Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca
Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

Computational Theoretical Physics @ICSC

Leonardo Cosmai (INFN - Sezione di Bari)
Michele Pepe (INFN - Sezione di Milano Bicocca)

INFN

ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

Workshop sul Calcolo nell'INFN, Palau, 20 maggio 2024

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50 YEARS OF QUANTUM CHROMO DYNAMICS

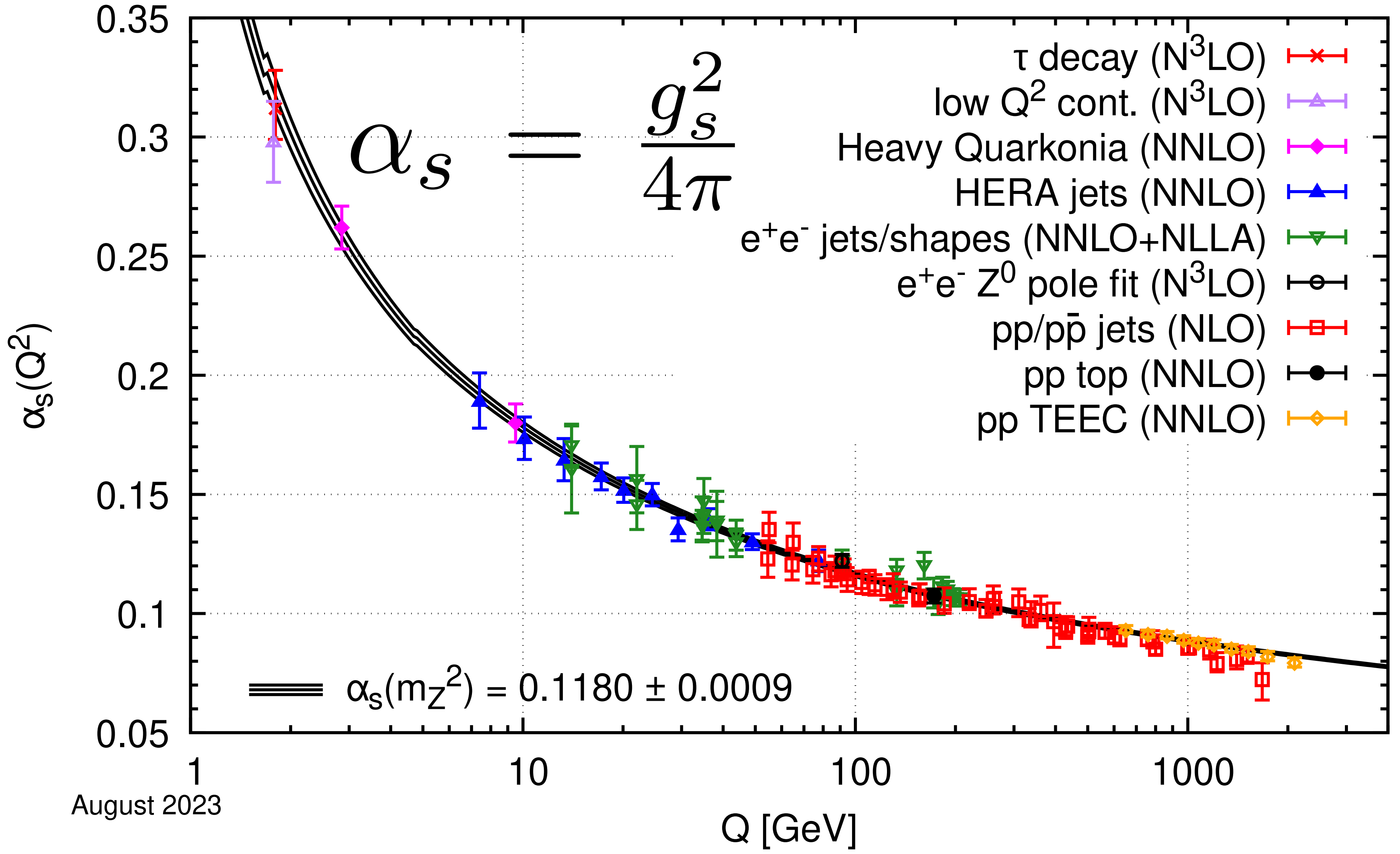
~ 1973

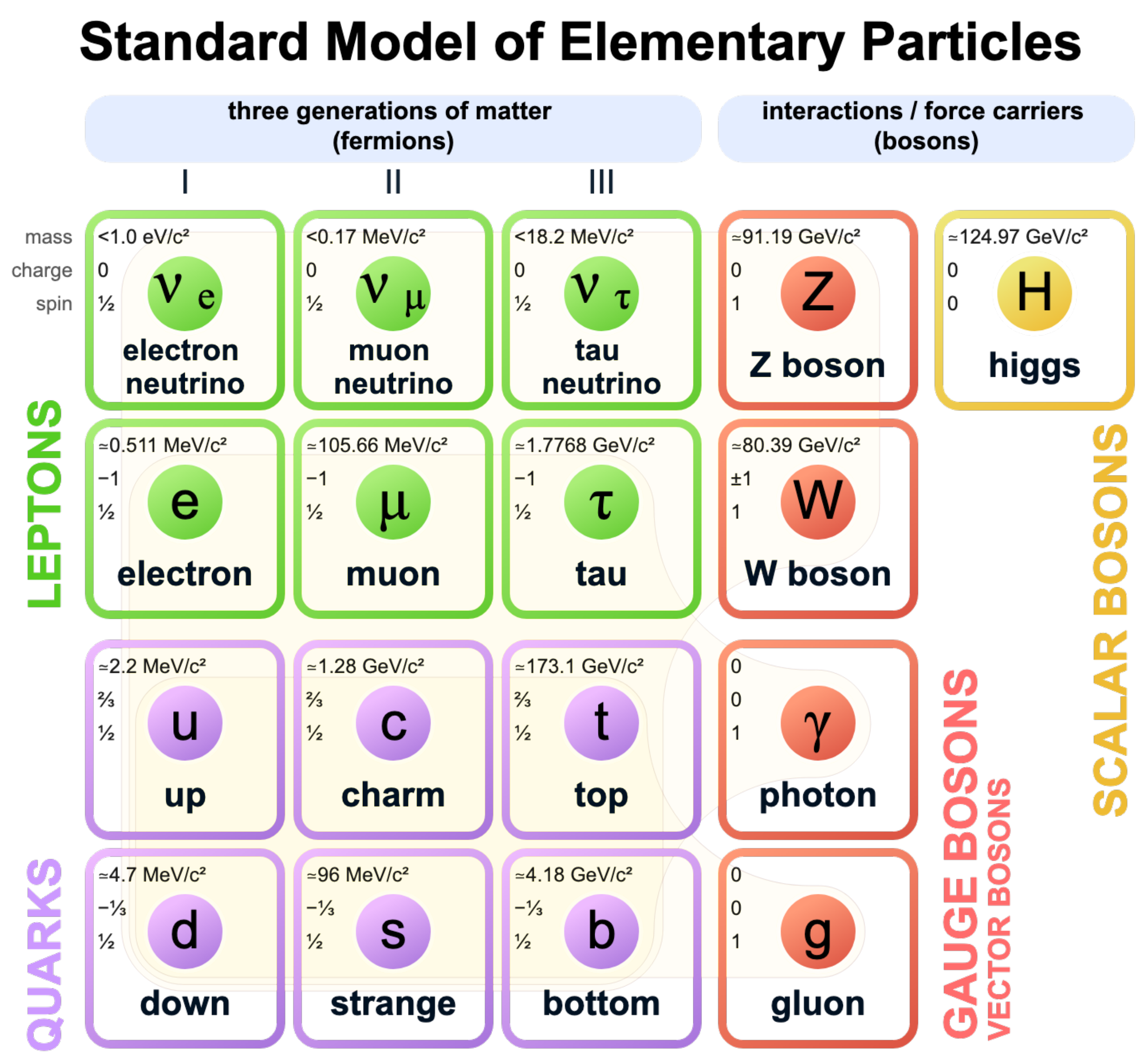
QCD

$$\mathcal{L} = \sum_q \bar{\psi}_{q,a}(i\gamma^\mu \partial_\mu \delta_{ab} - g_s \gamma^\mu t^C_{ab} \mathcal{A}^C_\mu - m_q \delta_{ab})\psi_{q,b} - \frac{1}{4} F^A_{\mu\nu} F^{A\,\mu\nu}$$

