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Fundamental Research and Space Economy: the Italian strategy in the new "High-Performance Computing, Big Data e Quantum Computing Research Centre"

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In the context of the Italian National Recovery and Resilience Plan (NRRP), the High-Performance Computing, Big Data e Quantum Computing Research Centre, created and managed by the ICSC Foundation, has been recently established as one of the five Italian "National Centres" to address designated strategic sectors for the development of the country, including simulations, computing, and high-performance data analysis, agritech, development of gene therapy and drugs via RNA technology, sustainable mobility, biodiversity. The focus of this specific National Supercomputing Centre is on maintenance and upgrade of the Italian HPC and Big Data infrastructure, as well as on the development of advanced methods and numerical applications and software tools to integrate computing, simulation, collection, and analysis of data of interest for research, manufacturing, and society, also through cloud and distributed approaches. In particular, in a hub-spoke set-up, the so-called "Spoke 2" is devoted to research at the frontiers of theoretical and experimental physics, mainly on experimental particle physics research, conducted with or without accelerating machines, as well as detectors studying gravitational waves, and more. The talk will present the organization and activity status of this spoke and elaborate on its scientific and technological contributions to the overall innovation ecosystem.

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1. Introduction

The landscape of modern scientific research, particularly in domains like High Energy Physics (HEP) and Astroparticle Physics, is increasingly reliant on computational power. The advent of next-generation experiments, capable of generating data at the exabyte scale, necessitates a paradigm shift towards collaborative and shared infrastructure models. In alignment with this imperative, Italy has recently invested considerable financial resources from the National Recovery and Resilience Plan (NRRP) to finance five large national research centers, for a total investment of about EUR 1.6 billions over 3-year research programs. One of these centres, called "High-Performance Computing, Big Data e Quantum Computing National Centre" (referred to as "National Centre" in the following), with a funding of about EUR 320 millions, is managed by the ICSC Foundation [1]. It focuses on modern IT technologies, and conducts R&D, nationally and internationally, for innovation in high-performance computing, simulations, and big data analytics. This aim is pursued through a state-of-the-art infrastructure for high-performance computing and big data management, which leverages existing resources and integrates emerging technologies. This ambitious project aims at deploying a long-term, sustainable, distributed research infrastructure acting as innovation accelerator for scientific research endeavours and industrial ecosystems in Italy. The launch of the National Centre was in September 2022. Among the multifaceted initiatives undertaken by the Centre, this paper specifically delves into the activities of one thematic area (called "Spoke 2", as explained in the next sections).

2. Organization of the National Centre

The National Centre activities are organized on the Hub and Spoke model: while a Hub focuses on management and coordination, the Centre has 11 Spokes on different areas of intervention and covering different domains and applications. In particular, Spoke 0 (with core activities centered in the Big Data Technopole in Bologna, Italy - see Fig. 1) is dedicated to the implementation, optimization and enhancement of the overall national infrastructure (both hardware and middleware), while the other 10 Spokes focus on specific research areas. An overall geo-localised view of the resources is displayed in Fig. 2 and the 11 Spokes are shown in brief in Fig. 3. Some details of each is provided in the following, with a deeper discussion on Spoke 2 activities from Section 3 onwards.

2.1 Spoke 0: "Supercomputing cloud infrastructure"

Spoke 0 oversees the coordination and execution of initiatives geared towards establishing a competitive federated infrastructure for High-Performance Computing (HPC) and Big Data. This entails bolstering the GARR-T [2] network to furnish dedicated connectivity for research and educational pursuits at speeds surpassing multi-terabit per second. The focus lies on enhancing computing facilities with a key emphasis on energy efficiency, expanding HPC and Big Data capabilities, and deploying open-source middleware to facilitate seamless access to distributed resources. Strategic planning has been attuned to addressing disparities in underserved areas to bridge the digital divide. Spoke 0's undertakings align with analogous endeavors both within Italy and across Europe. In the realm of HPC and Quantum Computing (QC), resources are co-funded

