

IL CALCOLO HPC NELLA FISICA TEORICA INFN: STATO E PROSPETTIVE

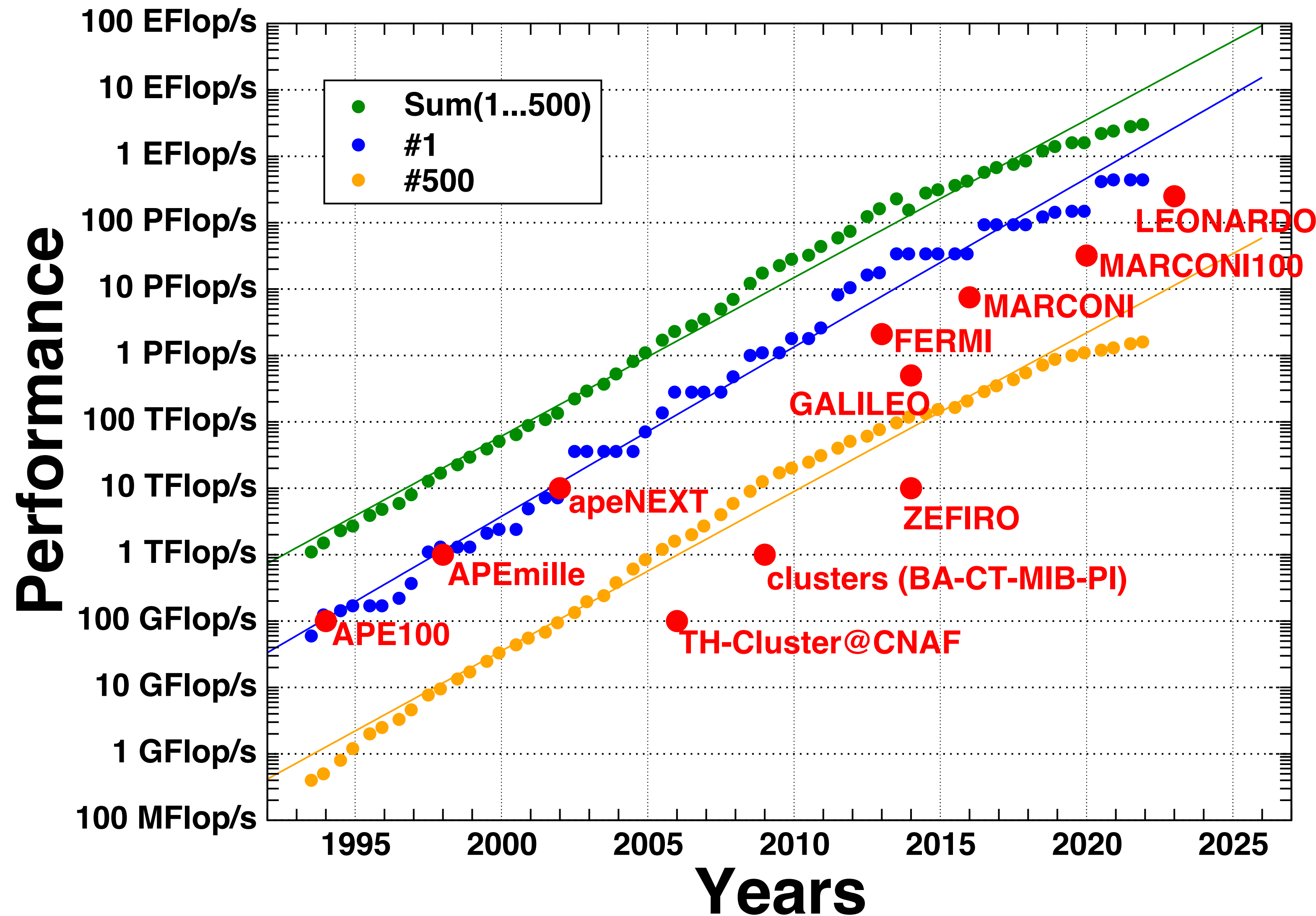
Leonardo Cosmai (INFN - Sezione di Bari)



Workshop sul Calcolo nell'INFN, Paestum, 23 maggio 2022



HPC & THEORETICAL PHYSICS @ INFN: A LONG HISTORY



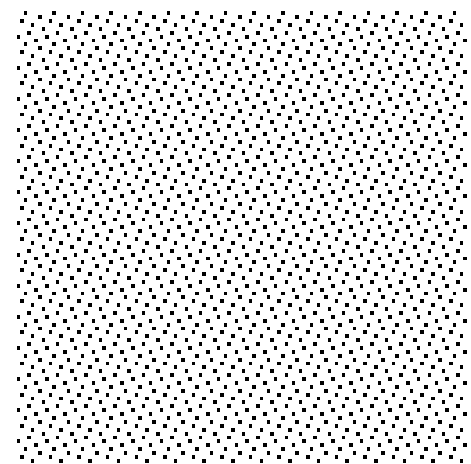
Storico:

- ~1985-1995: Cray 1M, Cray X-MP/12-48, Cray Y-MP, Cray T3D/64 (CINECA)
- ~1985-2010: APE, APE100, APEmille, apeNEXT
- ~2010-...: cluster locali (BA-CT-MIB-PI), cluster CSN4 (Zephiro)
- ~2012: nuova convenzione CINECA: BlueGene/Q (FERMI), IBM cluster (GALILEO), Lenovo cluster (MARCONI),...

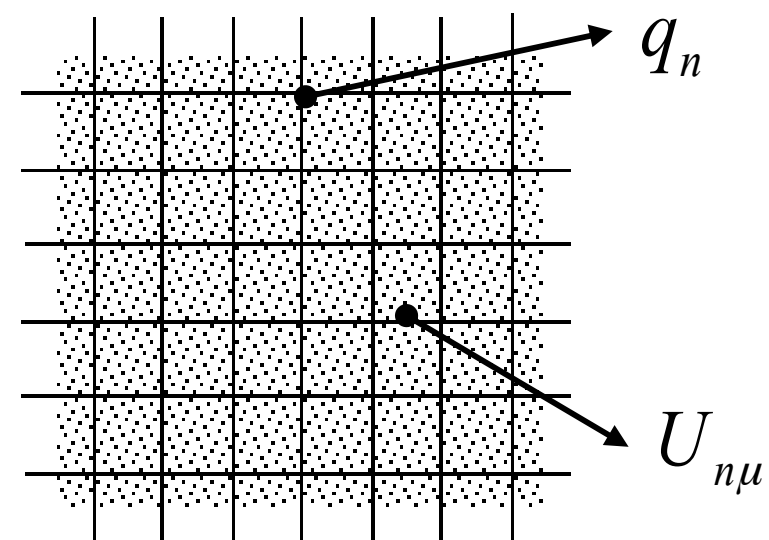
HIGH PERFORMANCE COMPUTING & LQCD: a paradigmatic use case

Formulation of QCD on a space-time lattice → a framework for understanding the dynamics of non-Abelian gauge fields