- *"A Tool Supporting Experimental Exploration"*
- *"A Tool for Astrophysics and Nuclear Technology"*
- *"A pointer to New Realities"*

(Frank Wilczek, arXiv:2403.06038v1)



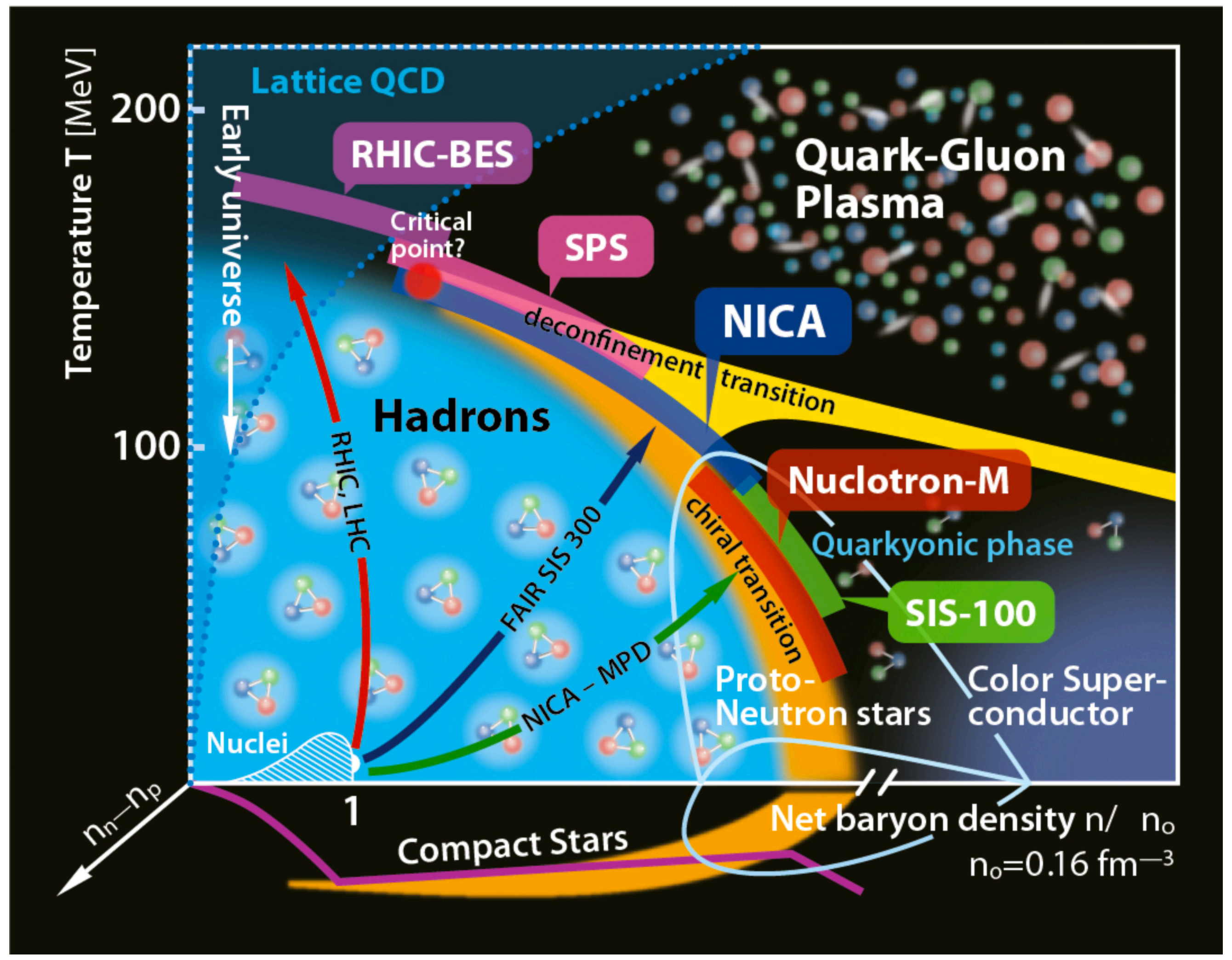


Theoretical calculations of the hadronic bound states properties require non-perturbative methods.

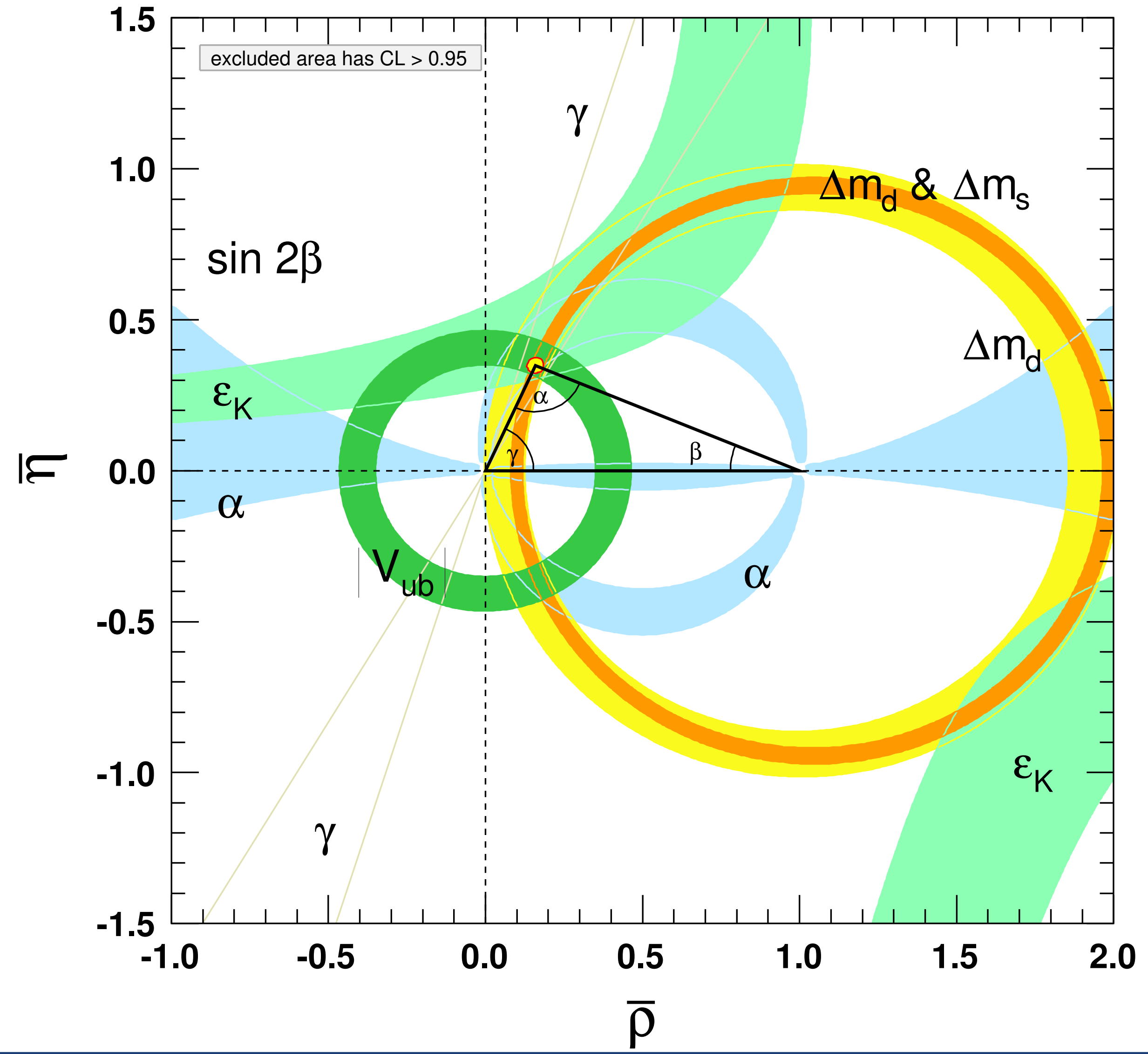
Lattice Quantum Chromodynamics (LQCD) is a tool to carry out such calculations.

