet libhepml libuuid llvm-ccompiler llvm-f77compiler meschach mxnet-predict numpy-c-api x11 oracle pacparser voda protobuf python3 qd f main sqlite sigcpp tauola headers tbb tensorflow-framework tensorflow-runtime tensorflow-xla compilO-pafccj3 toprex headers utm valgrind vdt headers xrootd xtensor boost system boost serialization boost program options boost python boost regex boost signals boost test cascade vami-cop photos pythia6 pcre cub cuda-api-wrappers cuda-cubias cuda-cusolver cuda-cusolver cuda-nov cuda-nover cuda-novine c cxxcompiler libtiff libungif llvm-analyzer-ccompil llvm-analyzer-cxxcomp mcdb opengl openldap oracleocci pyclang qtbase sip starlight tauola tensorflow-cc tkonlinesw toprex vdt boost\_chrono boost\_filesystem boost\_mpi cgal lhapdf classlib davix rootcling geant4core photospp geant4static graphviz lwtnn millepede gt3support rivet tkonlineswdb cgalimageio herwig rootmathcore rootrio pythia8 geant4vis thepeg pyquen gt rootrint rootrflx rootsmatrix rootx11 sherpa charybdis rootthread dire tauolapp geant4 geneva herwigpp jimmy gtdesigner rootgeom rootxmlio vincia rootcore evtgen roothistmatrix rootmath rootxml rootgpad rootfoam rootspectrum root rootminuit rootgraphics rootgui rootinteractive roothtml rootminuit2 dd4hep-core roofitcore mctester professor2 rooteg rootgeompainter rootrgl rootged rootguihtml rootmlp rootpy dd4hep dd4hep-geant4 roofit rooteve roottmva roostats rootpymva histfactory coral

• Note that **gcc** is there! CMS ships its own compiler, so dependency on the Linux host is only at the level of glibc.

So: what are the main drivers for the next 10 years of scientific computing for INFN?



#### 1. Infrastructure

- Renew infrastructures to be ready for the High Luminosity-LHC (HL-LHC) era, up to ~2035 or more
- Use more compact computing (from today's ~20 kW/rack to 80 or more)
- Lower the PUE (power usage effectiveness), be greener
- Extend and expand networking for a future-proof infrastructure

#### 2. Hardware, Software, Services

- Foster and simplify the utilization of more viable technologies (€/task or J/task), like GPUs, FPGA, down to Quantum when available
- Be more efficient, elastic and resilient
  - Pervasive use of geographically distributed storage ("the Datalake")
  - Abstract from physical machines, and form a national pool of resources and high-level services ("the Cloud")
  - Extend elastically to external providers such as traditional HPC or to other cloud providers ("dynamic federations")

#### The evolution of Infrastructure and of Higher-level Services must proceed together



## A founding milestone for us: INFN Cloud

#### INFN Cloud, <u>https://www.cloud.infn.it/</u>

- In **production** since March 2021.
- The **initial seed** of a National Datalake for research and beyond, building on (existing | renewed | new) e-Infrastructures.
- The **base of the evolution** of the INFN Distributed Computing vision.
- Built on a thin middleware layer running on top of *federated clouds*, decoupling physical and logical views via a service composition mechanism.
- The **INFN foundation** for the NRRP computing-related initiatives (more on this later).

This page collects all policies and procedures that have been validated by the INEN Cloud Project Management Board and that ar currently in place across the INFN Cloud infrastructure.

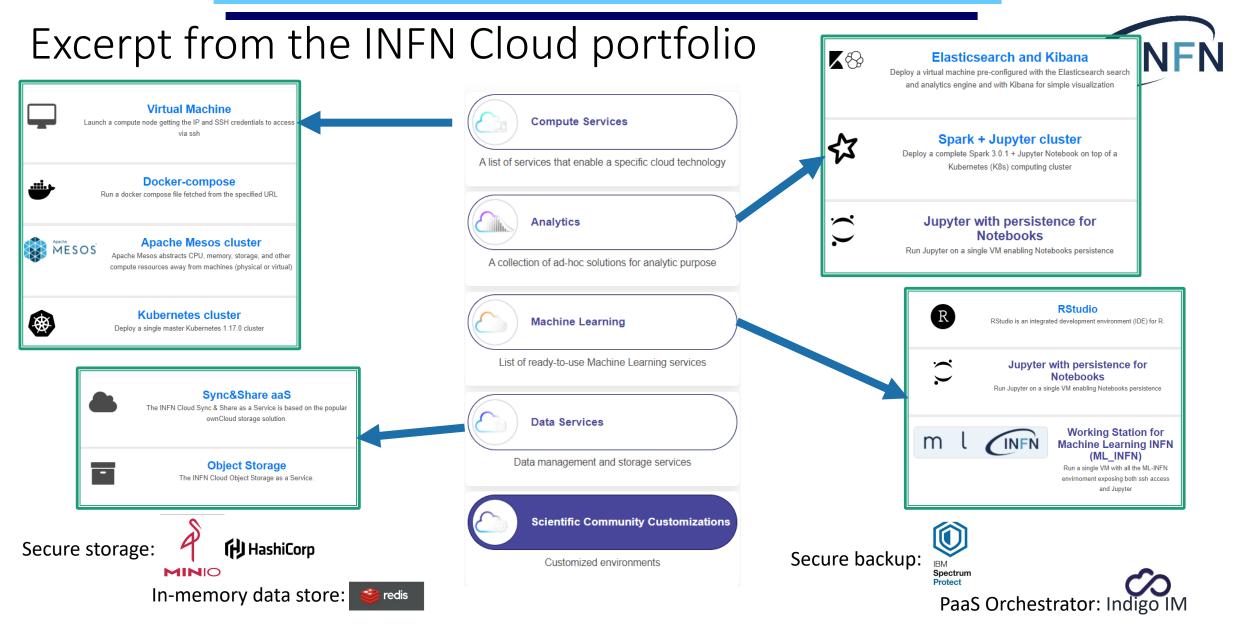
#### What is INFN Cloud

- A production-quality set of resources and solutions providing:
  - A core backbone, with ancillary and specialpurpose services.
  - A multi-site, federated Cloud infrastructure.
    - INFN Cloud can transparently federate INFN sites as well as public or private Clouds (e.g.: AWS, Google Compute Cloud, Microsoft Azure, and others)
  - A customizable portfolio of services accessible via web interfaces, terminal or API.
  - A fully distributed organization for the support and management of both infrastructure and services.
  - A set of rules that define access resources and policies, according to INFN, national and European laws.