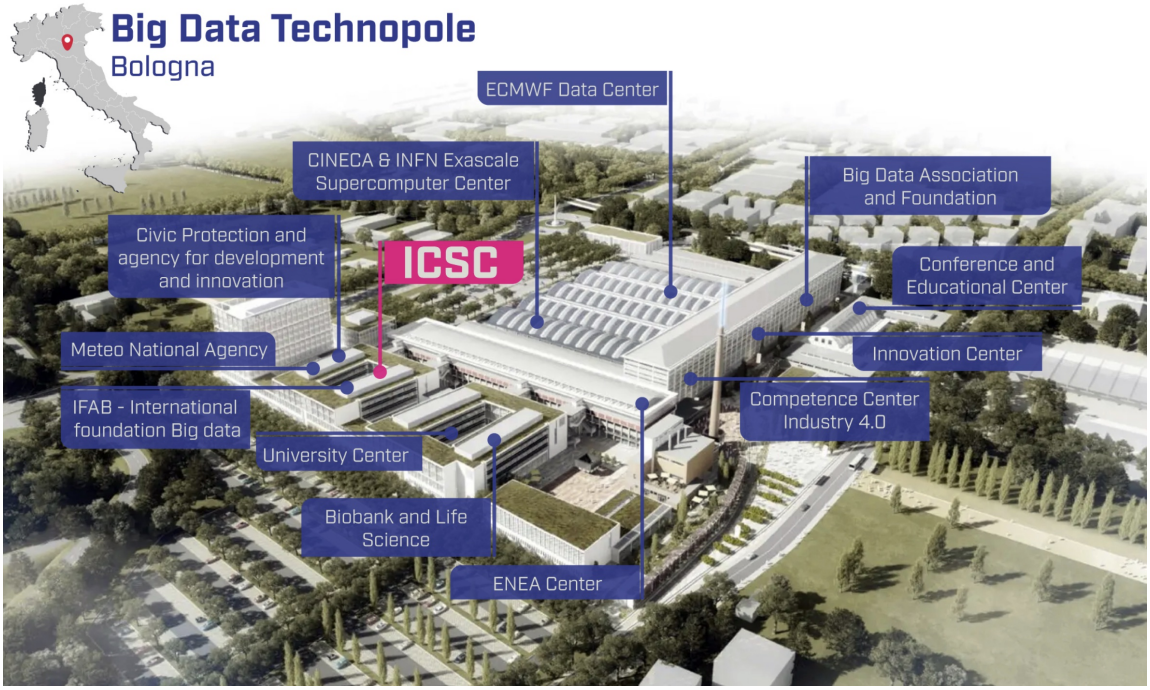

Figure 1: The Big Data Technopole in Bologna, Italy [1].

by the European initiative EuroHPC Joint Undertaking [3]. Activities associated with distributed computing management are integrated within the European Open Science Cloud (EOSC) framework [4]. The network forms part of the wider European GEANT network. Notably, the TeRABIT project [5], backed by the aforementioned NRRP on Research Infrastructures, aims to fortify the digital infrastructure of GARR [6], CINECA [7], and INFN [8] in synergy with Spoke 0. Under the stewardship of GARR, upgrades and enhancements are underway for the national research network, synergistically advancing terabit-scale connectivity across the nation. Incorporating new technologies affords users greater flexibility in managing connections, thereby enhancing their efficacy. Computing centers are being revamped, augmenting infrastructure capacity and energy efficiency, as well as bolstering computing power and data storage capabilities. CINECA plans to boost the Leonardo supercomputer's capacity by 30% and integrate it with a quantum computer. Similarly, INFN aims to enhance the computing capacity of its distributed system, making it accessible to diverse scientific domains. Furthermore, a national cloud federation is in development to streamline resource access for Italian and European researchers. Collaboratively developed services adhere to international standards established by entities such as EuroHPC, EOSC, and GAIA-X [9].

The Spoke also offers services and consultancy to empower researchers in optimizing the utilization of acquired resources and developing their skills. A specialized support team is being established to disseminate knowledge and enhance proficiency in distributed and high-performance computing, thus optimizing resource utilization.