Computational Challenges: *towards EXASCALE*

Study of QCD in extreme conditions



Precision studies of flavor physics, within and beyond the Standard Model



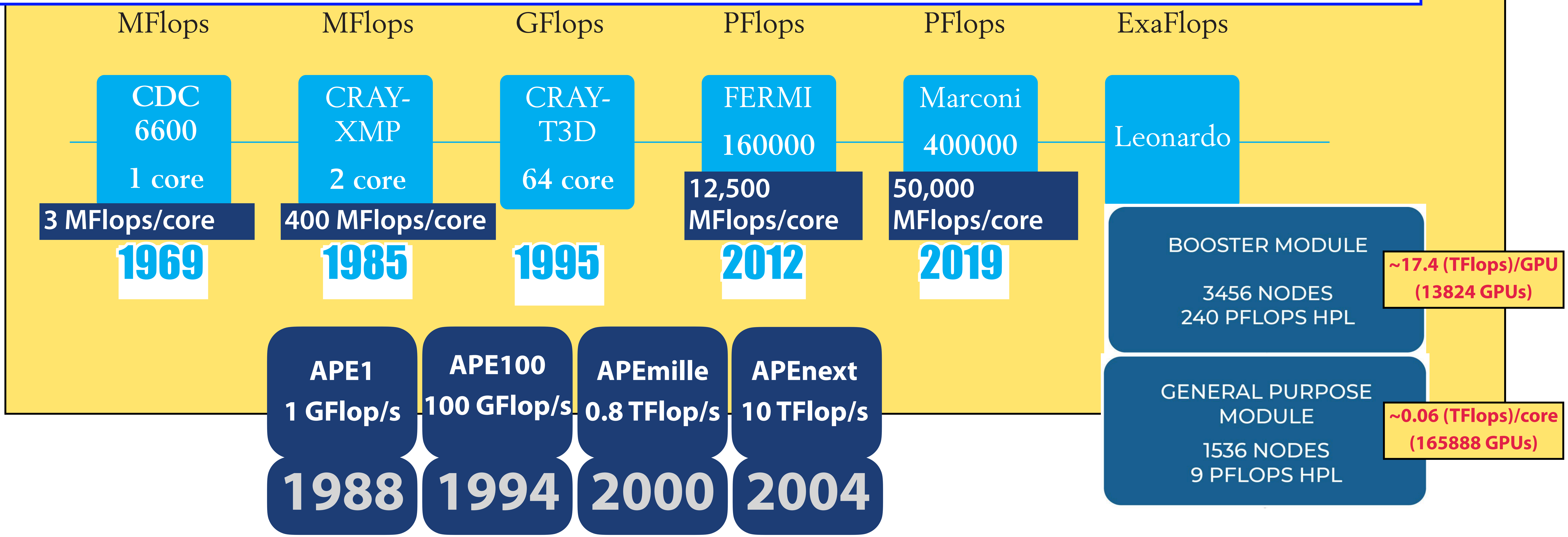
Lattice QCD

- Lattice QCD is an essential tool for obtaining precise first-principle theoretical predictions of the hadronic processes underlying many key experimental searches.
- As experimental measurements become more precise, lattice QCD will play an increasingly important role in providing the necessary matching theoretical precision.
- Achieving the needed precision requires simulations on lattices with significantly increased resolution.

A large number of computing nodes is required (up to $\mathcal{O}(10^5)$ cores. On the largest scales the challenge lies in efficiently and effectively exchanging data among the processors or nodes —> MPI, MPI+OpenMP.

The **development of numerical algorithms** is crucial: over the history of lattice gauge theory calculations, the improvement from algorithm development has been similar to the gain from Moore's law.

Example: timeline of the computing power (Cineca and INFN)



Not only brute force…

Developing computational strategies requires combining physical insight with an understanding of modern numerical mathematics and the capabilities of massively parallel computers.

Cineca-INFN agreement 2024

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Projects in Computational Theoretical Physics

Lattice QCD
- *LQCD123*
- *NPQCD*
- *QCDLAT*
- *SFT*
- *SIM*
- *GAGRA*

Cosmology and Astroparticle Physics
- *TEONGRAV* (*)
- *INDARK*
- *NEUMATT*

(*) talk B. Giacomazzo

Physics of Complex Systems
- *BIOPHYS*
- *FIELDTURB*
- *ENESMA*
- *LINCOLN*

Nuclear Physics
- *MONSTRE*
- *NUCSYS*

Condensed Matter
- *NEMESYS*

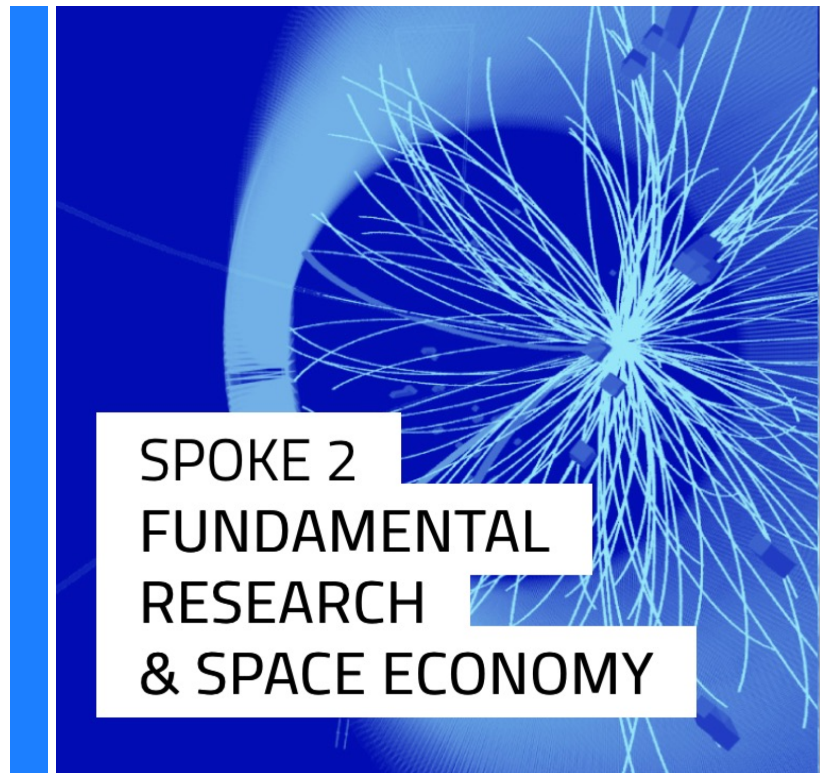
Particle Physics Phenomenology
- *QFTATCOL*
- *PML4HEP*

Quantum Information
- *QUANTUM*

Projects in Experimental Physics

- *ANNA*
- *BRAINSTAIN*
- *MIRO*
- *QUBIC*
- *EUCLID*
- *LHC*
- *LITEBIRD*
- *LSPE*
- *VIRGO*

ICSC —> SPOKE2 - WP1 (Theoretical Physics)



SPOKE 2 - FUNDAMENTAL RESEARCH & SPACE ECONOMY *(*)*

Lo Spoke 2 intende sviluppare e testare nuove soluzioni per rispondere alle sempre crescenti esigenze di calcolo delle nuove generazioni di esperimenti per la ricerca di base e favorire la condivisione delle conoscenze e delle tecnologie sviluppate in ricerca di base con i settori produttivi.