Space-time continuum



Space-time lattice

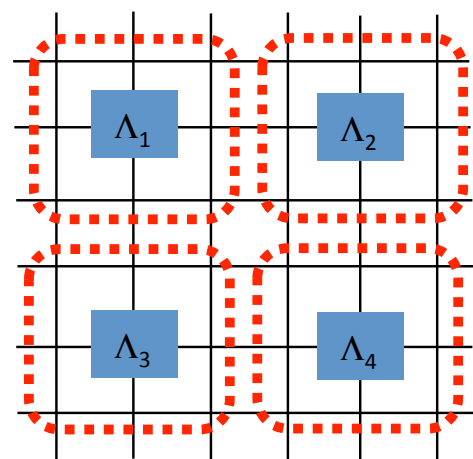


Lattice QCD drove the development of HPC hardware

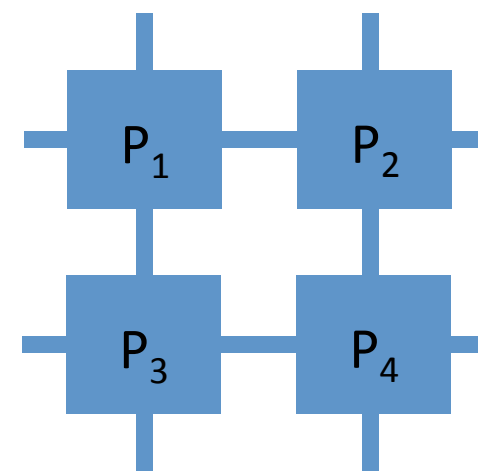
<i>name</i>	<i>year</i>	<i>authors</i>	<i>peak speed</i>
Columbia	1984	Christ-Terrano	-
Columbia-16	1985	Christ et al	0.25 GFlop/s
Columbia-64	1987	Christ et al	1 GFlop/s
APE1	1988	Cabibbo-Parisi	1 GFlop/s
Columbia-256	1989	Christ et al	16 GFlop/s
ACPMAPS	1991	Mackenzie et al	5 GFlop/s
QCDPAX	1991	Iwasaki-Hoshino	14 GFlop/s
GF11	1992	Weingarten	11 GFlop/s
APE100	1994	APE Collab.	0.1 TFlop/s
CP-PACS	1996	Iwasaki et al	0.6 TFlop/s
QCDSP	1998	Christ et al	0.6 TFlop/s
APEmille	2000	APE Collab.	0.8 TFlop/s
apeNEXT	2004	APE Collab.	10 TFlop/s
QCDOC	2005	Christ et al	10 TFlop/s
PACS-CS	2006	Ukawa et al	14 TFlop/s
QCDCQ	2011	Christ et al	500 TFlop/s
QPACE	2012	Wettig et al	200 TFlop/s

Massive parallelism and Lattice QCD

Space-time lattice

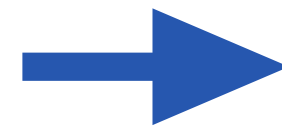


Processor array



HIGH PERFORMANCE COMPUTING & LQCD: a paradigmatic use case

Lattice QCD calculations typically require multidimensional integration over the gauge fields

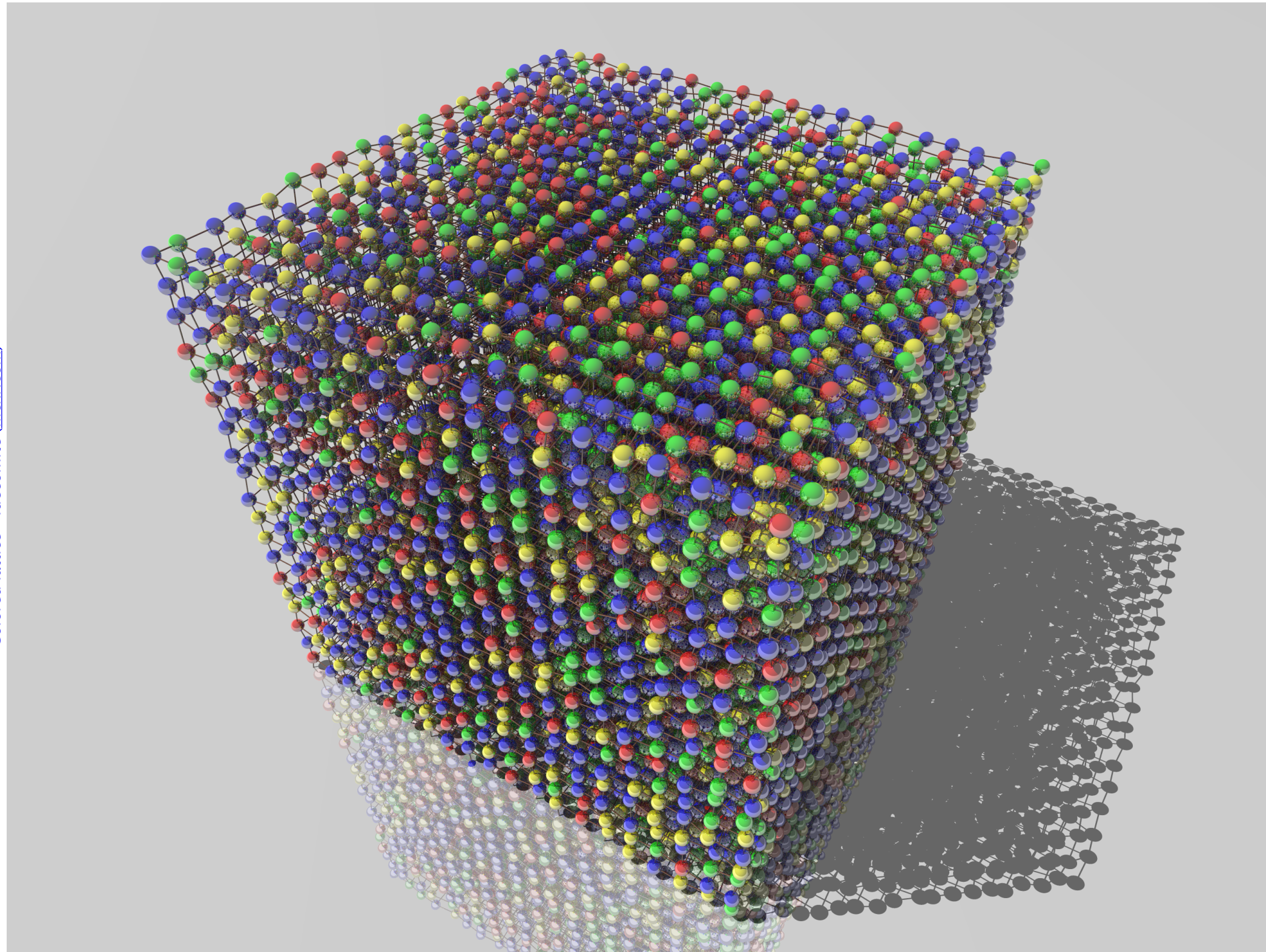


The integration dimension in state-of-the-art calculations is $\mathcal{O}(10^{10})$

Markov Chain Monte Carlo methods are used to perform the multidimensional integrations

Generation of ensembles of configurations with importance sampling via Monte Carlo methods is an essential step in numerical simulations of the path-integral of statistical mechanics systems and field theories.

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**.



"Colored lattice" fdecomite (flickr.com)

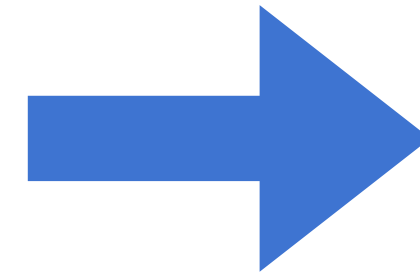
HIGH PERFORMANCE COMPUTING & LQCD: a paradigmatic use case

The Lattice QCD workflow

Monte Carlo sampling phase

$$P_{\text{eq}}(U) = \frac{1}{\mathcal{Z}} \text{Det}(M^\dagger M) e^{-S(U)}$$

- Generates an ensemble of gluon field configurations U distributed according to the QCD action (using the hybrid Monte Carlo algorithm): $\text{Cost} \propto V^{9/8} a^{-2}$
- This ensemble generation is serially dependent and represents a **strong scaling computational problem**.
- A large number of computing nodes is required. On the largest scales this becomes a **halo-exchange communication problem** since the local data bandwidths vastly exceed those of inter-node communication.