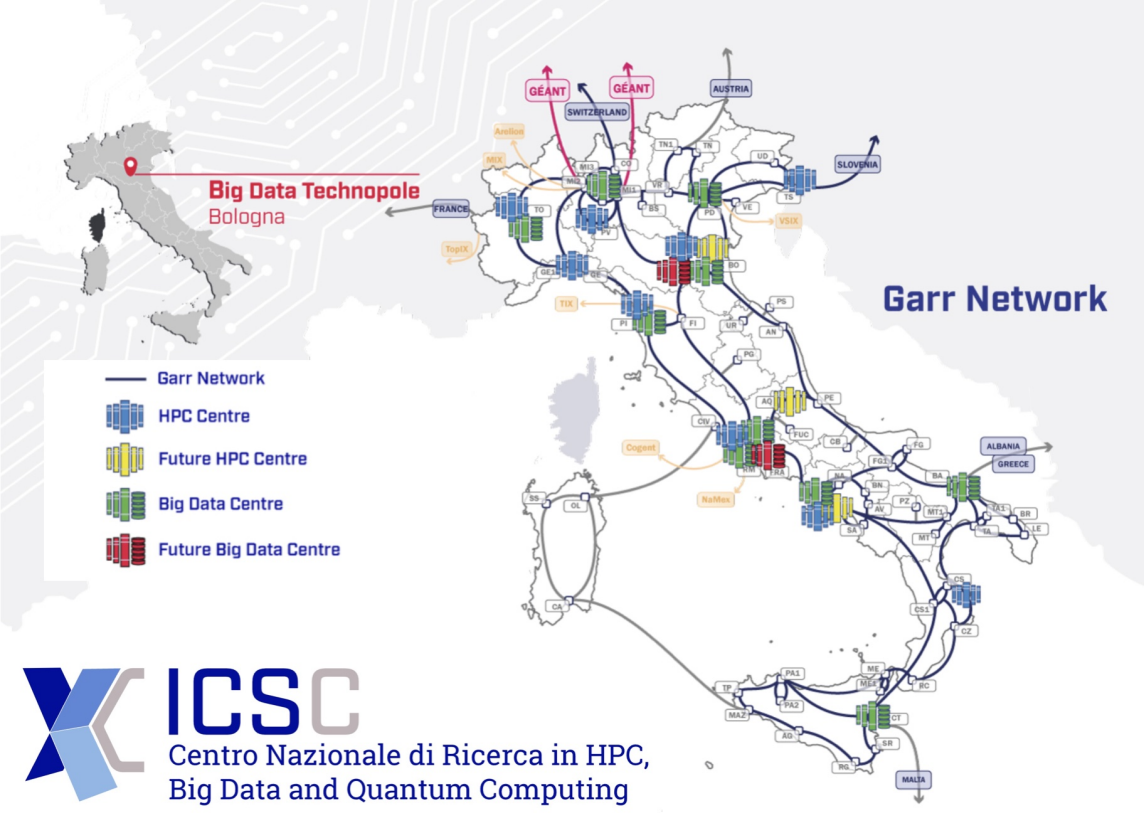

Figure 2: Infographics of the GARR map of ICSC resources [1].

2.2 Spoke 1: "Future HPC and Big Data"

Spoke 1 is structured around five scientific-technological "flagship projects", which serve as the operational hubs of research and involve collaboration from 15 universities (and research institutions) and 9 major industries. Additionally, 2 "living labs", i.e. physical facilities situated within leading universities (namely, University of Bologna and Torino).

The flagship projects are designed to enable research centers to combine their expertise and research outputs, fostering integration and cross-pollination, while also responding to the needs and requests of industrial partners. The living labs serve as repositories for scientific contributions from all flagships, with the goal of prototyping and demonstrating the most promising technologies, facilitating technology transfer, and ensuring the sustainability of Spoke 1's activities beyond the funding period supported by the NRRP. Furthermore, the living labs aspire to establish a nationally federated center with globally recognized expertise in hardware and software co-design. This aims to bolster Italy's leadership in the EuroHPC Joint Undertaking[3] and in the data infrastructure ecosystem for both scientific and industrial domains. In addition, open "cascade funding" calls are offered, which provide support to local SMEs, also contributing to these objectives, assisting Spoke 1 in fostering a robust HPC supply chain.