| INFN-Cloud Procedure to manage scheduled downtimes         INFN-Cloud Rules of Participation         INFN Cloud Security Recommendations         User Community Operation Level Agreement | Infra | astructure/Users<br>astructure/Users  | v.1.0<br>02/02/2022<br>v.1.2 |
|---|-------|---|------------------------------|
| INFN Cloud Security Recommendations   | Infra |   |                              |
|   |       |   | 19/01/2022                   |
| User Community Operation Level Agreement  | Use   | astructure/Users  | v.1.0<br>09/06/2021          |
|   |       | ers   | v.1.0<br>13/04/2021          |
| Welcome to the INFN Cloud Use Cases   | 8     | ers   | v.1.0<br>13/04/2021          |
| Documentation   |       | astructure  | v.1.0<br>13/04/2021          |
|   |       | ers   | v.2.0<br>29/09/2021          |
| 'ou'll find here useful information regarding the use-cases supported on the INFN Clo<br>nfrastructure.   |       | ers   | v.1.1<br>13/04/2021          |
| Table of Contents   |       | ers   | v.1.1<br>13/04/2021          |
|   |       | Search  | Q                            |
| Getting Started   |       | Training Co   | ontacts                      |
| How To: Create VM with ssh access   |       | training co   | intacts                      |
| How To: Deploy Sync&Share aaS   |       |   |                              |
| How To: Associate a FQDN to your VMs  |       |   |                              |
| <ul> <li>How To: Use the Notebooks as a Service solution</li> </ul>   |       |   |                              |
| <ul> <li>How To: Request to open ports on deployed VMs</li> </ul>   |       |   |                              |
| How To: Deploy a Kubernetes cluster   |       |   |                              |
| How To: Deploy an Apache Mesos cluster  |       |   |                              |
| <ul> <li>How To: Deploy a Spark cluster + Jupyter notebook</li> </ul>   |       |   |                              |
| How To: Deploy Elasticsearch & Kibana   |       | - 110000<br>- 1100001<br>- 01100001<br>- 01100100<br>- 01100100<br>- 01100100<br>- 01100100<br>- 01100100<br>- 01100100<br>- 0110000<br>- 011000<br>- 01000<br>- 010000<br>- 010000<br>- 01000<br>- 01000<br>- 01000<br>- 010000<br>- 0100 |                              |
| How To: Deploy RStudio Server   |       |   |                              |
| How To: Instantiate docker containers using custom docker-compose files   |       |   |                              |
| <ul> <li>How To: Instantiate docker containers using docker run</li> </ul>  |       |   | ~2                           |
| <ul> <li>How To: Access cloud storage from a scientific environment</li> </ul>  |       | 10 M  | اکر                          |
| How To: Request the "nomination to be system administrator"   |       |   | 6                            |
| How To: Request the "nomination to be system administrator" (italian version)   |       |   | 2                            |
| INFN is offering to its users a comprehensive and integrated set through its dedicated <b>INFN Cloud infrastructure</b> .   | of C  | Cloud service   | es                           |
| The <b>INFN Cloud portfolio</b> , available via an <b>easy-to-use web int</b> exploitable via command-line interfaces, is defined upon clear us   |       |   |                              |

Read more

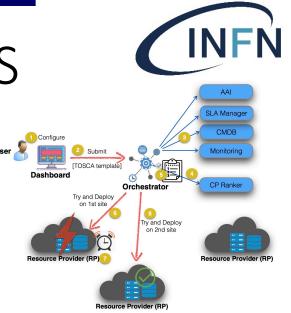
Join us



Selectable storage QoS levels: fast (SSD), normal (HDD), archive (tape-backed), remote replicas

Davide Salomoni

Ibergrid 2022



#### Architectural pillar: the INDIGO PaaS

- The INDIGO-DataCloud PaaS is rooted on:
  - 1. A distributed resource orchestration framework
  - 2. A standard—based **federated solution for identity** access management (INDIGO-IAM)
- In practice:
  - Following authentication, a user requests a service via a Dashboard, APIs, or a CLI.
  - The PaaS Orchestrator is contacted, and a series of ancillary services get involved (e.g. AAI, SLA Manager, Provider Ranker, Monitoring).
  - A deployment of the required service is scheduled and eventually delivered on one of the federated resource providers.
  - All services are described through an **Infrastructure as Code** paradigm, via a combination of TOSCA templates (to model an application stack), Ansible roles (to manage the automated configuration of virtual environments), and Docker containers (to encapsulate high-level application software and runtime).

## The INFN Cloud Backbone

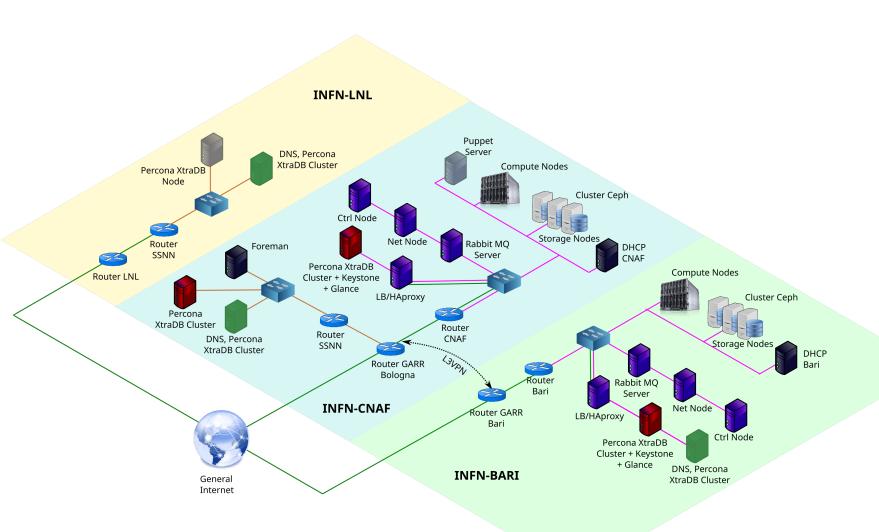


The INFN Cloud Backbone is a multi-site cloud infrastructure running both INFN Cloud Core Services and some user-level resources.