Hadronic observables are calculated on each sampled configuration U :

$$\langle \mathcal{O} \rangle \approx \bar{\mathcal{O}} = \frac{1}{N} \sum_U \mathcal{O}(U)$$

- High degree of trivial parallelism: computer interconnect limitations are more easily avoided by exploiting this trivial parallelism.

Physics goals:

calculations with ensembles of gauge fields with physical volumes V large enough to ensure that finite-volume effects are under control.

● Example at the *exascale frontier*:

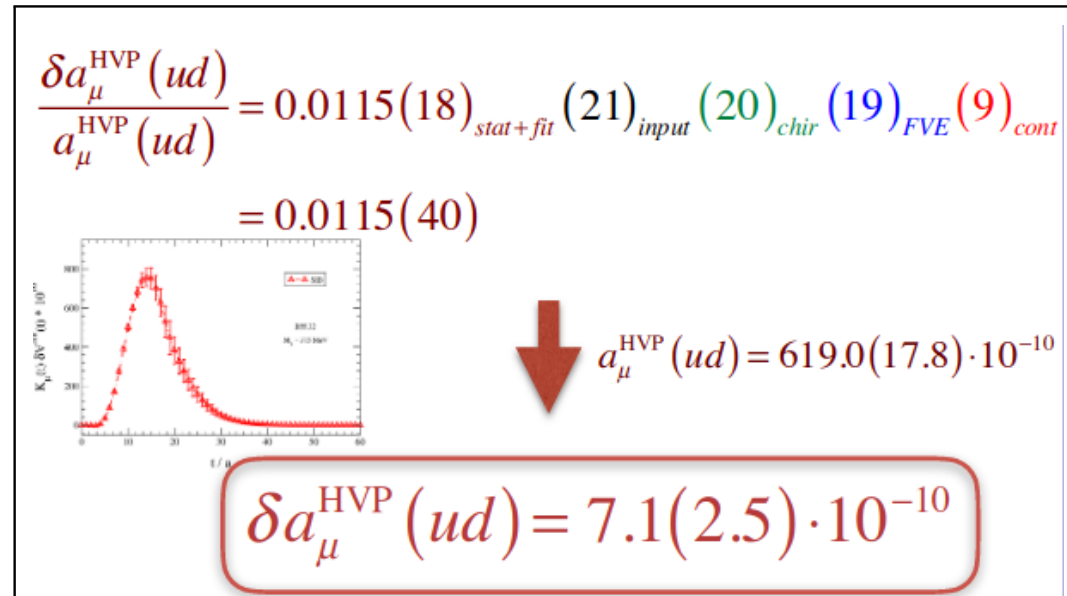
Simulation with up/down, strange, charm and bottom quarks at their physical masses with physical volume $V = (10 \text{ fm})^4$ at a lattice spacing $a = 0.04 \text{ fm}$ ($a^{-1} \sim 5 \text{ GeV}$) (lattice size $256^3 \times 512$)
 $\sim 12,000 \text{ Exaflop hours} = 12,000 \times (3600 \times 10^{18}) \text{ floating-point operations}$

AN OVERVIEW OF SOME PROJECTS IN LATTICE QCD

LQCD123 (F. Sanfilippo) r.n. V. Lubicz

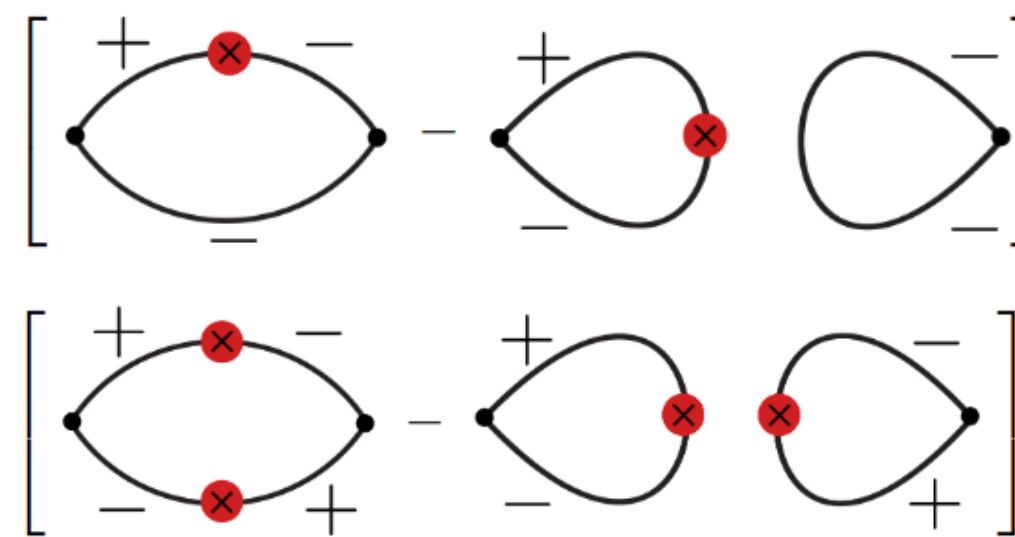
Physics activity: QCD + QED phenomenology

QED CORRECTIONS TO LEADING HADRONIC CONTRIB. (a_μ) OF $g_\mu - 2$
PRD99(2019) + update in progress

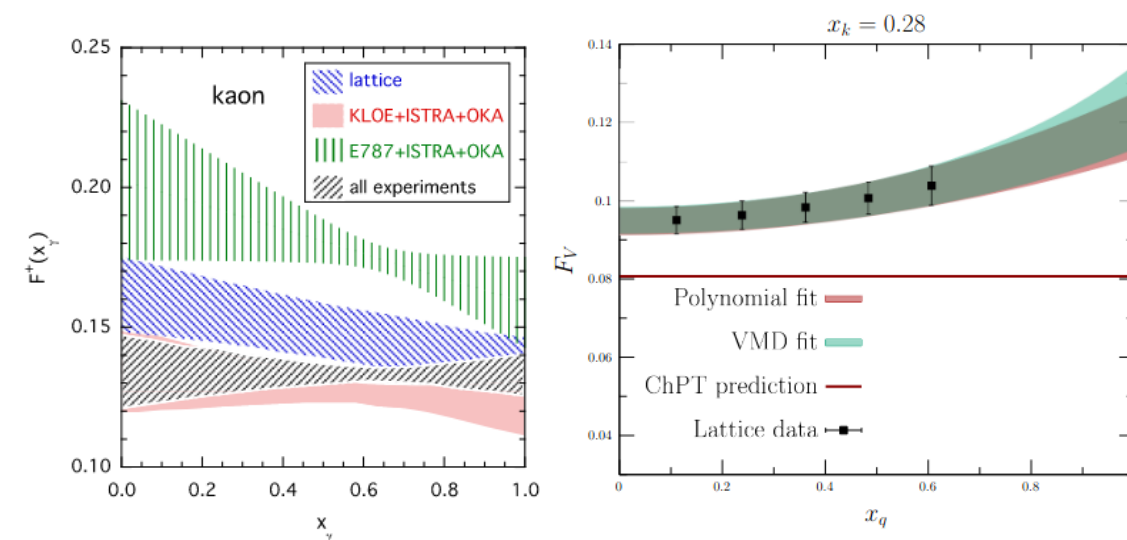


ℓ_7 low energy constant
PRD 104, 074513 (2021)