Among the activities, research areas cover: HPC developments; cloud computing and applications for Big Data Artificial Intelligence (AI); development of prototypes of innovative computing systems; analysis of system performances with a particular focus on energy efficiency;

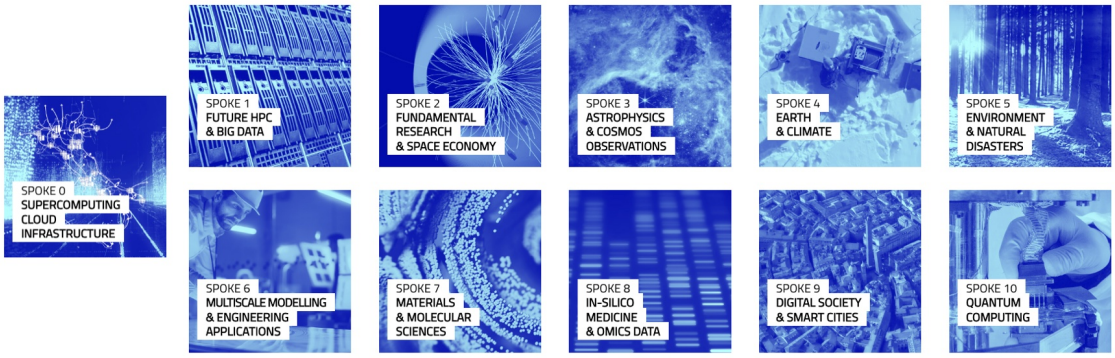

Figure 3: Spokes of the National Centre (see text for explanations) [1].

non-functional properties (such as energy, power, reliability, and performance portability); heterogeneous accelerations, encompassing architecture, tools, and software; workflows and I/O, cloud-HPC convergence and digital twins; confidential computing, trusted execution environment and federated learning; mini-applications and benchmarking.

Methodologically, FutureHPC advocates for open licenses (open hardware, open-source software, open standards) as catalysts for innovation. This model has already demonstrated substantial competitive advantages in terms of product quality and the sustainability of industrial business models. For example, the design of hardware, driven by the increasing popularity of the RISC-V instruction set, is progressively embracing an open approach for both instruction set specification and possible implementations.

2.3 Spoke 2: "Fundamental Research and Space Economy"

Spoke 2, as a special focus in this contribution, will be discussed from Section onwards.

2.4 Spoke 3: "Astrophysics and Cosmos Observations"

The primary objectives of Spoke 3 revolve around harnessing state-of-the-art solutions in HPC and Big Data processing and analysis to address challenges in: cosmology; stars and galaxies; space physics (Earth, solar and planetary); radio astronomy; observational astrophysics and time domain; high-energy astrophysics; cosmic microwave background; large-scale structure, clusters, and galaxies; multi-messenger astrophysics; numerical simulations and modeling. By also embarking on comprehensive outreach and training initiatives, Spoke 3 aims to cultivate a diverse and proficient talent pool within Italy, ultimately fostering the widespread utilization of high-performance and high-throughput cloud solutions across research institutions, academia, and private enterprises. Leveraging the opportunities presented by the NRRP, engagement with private stakeholders affiliated with the ICSC Foundation, who have shown interest in the project's activities, are prioritized.

All initiatives adopt a user-driven approach, ensuring close alignment with the community's needs. Furthermore, a co-design methodology will be employed for the development of selected applications. This entails integrating the requirements and expertise of scientists and community code developers with innovative software and hardware solutions envisioned by HPC and cloud

stakeholders. This collaborative effort also encompasses green computing approaches, promoting the synergistic and coordinated advancement of applications and technology.