The topology of the INFN Cloud Backbone simplifies the implementation of **geographic HA or failover** for its Core Services.

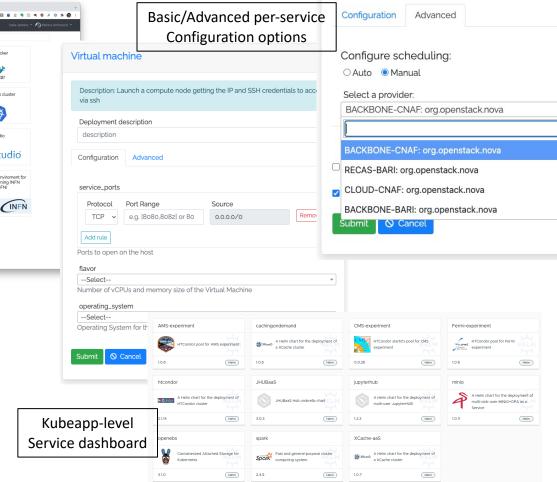
The backbone infrastructure is managed by the INFN Cloud Team with **extensive use of infrastructure automation tools**.

**Federated clouds** connect directly to the backbone.



## Status, Dashboards

| infn | Cloud Dashboard Deployments Advan       | iced + External Links + Users             | beta-testers *  |
|------|---|---|---|
|      | Virtual machine                         | Docker-compose                            | Run docker  |
|      | ·///                                    | s.  | docker  |
|      | Elasticsearch and Kibana                | Apache Mesos cluster                      | Kubernetes cluster  |
|      | kibana elastic                          | MESOS                                     | <b>(</b>  |
|      | Spark + Jupyter cluster                 | HTCondor cluster                          | RStudio   |
|      | Spark                                   | HICondor                                  | RStudio   |
|      | TensorFlow with Jupyter                 | Jupyter with persistence for<br>Notebooks | Computational environment for<br>Machine Learning INFN<br>(ML_INFN) |
|      | TensorFlow                              | Jupyter                                   | m l CINFN   |
|      | Working Station for CYGNO<br>experiment | Sync&Share aaS                            |   |
|      | C/GNO<br>Etpainer                       | 4   |   |
| -    | Per-user/pe                             | r-group                                   |   |
| /iew | of the mai                              | n dashboard                               | 4   |



#### **INFN Cloud Status**

This page shows the high level status of the INFN Cloud services.

2022-03-25 -> 2022-03-28 - Power shutdown @ CLOUD-VENETO

due to start in about 17 ho

| due to start in about 17 hours    |             |
|-----------------------------------|-------------|
| 1. INFN Cloud                     |             |
| Object Storage 💿                  | Operational |
| Backbone - Cloud Compute (Bari) 💿 | Operational |
| Backbone - Cloud Compute (CNAF) ③ | Operational |
| Authentication ⑦                  | Operational |
| 2. Federated Cloud - CloudVeneto  |             |
| CloudVeneto - Cloud Compute       | Operational |
| 3. Federated Cloud - ReCaS-Bari   |             |
| RECAS-BARI – Cloud Compute        | Operational |
| 4. Federated Cloud - Cloud@CNAF   |             |
| Cloud@CNAF - Cloud Compute        | Operational |
| 5. PaaS services                  |             |
| Infrastructure Manager ③          | Operational |
| Orchestrator 💿                    | Operational |
| CPR ()                            | Operational |
| CMDB 💿                            | Operational |
| Dashboard 💿                       | Operational |

Davide Salomoni

Ibergrid 2022

Virtual machine

SSH credentials to access via ssh

Deployment description

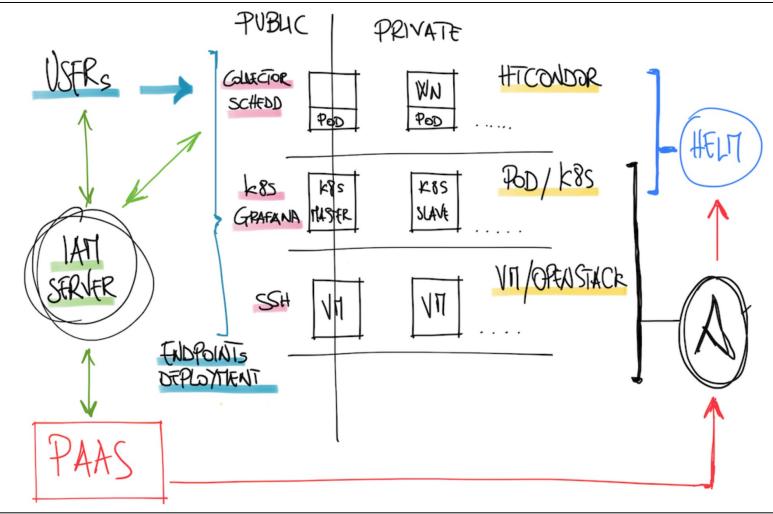
Description: Launch a compute node getting the IP and

Maintenance

## Examples of INFN Cloud services: on-demand HTCondor



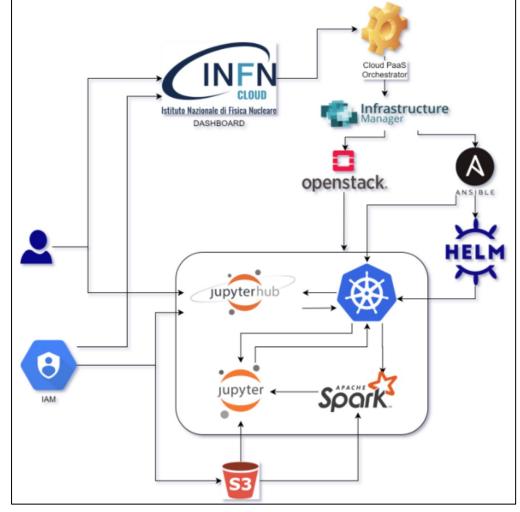
- This service instantiates a k8s cluster which is then used to automatically deploy an HTCondor cluster.
- HTCondor services are deployed using dedicated PODs.