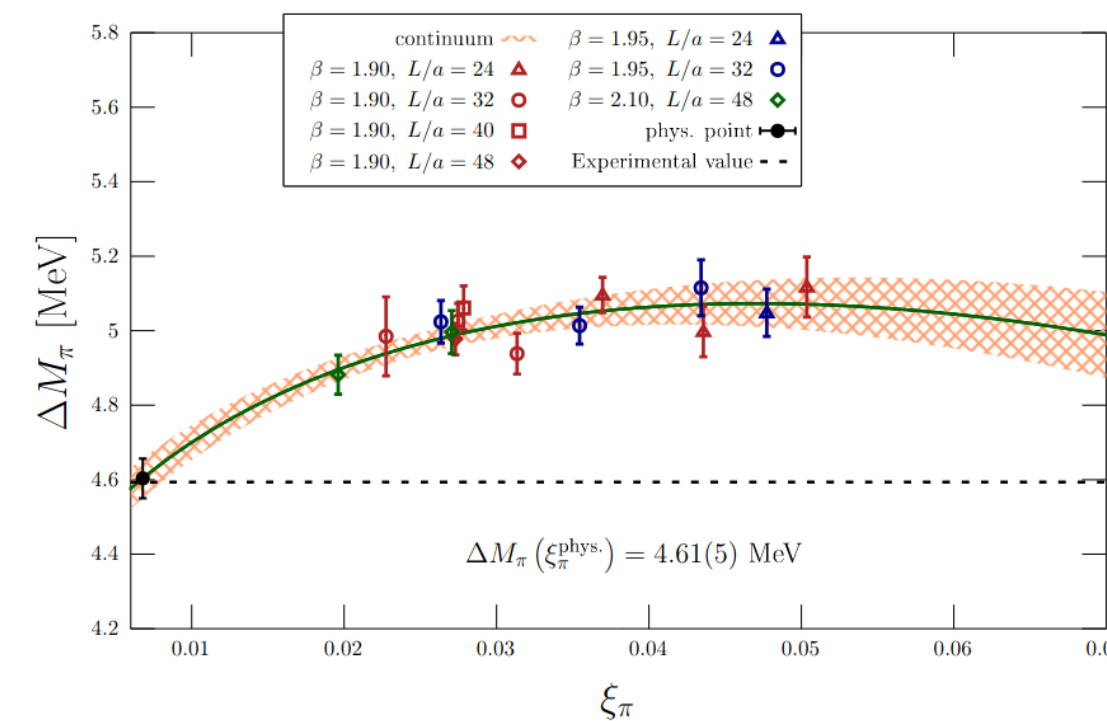
ISCRA22B - E π C



REAL & VIRTUAL PHOTON EMISSION
PRD103,1 (2021), PRD103,5 (2021)
and arXiv:2202.03833 (to appear on PRD)



$M_{\pi^+} - M_{\pi^0}$ theoretical prediction to $\mathcal{O}(\alpha)$
arXiv:2202.11970



Simulations within ETM collaboration: LQCD at the physical point

$N_f = 2 + 1 + 1$ Physical pion mass simulations - arXiv:2111.14710

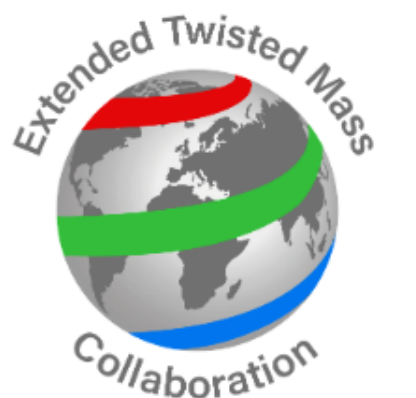
ensemble	β	V/a^4	a (fm)	$a\mu_\ell$	M_π (MeV)	L (fm)	$M_\pi L$
cA211.53.24	1.726	$24^3 \times 48$	0.0947 (4)	0.00530	346.4 (1.6)	2.27	3.99
cA211.40.24		$24^3 \times 48$		0.00400	301.6 (2.1)	2.27	3.47
cA211.30.32		$32^3 \times 64$		0.00300	261.1 (1.1)	3.03	4.01
cA211.12.48		$48^3 \times 96$		0.00120	167.1 (0.8)	4.55	3.85
cB211.25.24	1.778	$24^3 \times 48$	0.0816 (3)	0.00250	259.2 (3.0)	1.96	2.57
cB211.25.32		$32^3 \times 64$		0.00250	253.3 (1.4)	2.61	3.35
cB211.25.48		$48^3 \times 96$		0.00250	253.0 (1.0)	3.92	5.02
cB211.14.64		$64^3 \times 128$		0.00140	189.8 (0.7)	5.22	5.02
cB211.072.64		$64^3 \times 128$		0.00072	136.8 (0.6)	5.22	3.62
cB211.072.96		$96^3 \times 192$		0.00072	136.0 (0.3)	7.83	5.43
cC211.06.80	1.836	$80^3 \times 160$	0.0694 (3)	0.00060	134.2 (0.5)	5.55	3.78
cD211.054.96	1.9	$96^3 \times 192$	0.0576 (2)	0.00054	138.0 (0.5)	5.53	3.87

PRACE projects: PRA17-4394, PRA20-5171, PRA22-5171

Non perturbative renormalization,

Quark masses and meson decay constant determination

- Phys. Rev. D 104, 074515 (2021)
- Phys. Rev. D 104, 074520 (2021)



PRA17-4394: 45M core hours su MARCONI (KNL)

PRA20-5171: 76M core hours su Marconi100

PRA22-5171: 66M core hours su Marconi100

AN OVERVIEW OF SOME PROJECTS IN LATTICE QCD

NPQCD (M. D'Elia) r.n. L.Cosmai

Non-perturbative Quantum Chromodynamics

Research activities and HPC in NPQCD

1. QCD in extreme conditions

- finite temperature and density
- phase diagram in strong magnetic backgrounds
- color confinement and deconfinement
- topological properties and axion phenomenology