The activities are structured into Working Packages (WPs), as follows. WP1 is working on HPC codes enabling and optimization, focusing on redesigning, re-implementing, and optimizing codes to effectively utilize state-of-the-art HPC solutions, including accelerators and alternative architectures such as GPUs and ARM architectures. WP2 focuses on design of innovative algorithms, methodologies, codes toward exascale and beyond, identifying new innovative (and upgrading old) algorithms and methodologies to exploit and scale up to exascale and post-exascale architectures, and integrating these enhancements into codes, workflows, and pipelines. WP3 focuses on big data analysis, machine learning, and visualization applies advanced artificial intelligence and visualization solutions to large astrophysical data volumes, facilitating the convergence of HPC, High Throughput Computing (HTC), High-Performance Data Analytics (HPDA), and cloud tools on exascale platforms. WP4 focuses on big data management, storage, and archiving, and develops innovative frameworks to manage data and software with FAIR (Findable, Accessible, Interoperable, and Reusable) and Open Science principles. WP5 focuses on HPC services and access, by overseeing the management, maintenance, and deployment of an integrated environment, as well as providing tools for efficient development across all WPs, including the management and distribution of large datasets in a Data Lake national infrastructure, and facilitating high-rate analyses.

Additionally, WP0 provides managerial resources for the project, and all these WPs operate synergistically with one another and with private stakeholders affiliated with Spoke 3.

2.5 Spoke 4: "Earth & Climate"

Spoke 4 endeavors to establish an interdisciplinary network that integrates cutting-edge Earth system modeling components, providing the scientific community and users with versatile, dependable, and robust toolkits. The Spoke aims to construct a digital infrastructure seamlessly integrated into the national HPC and cloud architecture provided by the National Centre, with the objective of achieving several key goals: fostering the development and dissemination of Earth System Model (ESM) components (such as atmospheric, oceanic, sea ice, surface, vegetation, critical area, and human activity interaction models); managing and producing numerical simulations; creating an environment conducive to the digital infrastructure's evolution into a national resource accessible to the entire Italian research and educational community, as well as those engaged in climate forecasting and climate change initiatives. Ultimately, the infrastructure aims to position Italy as a frontrunner in cutting-edge climate research, while also advancing technologies aligned with the climate objectives outlined in the NRRP for digital and green transitions.

2.6 Spoke 5: "Environmental & Natural Disasters"

The advent of new state-of-the-art sensor technologies applicable across extensive geographical areas (Internet of Things, IoT) and the capacity to collect and analyze big data offer innovative avenues to address the complexities associated with scientific and social challenges globally, e.g. the depletion of the environment, the escalation of natural disasters and their correlation with climate change.

Spoke 5 collaborates closely with key industrial partners and endeavors to devise methodologies for monitoring both human-made physical structures (such as buildings and roads) and natural

environments (including waterways and slopes) to mitigate risks linked to their degradation. Leveraging the formidable computational capabilities of the National Centre, Spoke 5 aims to develop digital-twins virtual models of environments and infrastructures—to forecast their behavior concerning natural disasters or changes in environmental conditions. Spoke 5 assembles a diverse team of highly multidisciplinary researchers, spanning expertise from fundamental research in mathematics and physics to specialties in advanced computing, as well as research in earth sciences, civil engineering, and geo-environmental engineering. Ultimately, Spoke 5 is dedicated to translating research findings into tangible indicators of economic impact, proposing environmental monitoring solutions that benefit society at large.

2.7 Spoke 6: "Multiscale Modelling and Engineering Applications"

Spoke 6 delves into the exceptional capabilities offered by exascale computing and cutting-edge industrial-grade computing clusters to address multiscale challenges in science and technology of unprecedented complexity and magnitude. Leveraging HPC tools, ML and AI across various scientific and engineering domains will enable the development of digital twins and model-based design methodologies. This convergence of new methodologies and computing architectures is poised to foster innovation, enhance efficiency, and bolster safety across numerous critical engineering sectors, thus advancing the digital transition towards a cleaner and more sustainable future.

The primary objective of Spoke 6 is to sustain innovation across different Technology Readiness Levels (TRLs) in key engineering fields. These fields hold significant social, industrial, and economic implications for Italy, encompassing sustainability, life sciences, digital technologies for Industry 4.0, new materials, complex systems, and more.

Spoke 6 has 7 "flagship projects", and through the National Centre it is possible to support proof-of-concept demonstrators, addressing industrial challenges from core companies within the Italian industrial ecosystem, such as ThalesAlenia Space, Leonardo, Terna, Fincantieri, Autostrade per l'Italia, Ferrovie dello Stato, ENI, and Engineering. SMEs and associations are also engaged through the IFAB foundation.