## Examples of INFN Cloud services: on-demand Spark + Jupyter



- This service creates a Spark cluster ondemand, based on Kubernetes as resource manager and on JupyterHub for the user interface.
- The JupyterHub application, the Jupyter notebooks launched from it, the Spark driver and executors are all Docker containers orchestrated by a Kubernetes cluster deployed on a federated cloud (the box in the picture on the right). The components outside the box implement the workflow to instantiate the service.



## Examples of INFN Cloud services: managed services



- Several solutions are also provided by INFN Cloud as "centrally managed services". Among them:
- HARBOR Harbor as open-source registry
  - GitLab GitLab as DevOps platform
    - NextCloud as collaboration platform
    - Jupyter Notebook as a Service
    - Vault as identity-based secrets and encryption management system
      - CVMFS as software distribution service
  - wazuh. Wazuh as security monitoring platform
    - ... and others.

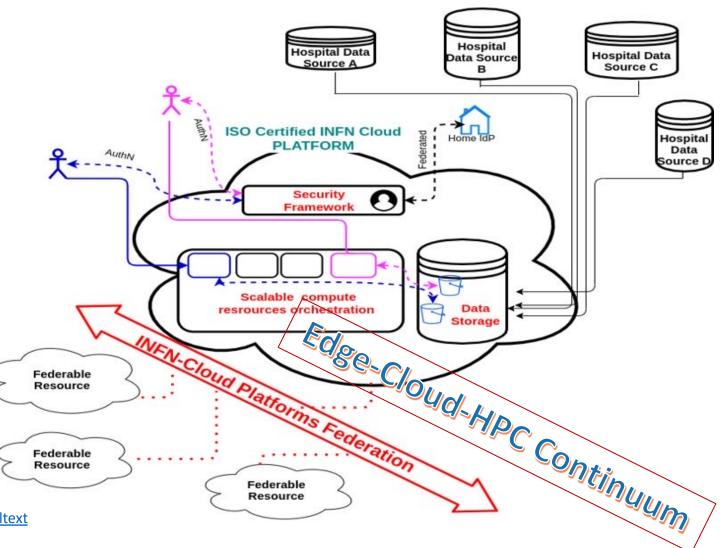
Jupyterhub

### The goal: a federated datalake

Multiple ways to ingest and process data are possible. For example, to handle sensitive data (e.g., in the nation-wide Health Big Data project), we are working on supporting these options:

- 1. Central harvesting of data generated remotely
- 2. Edge-level anonymization, followed by central ingestion and analysis of data
- **3. Edge-level feature extraction**, followed by central ingestion and analysis of features
- 4. Federated learning based on edgelevel training, followed by publishing of the trained methods and by inference performed either centrally or at other edge locations.

https://www.physicamedica.com/article/S1120-1797(21)00320-3/fulltext





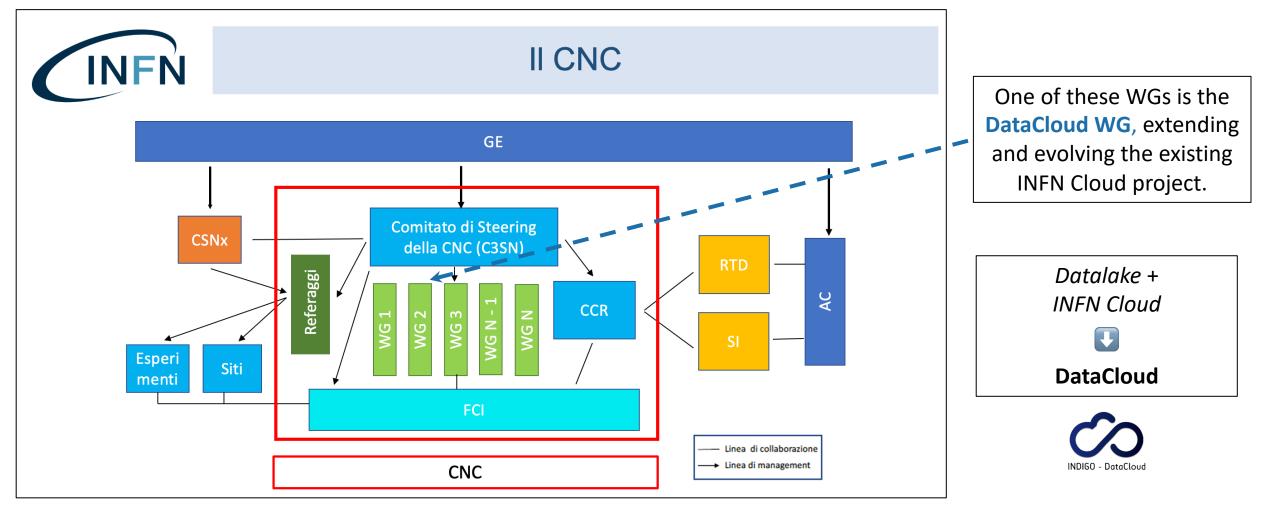
42



## Preparing for the future: the new INFN Computing Management Structure



## The New INFN Computing Structure





## The mandate of the DataCloud WG

- The DataCloud WG deals with several core activities related to computing @ INFN:
  - Development, implementation & management of the INFN Datalake architecture.
  - Development of ISO-Certified solutions. These have been seeing strong demand, thanks also to activities linked to the National Recovery and Resilience Plan (NRRP) and to various collaborations.
  - Support to users and to the management and operation of INFN Tier-x sites.
  - Development of new services.
- A key point of this WG is the **integration** between the traditional, WLCG-like Tier-x infrastructure and the "Cloud Native" model (currently represented by INFN Cloud).
  - Integration of what?  $\rightarrow$  Of resources, methods, people, solutions.