2. QCD-like theories (Large-N limit, universality)

3. Numerical approaches to quantum gravity (CDT)

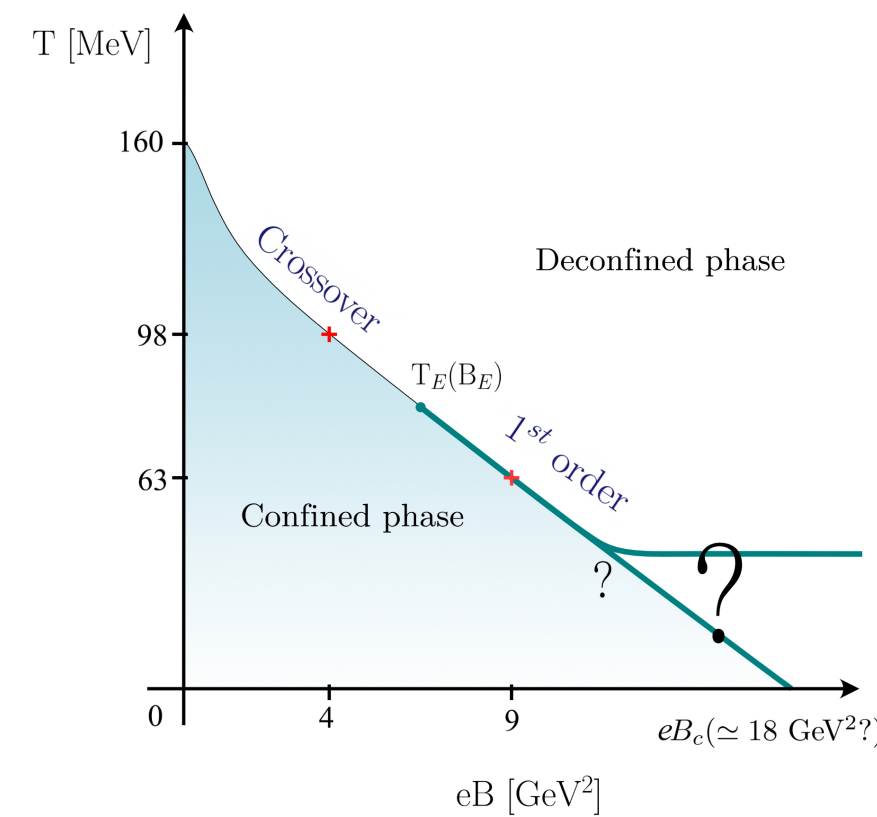
4. Exploratory exercises in Quantum Computing

Large scale HPC resources mostly dedicated to item 1)

Lists of PRACE and IS CRA-B projects:

- **PRACE:** AX TRO (call 13) and SISMAF (call 9)
- **IS CRA-B:** HP10BWSSLC, HP10BLQLBY, HP10BQMUVT, HP10B36BYO, HP10BA76RL, HP10BX8GQE, HP10BZV1G1, HP10BA5QTA, HP10BSRSMS, HP10B4P9OZ, HP10B9REXC, HP10B2J1PH, HP10CIN32X (last 4 in the last 3 years)

Highlights on most recent results

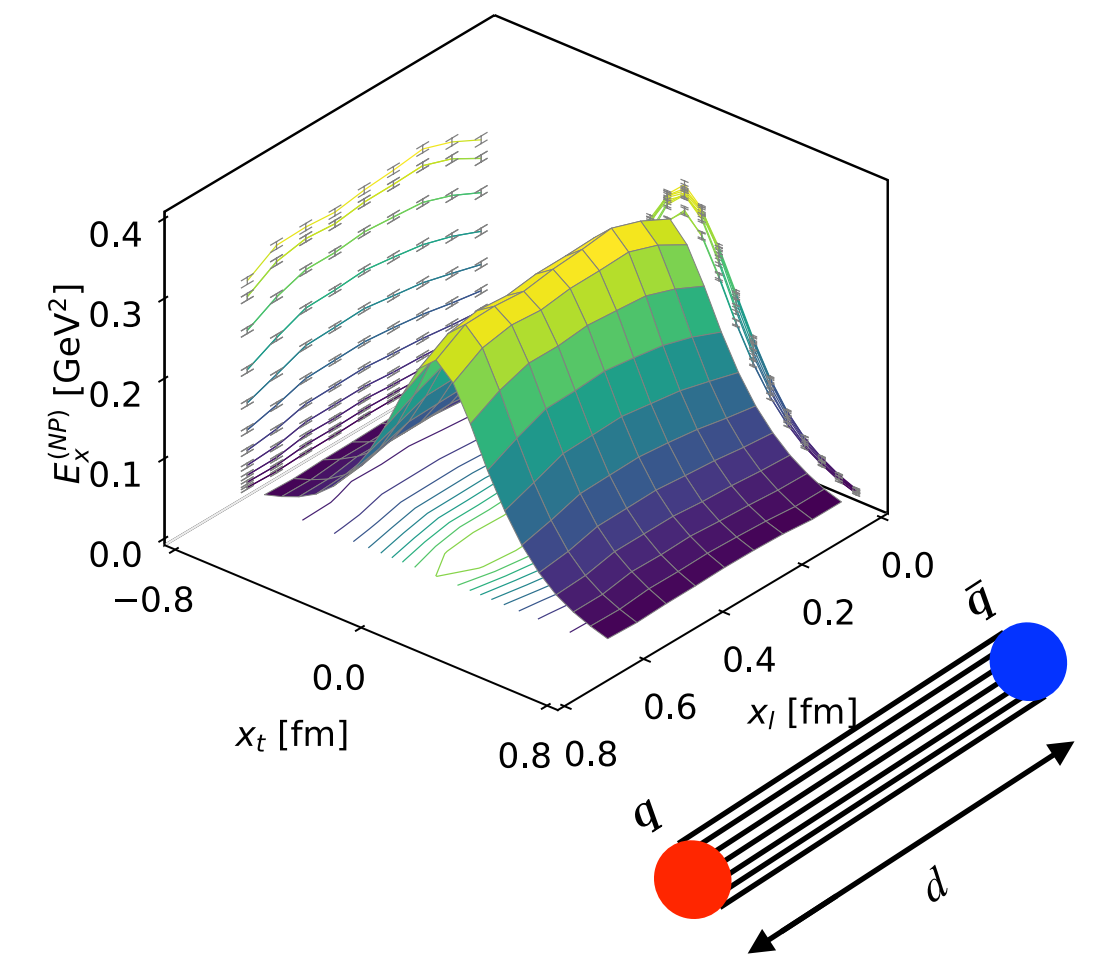


Critical endpoint found in the QCD Phase Diagram in a magnetic background

M. D'Elia, L. Maio, F. Sanfilippo and A. Stanzione, "Phase diagram of QCD in a magnetic background," Phys. Rev. D 105, 034511 (2022)

Editors' suggestion

based on NPQCD and Iscra-B QGPMF HP10B9REXC



The non-perturbative chromoelectric field obtained by subtracting the perturbative contribution