2.8 Spoke 7: "Materials and Molecular Sciences"

Historically, human civilization has progressed through the discovery of new materials and the exploration of novel applications for already known ones. However, the energy, environmental, and climate crises present new imperatives, signaling a shift in paradigm: being no longer sufficient to rely solely on the discovery and extraction of natural materials, the focus shifts now on designing artificial materials with tailored properties suited for specific applications and devising innovative processes to manufacture them. This transformation is propelled by the digital revolution, with computers capable of processing vast amounts of data per second, enabling the solution of fundamental equations governing material properties under realistic usage conditions. Among others, AI stands as a key tool to predict the intricate behavior of materials.

Spokes endeavors to strengthen Italy's leadership in developing, implementing, and disseminating high-performance scientific software for simulations of complex materials and molecular systems. It aims to optimize and expand the application spectrum of these software systems to address scientific, technological, and social challenges. Additionally, Spoke 7 facilitates access to

extensive computational resources for both public and private entities, enabling the application of new materials to emerging technologies.

2.9 Spoke 8: "In-Silico Medicine & Omics Data"

Spoke 8 primarily focuses on medical research, leveraging supercomputing for In-Silico Medicine and the analysis of vast datasets generated by omic sciences experiments (such as genomics, lipidomics, transcriptomics, etc). Specifically, Spoke 8 aims to pioneer new clinical trial methodologies through simulation techniques, with the objective of streamlining the time and cost associated with traditional clinical trials. Additionally, it seeks to develop a technological platform capable of analyzing big data using AI and ML algorithms. These endeavors are poised to deepen our understanding of numerous diseases, enhance diagnosis and prognosis capabilities, and facilitate drug discovery and the development of personalized medicine treatments. Through collaboration among various stakeholders, experimental practices in biomedical laboratories will be accelerated, leading to a reduction in animal testing. Moreover, the integration of precision and personalized medicine techniques into the healthcare sector will directly benefit patients in tangible ways.

2.10 Spoke 9: "Digital Society & Smart Cities"

Spoke 9 is geared towards relevant application domains within smart cities and digital societies. The Spoke channels its efforts into the 5 application domains. On "Health and Lifestyle", the Spoke leverages HPC and IoT technologies for e-Health, implementing digital twins for smart hospital and personal health record management, and deploying big data platforms for advanced territorial medicine management, among other initiatives. On "Mobility" the Spoke models citizen mobility patterns and large-scale crowding dynamics. On "Socio-economic analysis", the Spoke develops models for human behavior, learning, and adaptation, analyzing economic flows, devising novel approaches to identify and track disinformation and hate speech on social media, and monitoring urban crime, among other endeavors. On "Infrastructure and services", the Spoke focuses on avancing smart grid technologies, including innovative applications such as drone-based maintenance, optimizing radio coverage planning for wireless networks, conducting real-time monitoring, and performing risk analysis and forecasting for interconnected infrastructure. On "Environment", the Spoke monitors and forecasts environmental conditions, promoting biodiversity regeneration and managing urban ecosystems, and enhancing water cycle management, among other environmental initiatives.

2.11 Spoke 10: "Quantum Computing"

From a technological perspective, quantum computing holds immense promise in terms of speed and data management. Quantum computers have the capability to tackle complex problems that classical computers would struggle to solve within a reasonable timeframe — a phenomenon known as "quantum supremacy." However, despite the considerable anticipation surrounding potential applications and the emergence of new business models, achieving full technological maturity remains a distant goal. Overcoming challenges related to component reliability and the intricate nature of planning—issues that must be addressed to enable the practical utilization of quantum computers—is paramount. This forms the primary objective of Spoke 10, which will pursue 3 major lines of investigation: *i)* creating applications that leverage quantum computers as accelerators