#### The DataCloud WG structure NFN Projects WG The DataCloud WG WP2: User & Project Support New Technologies WP3: Resources, WG **WP1: Operations** Data Lake, **Sustainability WP7: Integrated** Management System, Legal Compliance Other WGs WP4: Security, WP6: R&D, Testbeds, **Policies** Use cases WP5: Middleware, **New Services External Activities** (DOMA, WLCG AuthZ, etc.)



## Opportunities: The Bologna Technopole

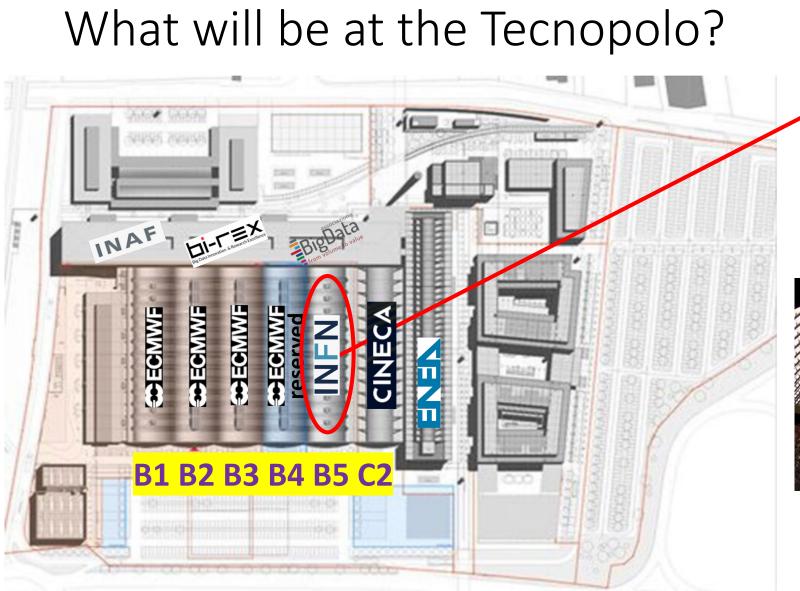
## The "Big Data Valley"

- In 2017, Bologna won a bid to host the "European Centre for Medium-Range Weather Forecasts" (ECMWF)
- The Emilia-Romagna region decided to repurpose the *"Manifattura Tabacchi \*"* area in Bologna to host a technology district, for ECMWF <u>and more</u>: the Tecnopolo

(\*a former tobacco factory)

How it will be







Each of the 6 "botti" (barrels) is ~5000m<sup>2</sup> of usable IT space



Same architect and design of the "Sala Nervi" in the Vatican



## The INFN + CINECA project

• ECMWF is up and running!





14 September 2021: new ECMWF data centre opens in Bologna, Italy

> See the "Datacenter Session" on 12/10 for more details





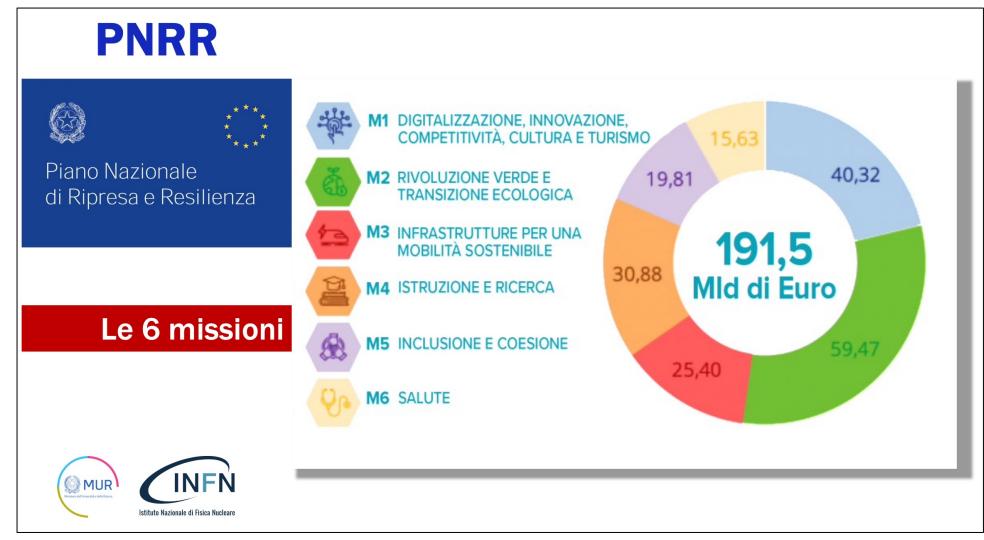
- The CINECA ("C2") and INFN ("B5") barrels are expected to be ready by:
  - ~October 2022 (CINECA)
  - ~mid 2023 (INFN)
- Two phases are expected:
  - Phase-1 (2023-2025): Leonardo + CNAF data center relocated. Total 13 MW.
  - Phase-2 (2025+): infrastructure up to 23 MW ready for post-exascale and for the next generation of scientific experiments.