M. Baker, V. Chelnokov, L. Cosmai, F. Cuteri, and A. Papa,

"The flux tube profile in full QCD", POS Lattice 2021

based on NPQCD and Iscra-B HP10BUL8OZ

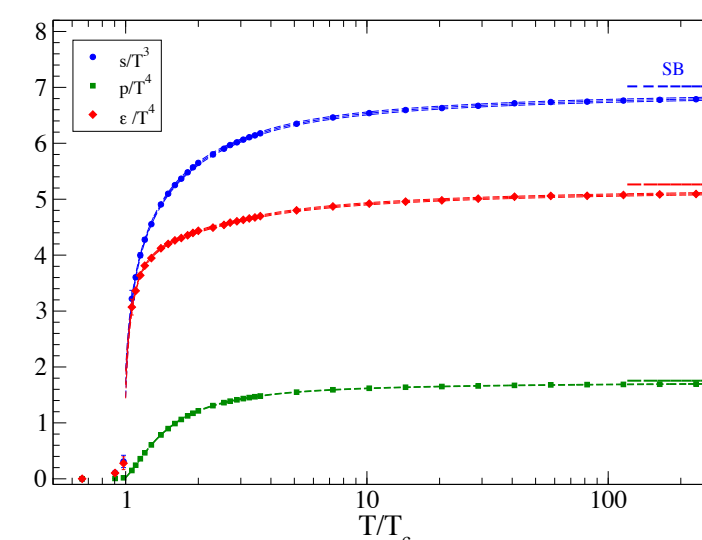
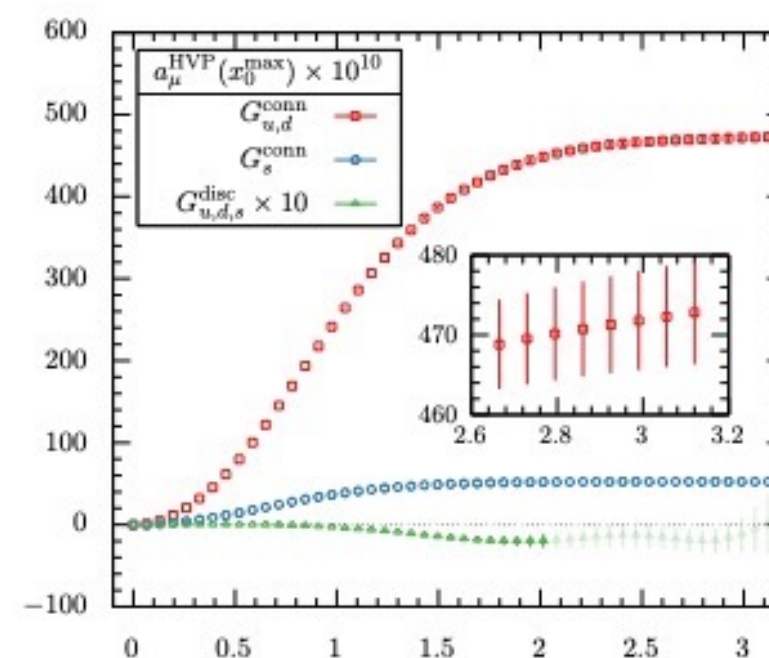
QC DLAT (L. Giusti)

r.n. L. Giusti

QC DLAT: Next generation lattice field theory for searching new phenomena in particle physics

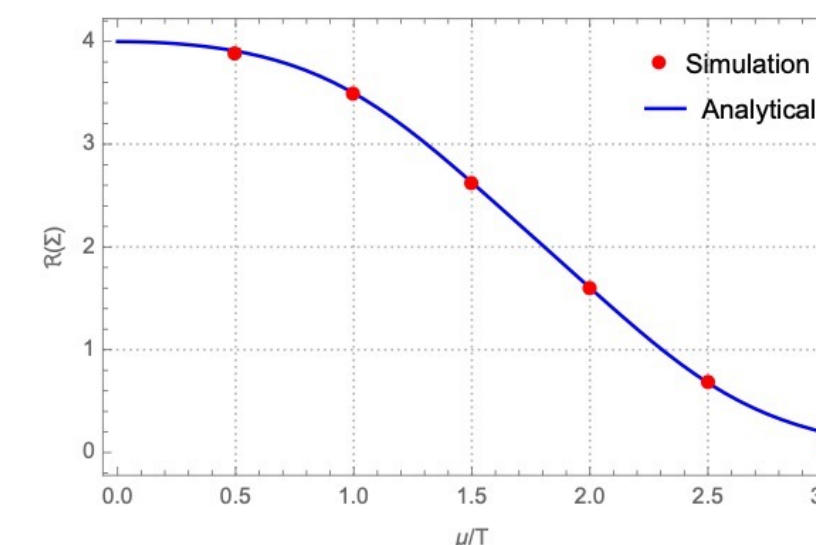
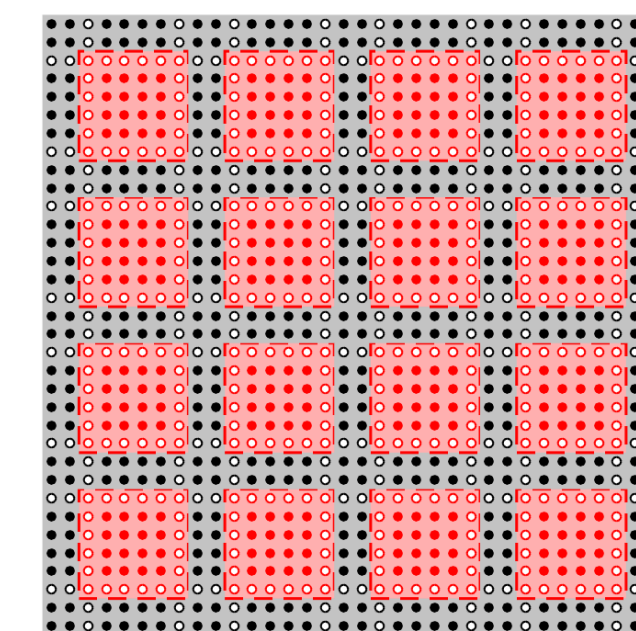
The Physics

- ❖ **Theme 1: QCD and flavour physics in the SM and beyond**
 $(g-2)_\mu$, $\Delta F=2$ in SM and beyond, CP violation in K, D and B mixing and decays
- ❖ **Theme 2: QCD at high temperature**
Equation of State, screening masses, transport coefficients, topology (axions)...
Study of QCD phase diagram by simulations with an imaginary chemical potential
- ❖ **Theme 3: Theoretical developments**
NP renormalization: quark masses, energy-momentum tensor, $\Delta F=2$ operators in SM and beyond, ..., NSPT, improvement, ...



Computational strategies (theme 4)

- ❖ Local factorization of determinant, multi-level integration with fermions, signal-to-noise ratio, master field simulations,...
- ❖ Development of algorithms for solving the sign problem in the presence of a non-zero chemical potential: simulations of toy-models in the Lefschetz thimble regularization
- ❖ Thermal field theories in a moving reference frame
- ❖ The challenge: HPC exascale, domain decomposition and factorization for the extreme parallelization of algorithms



Approximatively 180 MChours granted by PRACE and ISCRA

PRACE:

Title: EoSQCD – Equation of State of QCD
Allocation Period: 1.4.2019 -- 31.3.2020
Allocation: **80 MChours** SKL Marenostrum

Title: MLHVP - Multi-Level measurement of the Hadron Vacuum Polarization in Lattice QCD
Allocation Period: 01.04.2020 -- 31.03.2021
Allocation: **40 MChours** SKL JUWELS

Title: QCD2EW – Finite temperature QCD up to the Electro-Weak scale
Allocation Period: 01.10.2021 -- 30.09.2022
Allocation: **45 MChours** SKL JUWELS

Title: Lee-Yang edge singularities in QCD
Allocation Period: 1.10.2021-30.9.2022
Allocation: **1.6 MChours** Marconi100

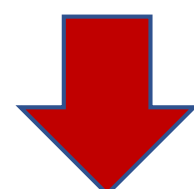
ISCRA:

Title: The anomalous magnetic moment of the muon with a multi-level algorithm
Allocation Period: 16.1.2019 -- 15.1.2020
Allocation: **14 MChours** KNL Marconi