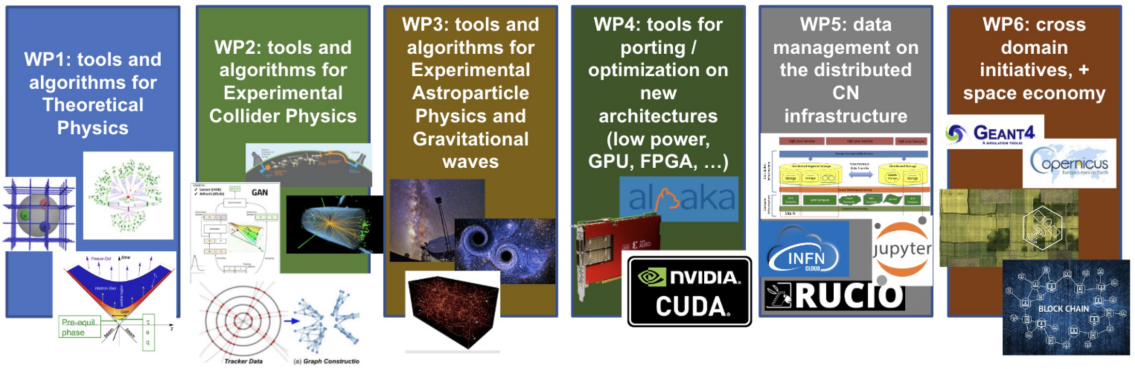

Figure 4: WP structure of Spoke 2 in the National Centre (see text for explanations) [1].

to solve otherwise intractable problems; *ii)* developing hardware and software tools to facilitate the planning of quantum computers and ensure their operational compatibility with traditional computing systems; *iii)* planning the development of large-scale and scalable quantum computers.

3. The focus on fundamental research in Spoke 2

In the realm of science, particularly in fundamental research, the demand for computing capabilities steadily escalates alongside the emergence of new generations of experiments, pushing the boundaries of knowledge ever further. Whether in theoretical or experimental physics, endeavors involving elementary particles, whether facilitated by particle accelerators or conducted with detectors probing gravitational waves, yield vast quantities of data. Despite varying timeframes, these realms of fundamental research encounter common challenges related to the scalability and efficiency, including energy efficiency, of computing infrastructure. Spoke 2 endeavors to address this imperative by devising and testing solutions tailored to both current and forthcoming experiments. This entails facilitating access to computing resources managed either by the National Centre or other entities. Furthermore, Spoke 2 endeavors to promote the dissemination of knowledge and technologies derived from basic research to industrial sectors, fostering the development of applications of national significance in the economic and industrial domains. In this context, synergies will emerge with the burgeoning Space Economy, with direct ties to data from Mirror Copernicus, a national program supporting operational services under the Space Economy strategic plan. This initiative aligns with the European Copernicus Earth observation program, dedicated to monitoring the planet and its environment.

The advancement of algorithms and computing solutions will be shared across various scientific and production domains within the National Centre, contributing to broader and more interdisciplinary scientific advancement. The outcomes will be readily accessible to the Italian ecosystem through dissemination and technological transfer initiatives.

In Spoke 2, two classes of WPs are defined: "scientific" WPs (WP 1,2,3) - which analyze the needs of each (sub-)domain, and pose open problems for which advanced computing solutions are seeked - and "technological" WPs (WP 4,5,6) - which harvest / investigate technical solutions in

computing, on the National Centre infrastructure and beyond, to provide ad-hoc support / training, while at the same time proposing these to a larger audience, including interested industries.

The plan of work is outlined in the following. All the project activities iplement a standard 4-phases plan over the 3-year period of NRRP funding. The first phase is the *planning and identification phase*: the first year of the project has been dedicated to a landscape recognition for interesting state-of-the-art use case. The outcome is a work plan identifying the activities on which the core part of the project would be focusing - in particular, algorithms and services to be accomplished. The second phase is the *realization phase*, in which the actual development is performed via the staff/hired personnel; the outcome is usable algorithms/services, documented (alpha/beta level) and ready to be tested on a larger scale. The third phase is the *validation phase*, in which the outcomes of the realization phase are verified in testbeds and proofs of concept, and benchmarked in order to assess their adherence to the specifications. The fourth phase is the *wrap-up phase*,in which results are analysed and consolidated in reports and white papers to be used as guidelines for similar use cases.