(*) talk T. Boccali

Use cases

- UC2.1.1 "Multilevel Hybrid Monte Carlo for Lattice QCD"
- UC2.1.2 "QCD under extreme conditions"
- UC2.1.3 "Advanced Calculus for Precision Physics (ACPP)"
- UC2.1.4 "Large Scale Simulations of Complex Systems"

- WP1: tools and algorithms for Th. Physics
- WP2: tools and algorithms for Collider Physics
- WP1: tools and algorithms for AstroParticle Physics
- WP4: Boosting the computational peformance
- WP5: Distributed Datalake
- WP6: Cross Domain Initiatives

UC2.1.1 Multilevel Hybrid Monte Carlo for lattice QCD

Development, test and validation of a fully optimized parallel code for simulating QCD with a multi-level Hybrid Monte Carlo (HMC), obtaining a dramatic improvement of the signal to noise ratio even in the case of full QCD, with the aim to compute many correlation functions with an unprecedented precision.
The code will implement an MPI+openMP parallelization so as to run efficiently up to approximately 100,000 cores or more simultaneously (the real limit being the resources the ICSC will be able to provide).

UC2.1.2 QCD under extreme conditions

The main purpose of the present use case is to extend that strategy to compute the Equation of State of QCD. To accomplish this task, we need to define the numerical techniques and prepare an efficient parallel code that can be run on large HPC systems. Since the numerical simulations are computationally very demanding, the code has to run efficiently and scale up to 5,000-10,000 cores.

UC2.1.3 Advanced Calculus for Precision Physics (ACPP)

The Advanced Calculus for Precision Physics (ACPP) use case aims at supporting the phenomenology analyses for prospects of detection and observations of new physics events or weaker signals that require an enhancement of sensitivity within advanced collider physics programs (CERN, Fermilab, etc.), as well as within current and future gravitational waves (GW) detectors (LIGO-VIRGO-KAGRA, ET, LISA, etc.) in the next three decades.

- Developing software and tools for the efficient, automatic evaluation of multi-loop scattering amplitudes, making use of advanced analytic and numerical methods;
- Exploring new computational architectures to improve the events generation, the evaluation of hadronic cross sections, and the data fits for collider phenomenology;
- Developing codes for describing hadronic production and decay of new particles, as well as to include new physics effects in the study of Higgs boson and top-quark phenomenology;
- Developing softwares that combines new methods and advanced computing techniques of particle physics and cosmology.

UC2.1.4 Large Scale Simulations of Complex Systems

Development, test, and validation of an optimized parallel Lattice Boltzmann (LB) solver specifically designed for simulating 3D multiphase active droplets.
Generalization of the LB algorithm to handle three spatial dimensions, enabling to us accurately capture the complex dynamics of the active droplets.
To ensure computational efficiency and handle large-scale simulations, we will leverage the MPI standard and implement domain decomposition techniques.

Computing resources for development and test of the codes —> ICSC RAC

Computing facilities 2024

LEONARDO-booster

3456 nodes   240 Pflops HPL

1 x CPU Intel Xeon 8358 32 cores, 2,6 GHz
512 (8 x 64) GB RAM DDR4 3200 MHz
4 X Nvidia custom Ampere GPU 64GB HBM2
2 x NVidia HDR 2×100 Gb/s cards

LEONARDO-GP

1536 nodes   9 Pflops HPL

2x Intel Sapphire Rapids, 56 cores, 4.8 GHz
512 (16 x 32) GB RAM DDR5 4800 MHz
3xNvidia HDR cards 1x100Gb/s cards
8 TB NVM

LISA-GPU (> 100 PFlops HPL)

LISA-CPU (> 6 PFlops HPL)

GALILEO100

528 computing nodes each 2 x CPU Intel CascadeLake 8260, 48 cores/node
Peak Performance: ~2 PFlop/s

MARCONI-A3

Nodes: 2982
Processors: 2 x 24-cores Intel Xeon 8160 (SkyLake) at 2.10 GHz
Cores: 48 cores/node
RAM: 196 GB/node
Peak Performance: ~8 PFlop/s

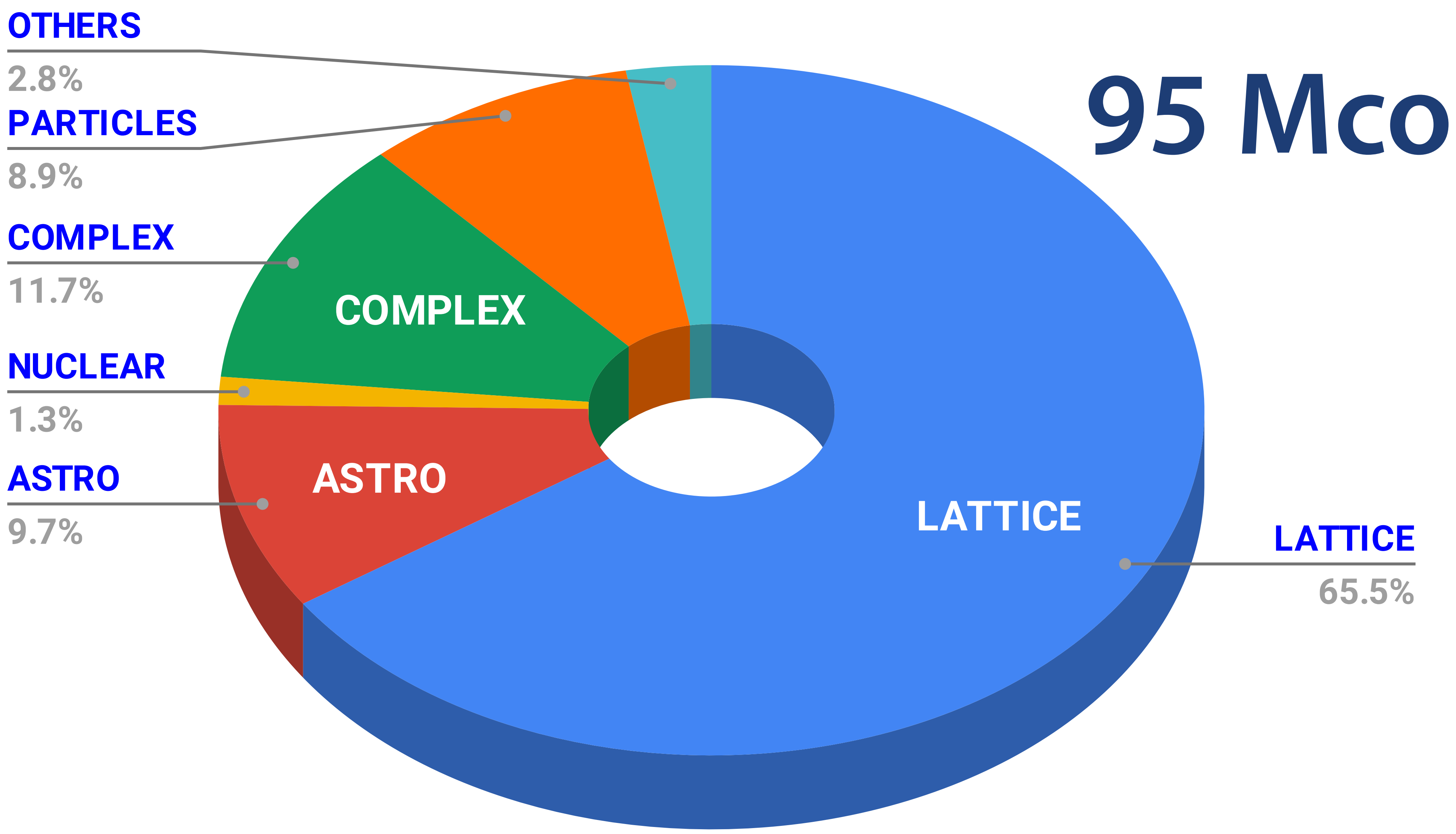
HPC bubbles

HPC systems in a selected number of sites, equipped with CPUs, GPUs (Nvidia H100), FPGA, fast storage, Infiniband
~10 M€ investment in TeRABIT