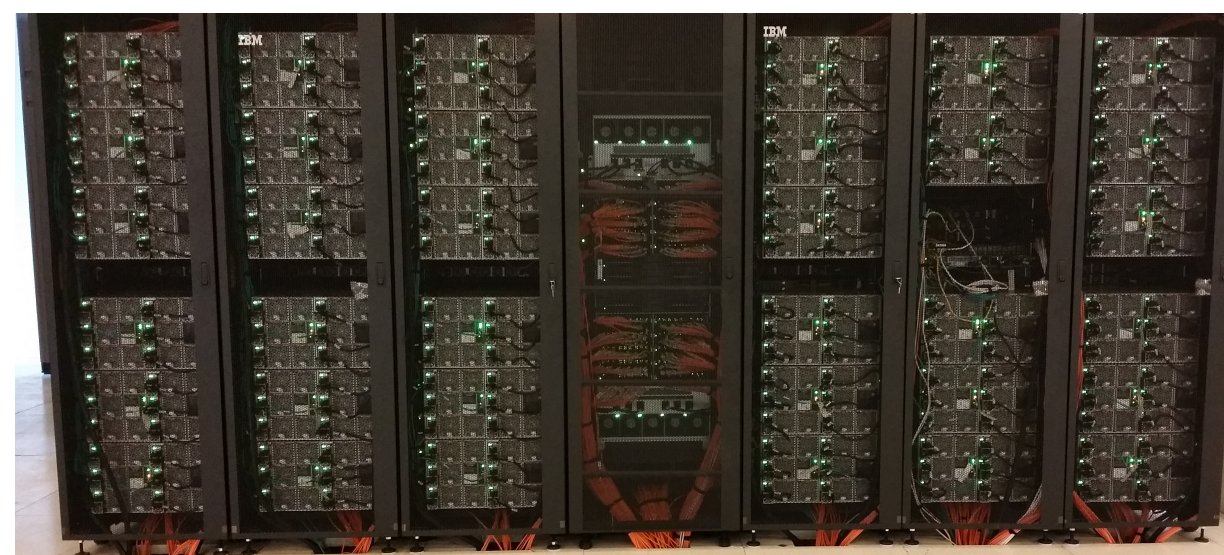
Title: LqcdPADE
Allocation Period: 27.10.2021-26.10.2022
Allocation: **0.64 MChours** Marconi100

Dall'R&D alle simulazioni su grande scala


HPC piccolo: R&D algoritmi. **O(0.1M€)**. In casa.



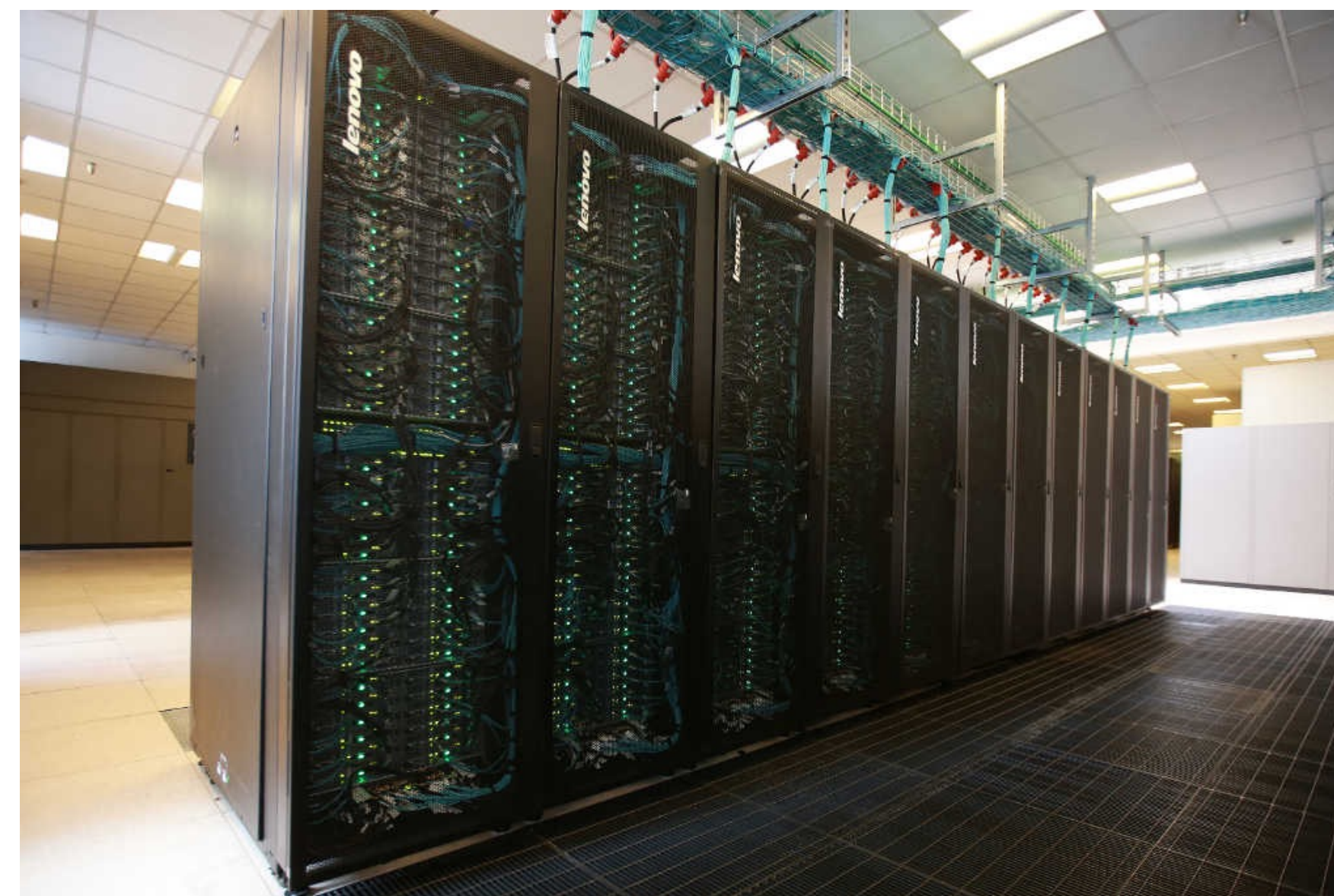
HPC medio: R&D, studi di fattibilità. **O(1M€)**.
Convenzioni: INFN/Cineca



HPC grande (top 500): produzione. **O(10M€) → O(100M€)**
con Leonardo (CINECA).

Bandi competitivi Europei e Nazionali, Bicocca ultimi 2 anni:
4 PRACE , 2 ISCRA  per 180 MChours (~1.8 M€)

Coordinated Lattice Simulation (CLS): condividiamo dati a
livello Europeo () nata al CERN nel 2008,
QC DLAT membro fondatore.



SFT (M. Panero)

r.n. G. Mussardo

INFN_SFT: Statistical Field Theory

Research focus: Strongly interacting quantum theories describing *condensed matter* and *elementary particles*:

- Statistical field theories in and out of equilibrium
- Entanglement in quantum systems
- Topological phases of matter
- Conformal field theory
- Integrable models

HPC-intensive activities:

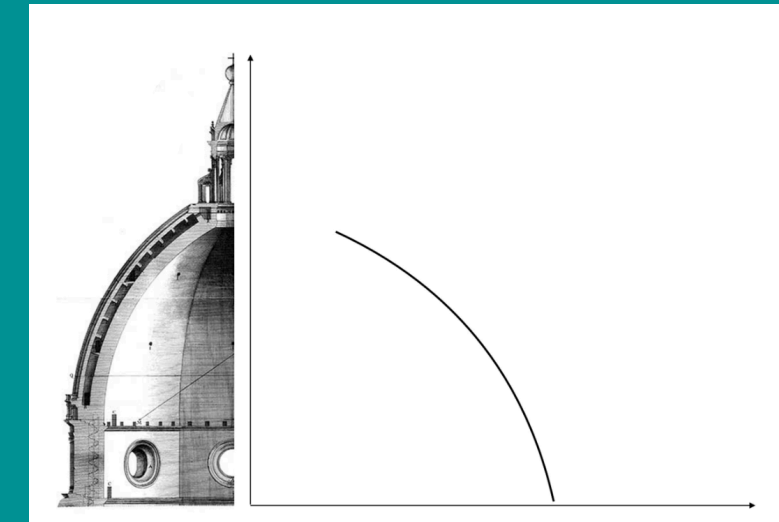
- Conformal field theory and conformal perturbation theory vs. Monte Carlo simulations of lattice gauge theories
- Lattice simulation of topological objects in statistical models
- Free energies from non-equilibrium Markov-chain Monte Carlo & machine learning for lattice field theory
- Strong dynamics with matter fields in multiple representations: lattice simulation of SU(4) lattice gauge theory for new physics beyond the Standard Model