Among the technologies in place within the Spoke 2 activities, on the software side machine learning is looked at as a potential substitute for hand-written algorithms. Massive initiatives are active on porting of codes to GPU systems (with heterogeneous frameworks), FPGA systems (with HLS or direct programming), low power architectures (ARM today, possibly RISC-V in the near future). Scientific codebases are being adapted towards distributed computing paradigms (e.g. to be "data-lake compatible") and ability to seamlessly exploit generic data management tactics, scalable data access solutions, containerization, exploitation of single node to multinode (MPI, etc), and more. Additionally, on the hardware side instead, Spoke 2 is working to deploy generally accessible pilots with FPGA, deploy generally accessible pilots with ARM and RISC-V, deploys clusters accessible via cloud technologies, all managed via a central data management system.

Spoke 2, within each of the existing WPs, has identified a set of (about 20) "flagshipt projects", each aiming at demonstrating a technology and/or a new approach in a scientific domain. The major ones are outlined in the following:

- WP1: "Multilevel Hybrid Monte Carlo for lattice QCD", "QCD under extreme conditions", "Advanced Calculus for Precision Physics", "Large Scale Simulations of Complex Systems"

- WP2: "Advanced ML - Flash Simulation and bleeding edge applications", "Porting Algorithms on GPU", "Ultra-fast algorithms running on FPGAs", "Validation of HEP reconstruction code on ARM", "Quasi interactive analysis of big data with high throughput"

- WP3: "Frequency Hough (FH) Transform analysis on Gravitational Waves (GW) continuous sources", "Efficient use of ML and GPUs in cosmological data analysis: from theory to likelihood to statistical inference", "Inference of cosmological and astrophysical population properties from GW observations with and without electromagnetic counterparts", "Development of innovative analysis techniques using realistic simulations of the upgraded Auger Observatory within the context of a ML environment", "Detection and classification of SSO in Euclid Simulated data", "Pipeline optimization for space and ground based experiments", "Hydrodynamical simulations to test the nature of dark matter".

- WP4 and WP5 do not have specific flagships, but participate to most of the other flagships, with themes like GPU /FPGA utilization, low power computing with ARM, high rate analysis solutions on the data lake; ML at large scale; fast simulations via generative networks.
- WP6: "Enhancing Geant4 Monte Carlo Simulations through ML Integration", "Fast Extended Computer Vision", "AI algorithms for (satellite) imaging reconstruction"

4. Spoke 2: from Research to Industry

The interest of industrial partners in the Spoke 2 activities lies in the technological side, as Spoke 2 researchers can share the platforms, the solutions and the expertise. The Spoke has additionally funded more than EUR 2 millions on "Innovation Funds", i.e. projects to be conducted in partnership between Spoke 2 and large enterprises, and about EUR 3.2 millions on "Cascade Calls", i.e. projects between research groups and SMEs. Some examples of Innovations Funds are shown below, listing the name(s) of the companiy(ies) involved, and the title of the running project(s):

- ENI: "Testing HEP workflows on a industrial data center", "Predictive maintenance on ENI industrial plants", "Physics-inspired ML for the exploitation of natural resources"
- Leonardo, TASI: "Interoperable Datalake: Data management + Block Chain pilot for data from space economy"
- Unipol: "Merging data and Al for improving Seismic Risk assessment and Management in populated areas"
- UnipolSAI, SOGEI: "Monitoring of alert and hurban vulnerability for fast response and assurance evaluation"
- Intesa Sanpaolo: "Correlations between satellite images and budget in agricoltural enterprises", "Fraud detection as anomaly search on financial streams"
- IFAB, SECO, Coldiretti, and more: "Digital Twins for Precision Agricolture"
- IFAB, Bonfiglioli, Tampieri, SECO, and more: "Edge AI Anomalv Detection System for Critical Environments"

5. Conclusions

The National Center for HPC, Big Data and Quantum Computing is a unique opportunity for research in Italy, in building a modern, shared and sustainable infrastructure for research, expanding to the involvment of industrial partners. In particular, the initiatives in Spoke 2 are aligned with the most crucial scientific and technical needs of the High Energy Physics and Astroparticle Physics community. The efforts include training initiatives to form the next generation of scientists in Italy, versed in modern technologies, to grow a strong and skilled community able to contribute to complex scientific and societal challenges.

6. Acknowledgements

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