Resource allocation 2024 (TH)

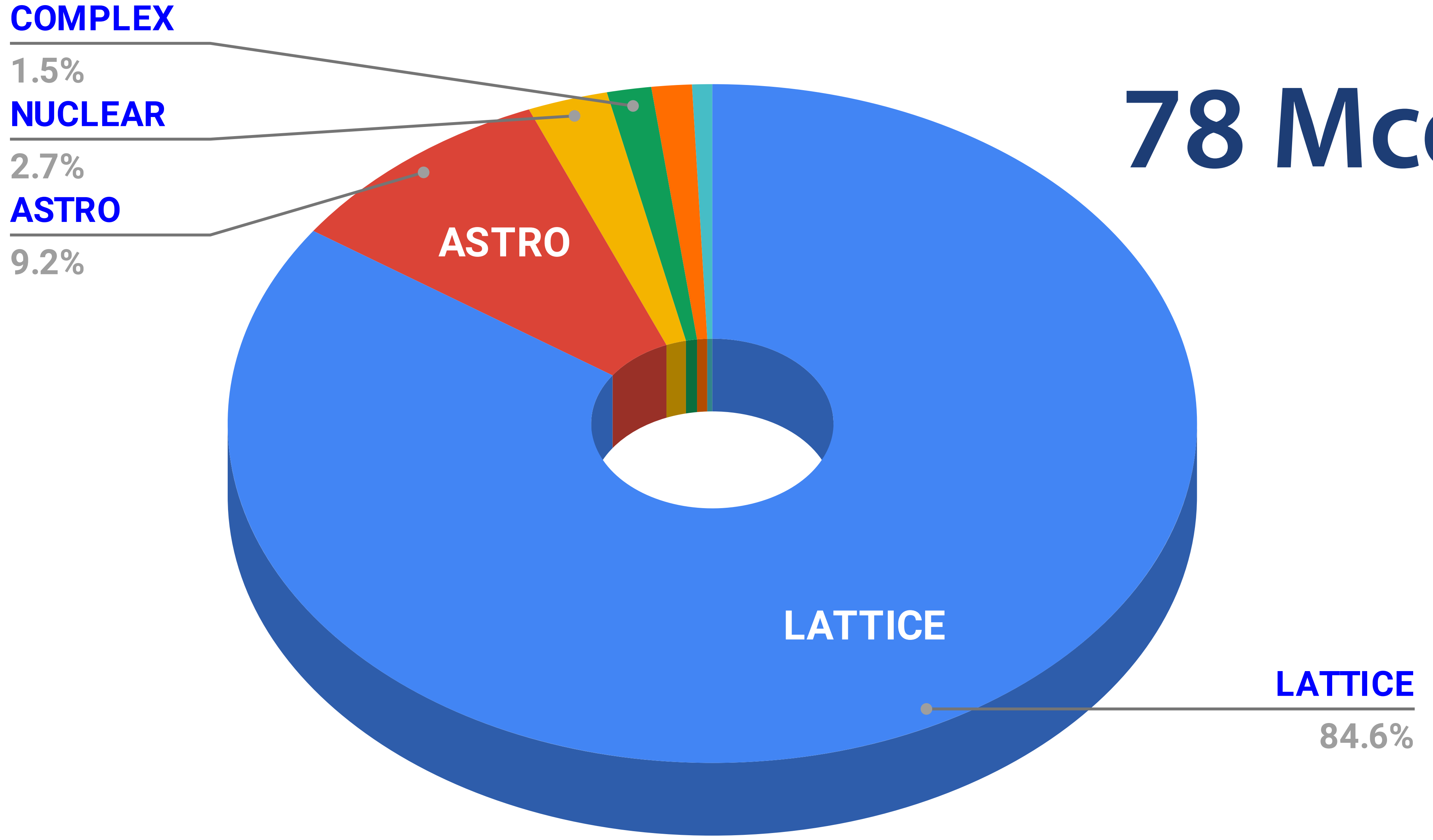
LEONARDO-booster

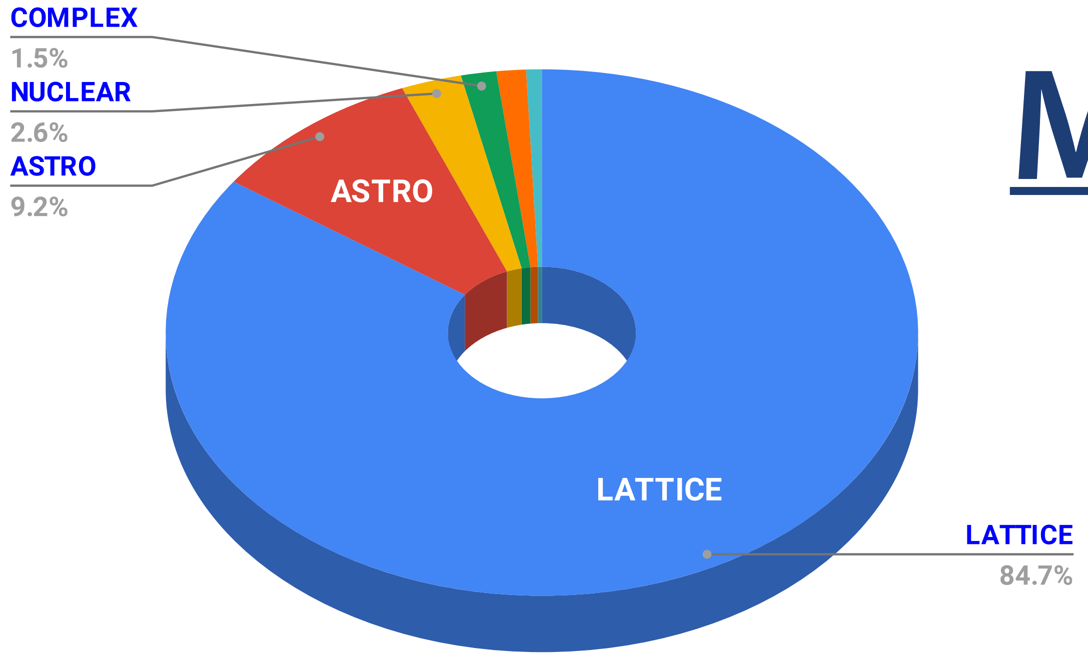
95 Mcoreh



LEONARDO-GP

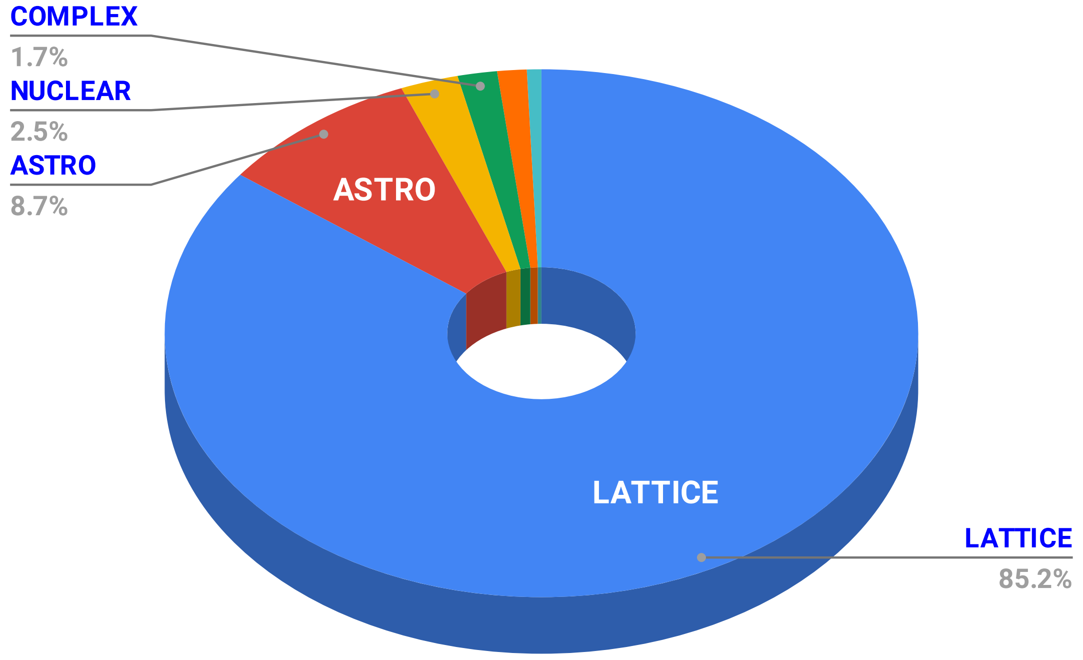
78 Mcoreh





MARCONI-A3

14 Mcoreh



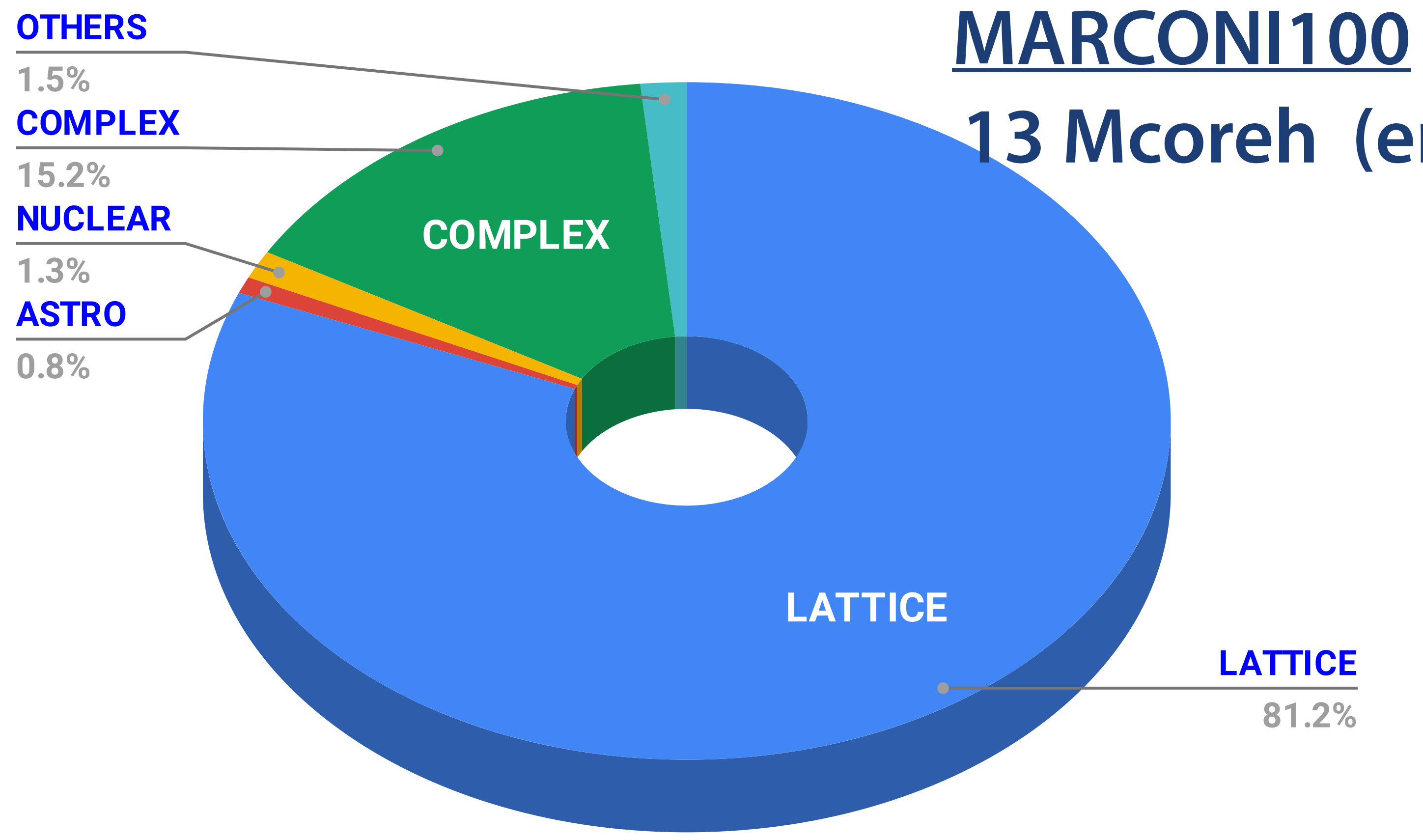
GALILEO100

5.6 Mcoreh

Computing Resource Use in 2023

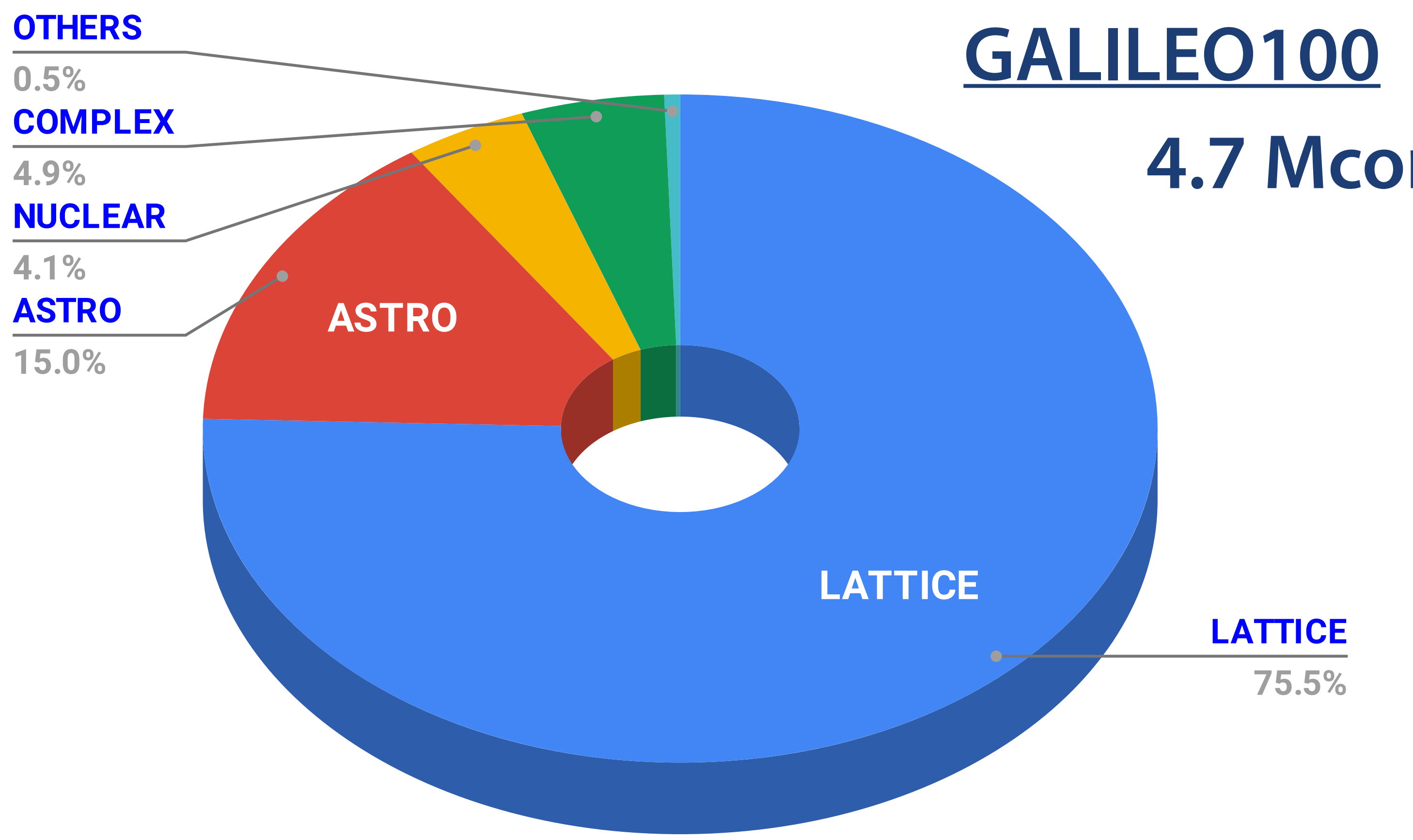
MARCONI100

13 Mcoreh (end June 2023)



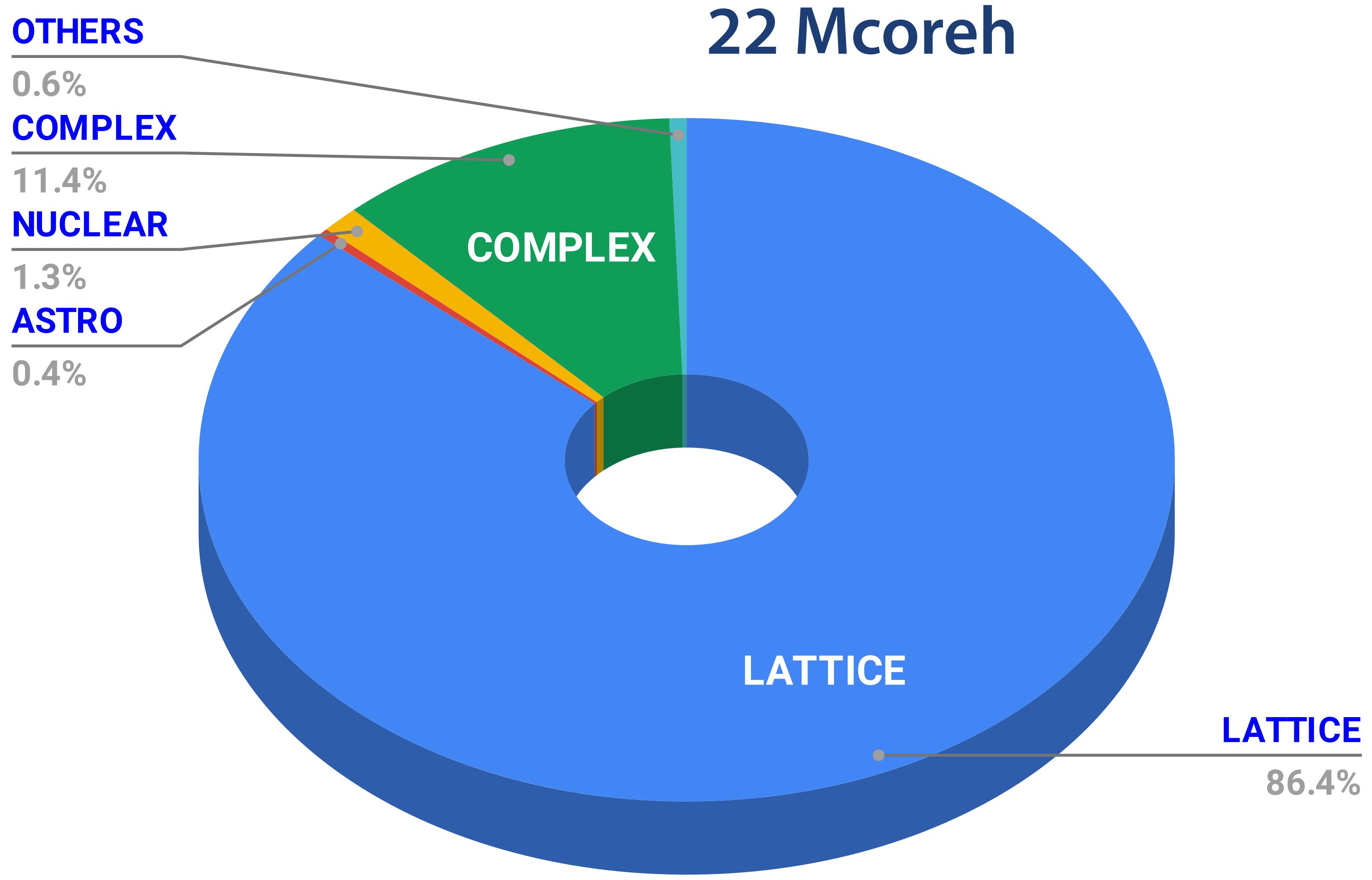
GALILEO100

4.7 Mcoreh



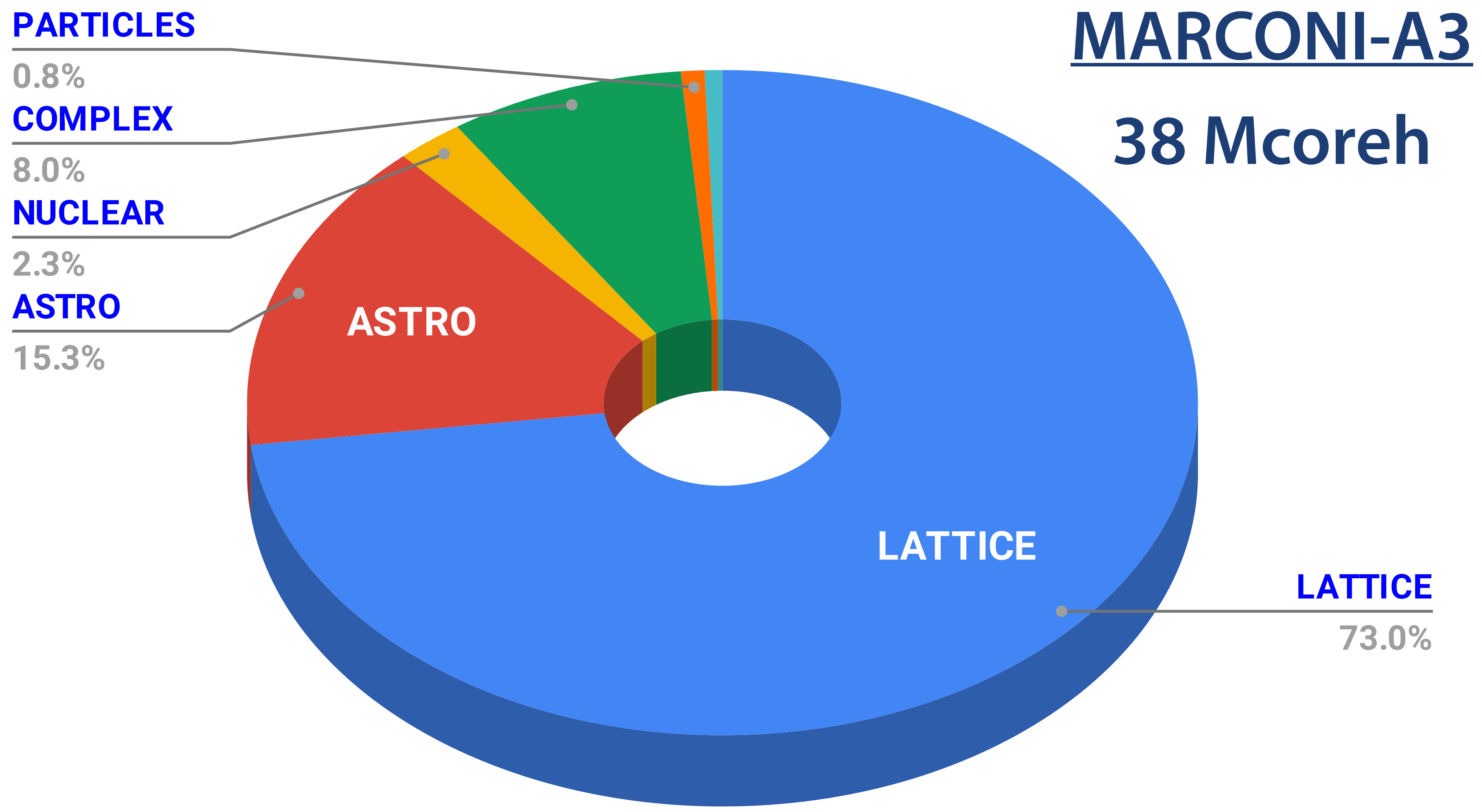
LEONARDO-booster

22 Mcoreh



MARCONI-A3

38 Mcoreh



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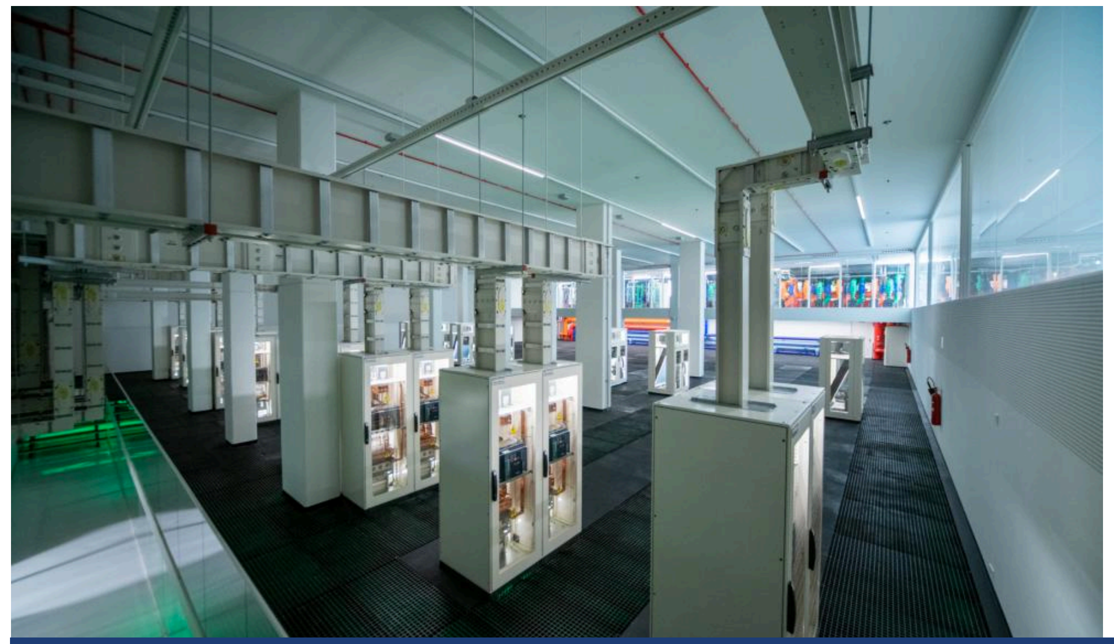
Other potential resources: EURO-HPC JU