## Opportunities: The Italian National Recovery and Resilience Plan (NRRP)

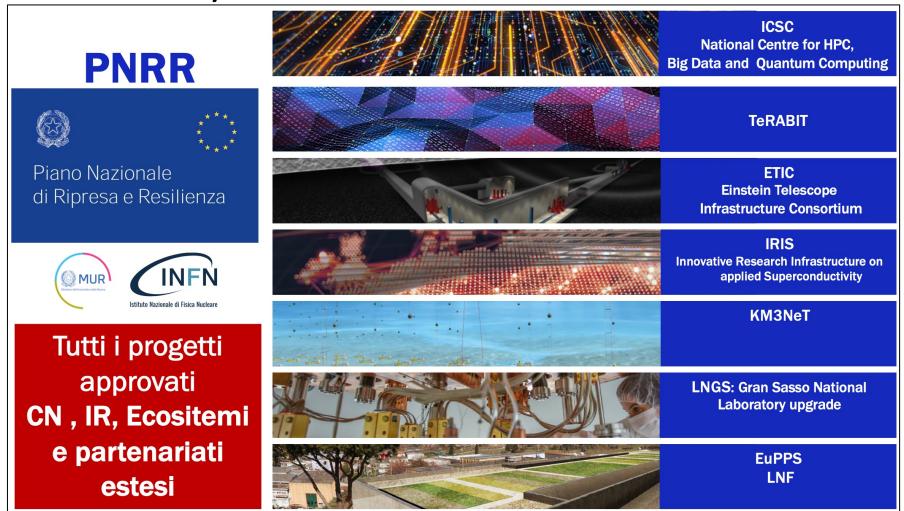


## The NRRP Budget



# Some NRRP projects already approved and led by INFN...











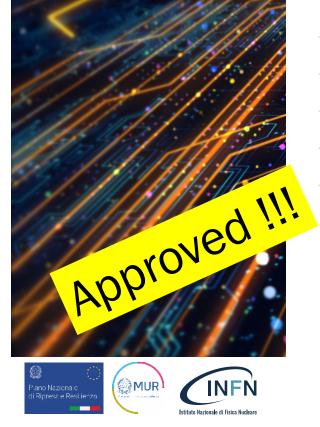
### **Centro Nazionale HPC, Big Data e Quantum Computing**





#### ICSC Centro Nazionale HPC,

Big Data e Quantum Computing



#### Cloud national infrastructure for supercomputing. Hub & Spoke organization: 10 vertical spokes for technology developments and software applications

**320 + 41 M€** Total Budget

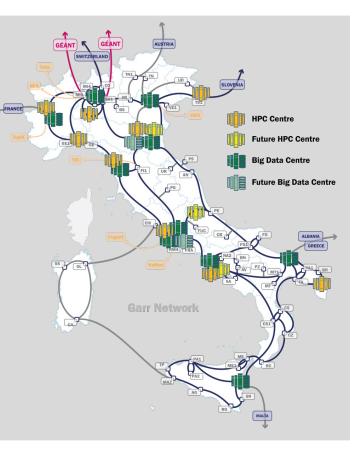
**139 M€** Cloud Infrastructure

32 M€ Open Call

32 M€ Innovation & TT

#### 42% investment South Regions

- 34 MUR Universities and Research institutions
- 15 Private Companies
- 1575 Researchers and engineers
- 250 New Temporary positions
- 250 New PhD
- 40 % Female



INFN

#### Public Research Institutions Founding Members: a pervasive initiative throughout Italy



RB

#### Solo HUB



UNIVERSITÀ DI PARMA



BITTOTO FRAMMO

#### Private companies Founding members: **strategic players for digital transformation**



Highly-qualified group of large leading companies covering most of the strategic industrial sectors involved by digital transformation in Italy

#### fondazione innovazione urbana

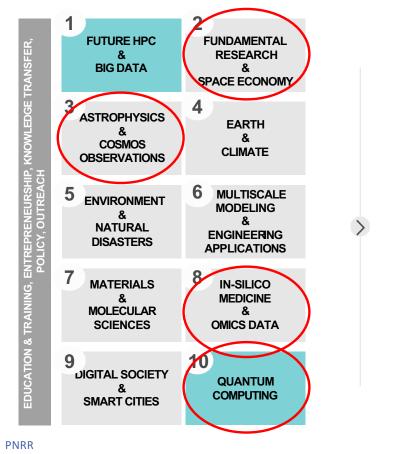
Strategic partner to implement and develop the digital twin pilot case of an urban complex system

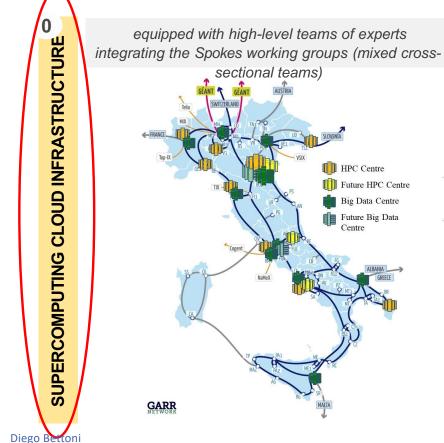
**IFAB** INTERNATIONAL FOUNDATION BIG DATA & ARTIFICIAL INTELLIGENCE FOR HUMAN DEVELOPMENTE

Industry-driven not-for-profit international organization aimed at: (1) aggregating companies, including SMEs, to engage with ICSC through a structured partnership, (2) funding research and innovation projects, (3) promoting the Big Data Technopole