https://eurohpc-ju.europa.eu/supercomputers/our-supercomputers_en

EuroHPC Joint Undertaking

LUMI supercomputer
375 PFlop/s - FINLAND

- LUMI-G (accelerated partition)
  2978 nodes with 4 AMD MI250x GPUs and a single 64 cores AMD EPYC "Trento" CPU.
  379.70 PFlop/s HPL
- LUMI-C (CPU partition)
  2048 CPU-based compute nodes (128 cores/node AMD EPYC)

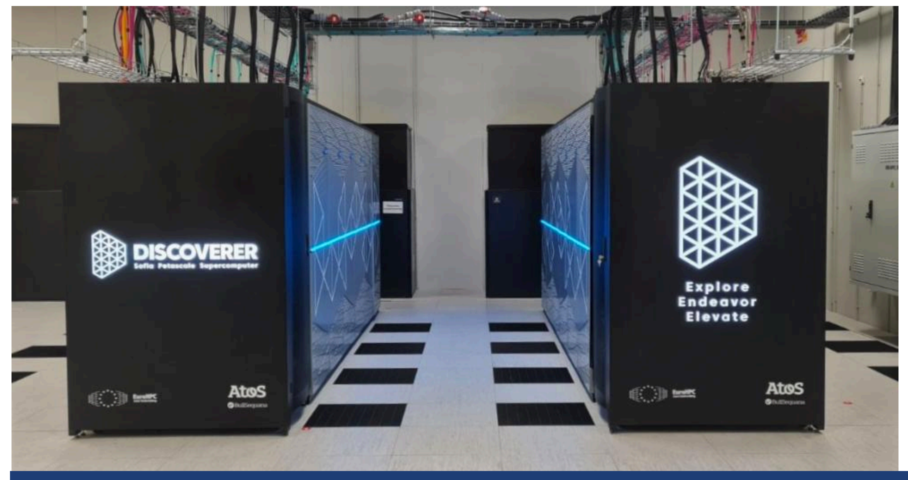


MARENOSTRUM 5
275 PFlop/s - SPAIN

- MareNostrum 5 ACC (Accelerated Partition)
  1120 nodes based in Intel Sapphire rapids (64 cores/node) and Nvidia Hopper GPUs (4 GPUs/node). 230 PFlops HPL
- MareNostrum 5 GPP (General Purpose Partition)
  6408 nodes based in Intel Sapphire rapids (112 cores/node). 45 PFlops HPL

HPC Vega IZUM
6.92 PFlop/s - SLOVENIA

MELUXINA supercomputer
12.81 PFlop/s - LUXEMBOURG



DISCOVERER supercomputer
4.51 PFlop/s - BULGARIA

DEUCALION supercomputer
7.22 PFlop/s - PORTUGAL

KAROLINA supercomputer
9.59 PFlop/s - CZECH Republic

…and the first European exascale computer, Jupiter, is underway in Germany (Jülich Supercomputing Centre).

Compute partitions:

- Booster Module (highly-scalable GPU accelerated)
- Cluster Module (general-purpose, high memory bandwidth)

1 Exaflop sustained performance

#EuroHPC
Joint Undertaking

The European High Performance Computing Joint Undertaking (EuroHPC JU) will pool European resources to develop top-of-the range exascale supercomputers for processing big data, based on competitive European technology.

Member countries are Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Montenegro, the Netherlands, North Macedonia, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden and Turkey.

EuroHPC Joint Undertaking

Conclusions

- Computational theoretical physics @INFN: a rich and enduring tradition. Researchers in this field are working on a wide range of projects, including lattice QCD, high-energy physics (HEP), astroparticle physics, nuclear physics, complex systems, and quantum computing.
- Challenge: Ensuring the long-term sustainability of efforts to maintain and enhance codes and algorithms.
- The availability of cutting-edge computing resources is vital for maintaining competitiveness on an international scale.