## The ICSC will include ten **thematic Spokes** and one **Infrastructure spoke**

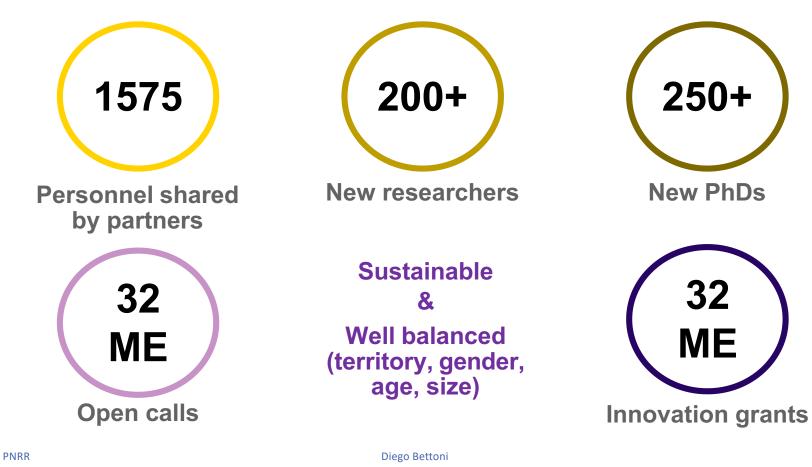




10



#### ICSC: Main figures over the next 3 years



11

### NRRP: TeRABIT



- Complementing ICSC, TeRABIT (Terabit network for Research and Academic Big data in ITaly) is a 41M€ NRRP approved project to create a distributed, hyper-networked, hybrid Cloud-HPC computing environment.
- This will be done by integrating and upgrading three leading digital Research Infrastructures: GARR-X, PRACE-Italy and HPC-BD-AI (the INFN computing infrastructure).
- Specifically, INFN targets TeRABIT to expand INFN Cloud for the creation of distributed "HPC Bubbles".
  - The aim is to realize a scalable open Edge-Cloud Continuum, integrating Al technologies. Through this architecture, we will be able to dynamically and efficiently ingest, process and re-process data at multiple locations ("keep computing close to data production whenever possible and sensible").



## Opportunities: Health-related Initiatives

### EPIC Cloud



Enhanced Privacy and Compliance Cloud – The INFN Cloud partition located at CNAF for personal and confidential data processing

- Motivation: the GDPR states that Clinical and medical data (in particular genomic) is personal data (it fits in the Art.9 special categories of personal data).
  - Genomic data is mostly impossible to be anonymized ightarrow GDPR shall always be applied
  - ISO/IEC 27001 is the main certification mechanism compliant with GDPR requirements (Art. 43, 58, 63)
- In order to comply with the requirements of health research projects INFN is involved in, we created **a region of the INFN Cloud infrastructure**, applied specific organizational and technical security measures, and certified it ISO/IEC 27001, 27017, 27018.
  - This is the **EPIC Cloud**: a reference Cloud implementation for the treatment of sensitive data at INFN.

See the presentation on EPIC on 11/10 for more details

From the Data Controller side, the fact that EPIC Cloud is ISO-certified is a way to demonstrate that processing is performed in accordance with the GDPR.

## ACC / Health Big Data

Alleanza Contro il Cancro

The National Oncology Network founded in 2002 by the Ministry of Health, joined by 51 IRCCS, ISS, AIFA, INFN and Politecnico di Milano and several patients' associations to perform translational research in the field of cancer research.

- Genomic pseudonymized data
- GDPR applies
- Italian Data Protection Authority rules apply



https://www.alleanzacontroilcancro.it/en/





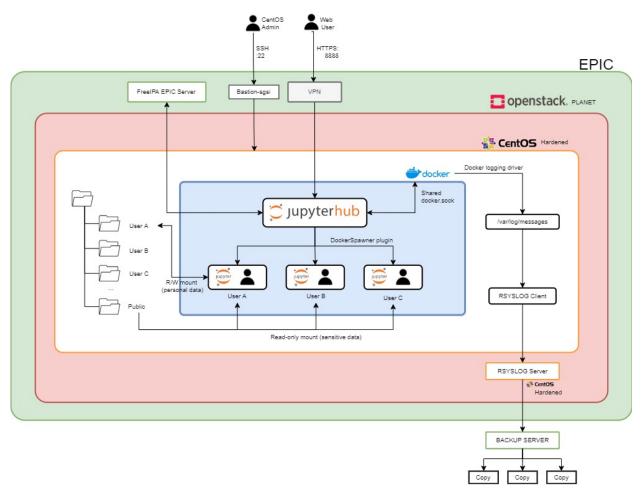


## PLANET

Pollution Lake Analysis for Effective Therapy

An INFN-funded research initiative, aiming to implement an observational study to assess a possible statistical association between environmental pollution and Covid-19 infections, symptoms and course.

- Data:
  - Pseudonymized clinical data (Covid-19 and Electronic Health Records from several hospitals)
  - Atmospheric data, population density, urban vs rural environment, mobility, socio-economic conditions
- Regulated by GDPR, Italian Data Protection Authority and by a convention between INFN and the Italian Istituto Superiore di Sanità.
- Container-based platform
- Data processing through a JupyterHub service
- 2FA for both analysis and infrastructure access



### **INFN-AIFM** collaboration



Physica Medica xxx (xxxx) 1-11



1 10 tor Ben

European Journal of Medical Physics

To support the development and largescale validation of Al-based tools for medical applications a joint effort has been conducted by the Medical Physics and High Energy Physics communities.

- Design of a dedicated computing infrastructure.
- The goal is to support the development and extensive validation of Al-based tools for precision medicine in the field of diagnostic and therapeutics.



#### Contents lists available at ScienceDirect Physica Medica journal homepage: www.elsevier.com/locate/ejmp

Invited commentary

Enhancing the impact of Artificial Intelligence in Medicine: A joint AIFM-INFN Italian initiative for a dedicated cloud-based computing infrastructure

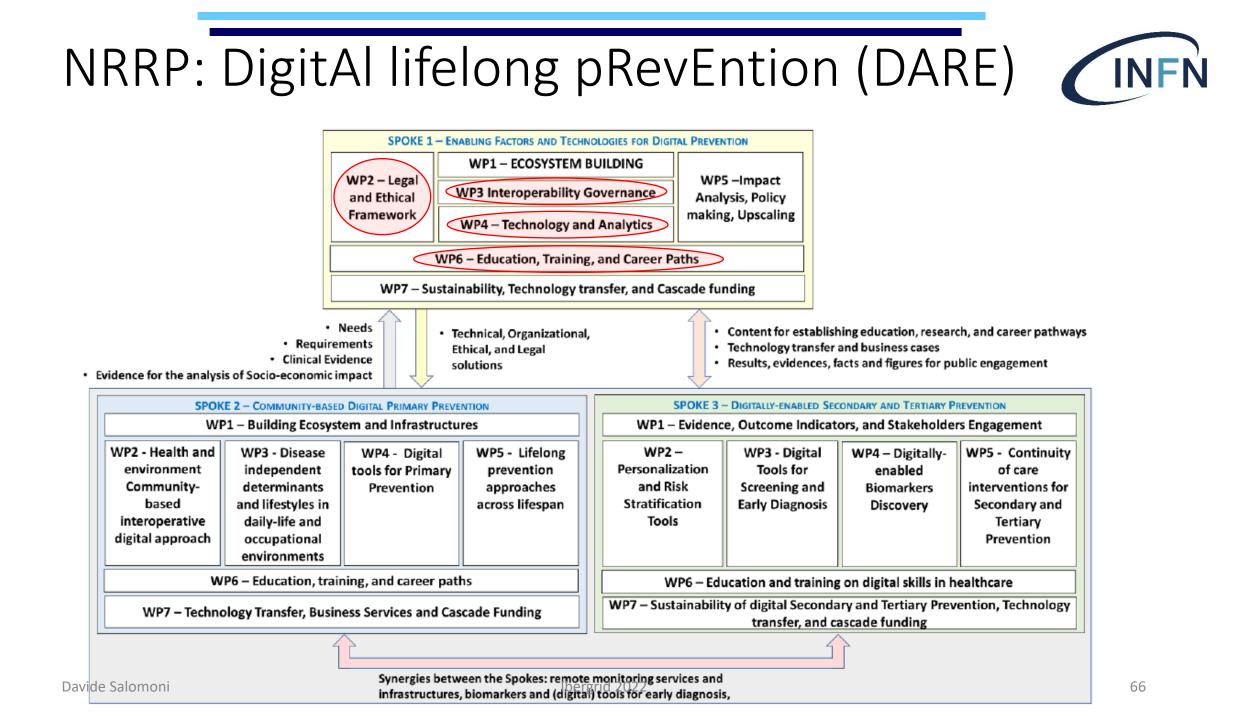
ARTICLE INFO

#### ABSTRACT

Keywords: Artificial intelligence Decision support systems

Computing infrastructure Distributed learning

Alessandra Retico<sup>a</sup>, Michele Avanzo<sup>b</sup>, Tommaso Boccali<sup>a</sup>, Daniele Bonacorsi<sup>c,d</sup>, Francesca Botta<sup>e</sup>, Giacomo Cuttone<sup>f</sup>, Barbara Martelli<sup>g</sup>, Davide Salomoni<sup>g</sup>, Daniele Spiga<sup>h</sup>, Annalisa Trianni<sup>i</sup>, Michele Stasi<sup>j</sup>, Mauro Iori<sup>k,\*</sup>, Cinzia Talamonti<sup>l,m</sup> Artificial Intelligence (AI) techniques have been implemented in the field of Medical Imaging for more than forty years. Medical Physicists, Clinicians and Computer Scientists have been collaborating since the beginning to realize software solutions to enhance the informative content of medical images, including AI-based support systems for image interpretation. Despite the recent massive progress in this field due to the current emphasis on Radiomics, Machine Learning and Deep Learning, there are still some barriers to overcome before these tools are fully integrated into the clinical workflows to finally enable a precision medicine approach to patients' care. Nowadays, as Medical Imaging has entered the Big Data era, innovative solutions to efficiently deal with huge amounts of data and to exploit large and distributed computing resources are urgently needed. In the framework of a collaboration agreement between the Italian Association of Medical Physicists (AIFM) and the National Institute for Nuclear Physics (INFN), we propose a model of an intensive computing infrastructure, especially suited for training AI models, equipped with secure storage systems, compliant with data protection regulation, which will accelerate the development and extensive validation of AI-based solutions in the Medical Imaging field of research. This solution can be developed and made operational by Physicists and Computer Scientists working on complementary fields of research in Physics, such as High Energy Physics and Medical Physics, who have all the





## Final considerations



## Some recurring keywords

- Integration between the "traditional" infrastructural and the "Cloud Native" models.
  - But integration of *what*? Of <u>resources</u>, <u>data sources</u>, <u>methods</u>, <u>people</u>, <u>solutions</u>.
- **Continuum** between edge, cloud and HPC, in the recognition that "one size (even if big, or *Exascale*) does not fit all".
- Simplification for what regards [secure] data access, use and reuse. No matter where the resources are, no matter what the vertical domain is.
- **Continuous learning, innovation and adaptation**, if we want to profit from opportunities such as those offered by NRRP funds and by the increasing number of scientific collaborations.

## Conclusions: the Background



1. INFN is **revisiting and expanding its computing infrastructure, management structure and expertise** to tackle the challenges expected in the next 10+ years in several scientific domains.

2. We have **identified many initiatives and projects** that, at multiple levels, are in line with the INFN mission to serve science. The Bologna Technopole and NRRP funds are precious opportunities here.



## Conclusions: the Foreground

- 3. Our overall technological approach is to try and **abstract from where resources are, leveraging** *aaS* models to build a scalable [trans-]National federated structure integrating know-how, people, hardware, solutions.
- 4. While doing so, INFN has the ambition to create and operate a vendor-neutral, open, scalable and flexible "data lake" that serves much more than just INFN users and experiments. This should be a key asset for fundamental, applied and industrial research in Italy and beyond.



### Conclusions: the Synthesis

5. However, all these tasks cannot easily be performed by a single country, let alone a single institution. We need to keep on working collaboratively, sharing know-how and ideas. Initiatives such as Ibergrid are instrumental in facilitating this (many thanks to the organizers!).

## Also at Ibergrid 2022

- Barbara Martelli, "EPIC Cloud: a secure, GDPRcompliant, open-source cloud platform for life-science applications" → 11/10, 13:30-14:00
- Session on INDIGO-DataCloud  $\rightarrow$  11/10, 13:30-15:30
- Davide Salomoni, "The INFN infrastructure at the Bologna Technopole" → 12/10, 11:18-11:27
- For more information on these slides: <u>davide@infn.it</u>.