SIM (M. P. Lombardo)

r.n. V. Greco

SIM

Research Topics



Critical and pseudocritical behaviour in QCD

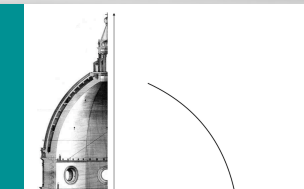
Phenomenology of the Quark Gluon Plasma

QCD axions and topology of strong matter

Dense matter: methods and models

Machine Learning for phase transitions

Compute grants* during the past three years



2022 – 2025 UK STFC DIRAC PPTM303 - Extreme QCD: Quantifying the QCD Phase Diagram III
2019 – 2021 ISCR High Performance Computing Allocation PCHSHT – Patterns of chiral symmetry at high temperatures
2016–2019 PRACE High Performance Computing Time Allocation – Extreme QCD, quantifying the QCD Phase Diagram

**M.P. Lombardo is excluded from European compute grants as chair of the EuroHPC panel on fundamental physics and universe, and member of the PRACE AC 2017–2022*

NOT ONLY LATTICE QCD...

Theoretical Physics projects that make use of HPC

- **Lattice QCD**
 - LQCD123 (*F. Sanfilippo*)
 - NPQCD (*M. D'Elia*)
 - QC DLAT (*L. Giusti*)
 - SFT (*M. Panero*)
 - SIM (*M.P. Lombardo*)
 - GAGRA (*M. Papinutto*)
- **Cosmology and Astroparticle Physics:**
 - INDARK (*M. Lattanzi*)
 - NEUMATT (*R. De Pietri*)
 - TEONGRAV (*B. Giacomazzo*)
- **Condensed matter:**
 - NEMESYS (*A. Sindona*)
- **Standard Model Phenomenology:**
 - QFTATCOL (*C. Carloni Calame*)
- **Nuclear Physics:**
 - MONSTRE (*N. Itaco*)
 - NUCSYS (*M. Viviani*)
- **Physics of the Complex Systems:**
 - BIOPHYS (*S. Morante*)
 - ENESMA (*C. Presilla*)
 - FIELDTURB (*G. Boffetta*)
- **Quantum Information:**
 - QUANTUM (*S. Montangero*)

Experimental Physics projects that make use of HPC

- EUCLID (*M. Tenti*)
- LSPE (*F. Piacentini*)
- VIRGO (*S. Mapelli*)
- LHC (*T. Boccali*)

HPC @ INFN



COSMOLOGY AND ASTROPARTICLE PHYSICS

TEONGRAV (*B. Giacomazzo*)

Hydrodynamics and magnetohydrodynamics simulations using state of the art codes in both the Newtonian and the General Relativistic regime

TEONGRAV

TEONGRAV members run simulations on several HPC clusters, including also Marconi A3, Marconi 100, and Galileo 100 at CINECA.

Projects includes both analysis of observational data and numerical simulations of compact objects.

In the field of numerical simulations of compact objects, TEONGRAV performs hydrodynamics and magnetohydrodynamics simulations using state of the art codes in both the Newtonian and the General Relativistic regimes. Main recent projects include:

- Model the gravitational wave emission from horizonless, multicenter geometries within the “fuzzball” paradigm of string theory (Roma 1)
- Model gravitational and electromagnetic emission from neutron stars (Firenze, Milano-Bicocca, Padova, TIFPA, Trieste)
- Accretion disks around Kerr black holes (Firenze)
- Simulations of binaries neutron stars beyond General relativity (Trieste)
- Exploring the dynamics of massive black hole binaries embedded in circumbinary discs (Milano-Bicocca)
- Model electromagnetic counterparts of supermassive black hole mergers (Milano-Bicocca)
- Model dynamical evolution and formation of stellar-mass and supermassive black holes via N-body simulations (Milano-Bicocca, Padova)

Analysis of observational data and numerical simulations of compact objects

TEONGRAV

In the field of data analysis, main recent projects include:

- Develop efficient data analysis strategies which use gravitational-wave observations of binary neutron stars to test the nuclear equations of state of neutron star matter (Roma 1, GSSI).
- Exploit multimessenger observations to constrain fundamental properties of hadron interactions within the neutron star cores (Roma 1, GSSI).
- Inference of nuclear equation of state properties and nucleosynthesis yields from compact binary mergers (TIFPA)
- Machine learning techniques to analyze gravitational waves from black hole binaries (Milano-Bicocca)
- Model selection for detector characterization in Pulsar Timing Arrays (Milano-Bicocca)
- Inferring population distribution parameters using non-parametric methods (Milano-Bicocca)

2019: 2 IS CRA B ed 1 IS CRA C (totale 4.2 M core hours)
 2020: 2 IS CRA B, 2 IS CRA C, 1 PR ACE (totale 16.8 M core hours)
 2021: 2 IS CRA C e 2 DE CI (totale 4.4 M core hours)
 2022: 4 IS CRA C (totale 0.4 M core hours)

COSMOLOGY AND ASTROPARTICLE PHYSICS

INDARK (*M. Lattanzi*)

dark energy and matter, axions,
neutrinos, modified gravity

Markov Chain Monte Carlo codes
interfaced with Boltzmann codes

ATTIVITÀ HPC IN INDARK

InDark è l'IS che si propone di studiare il modello cosmologico standard e le sue estensioni, e le connessioni con la fisica delle particelle. Si occupa di **inflazione**, **materia ed energia oscure**, **neutrini** e altre **relic cosmologiche leggere** (e.g. **assioni**), e **gravità modificata**.

A questo scopo, in InDark si utilizzano risorse HPC per:

- *Esplorazione dello spazio dei parametri di modelli cosmologici*
 - codici paralleli Markov Chain Monte Carlo interfacciati con codici Boltzmann.
 - applicazioni per es. alla stima dei parametri del modello cosmologico standard e delle sue estensioni, inclusi: proprietà dei neutrini, assioni e altre light relics; birifrangenza cosmica; storia di reionizzazione.
 - Inferenza "Likelihood-free" (i.e. basata su simulazioni) per stimare parametri di nongaussianità primordiali.
 - Applicazione a dati reali e a dati simulati di esperimenti futuri
- *Implementazione di algoritmi per la stima dello spettro da mappe di osservabili cosmologiche*
 - Test, validazione e produzione di codici paralleli per stime dello spettro di potenza e di statistiche di ordine più alto (es. bispettro).
 - Estrazione di informazione dalla polarizzazione del fondo cosmico di microonde, inclusa la ricerca di effetti di violazione di parità;
 - Studio di estimatori di nongaussianità primordiali dalla distribuzione di materia, validati su simulazioni N-body.

- **EuKey: 33333 Standard Hours**
- **EuNuComp: 32000 Standard Hours**
- **DZSH: 75000 Standard Hours**
- **DZS: 50000 Standard Hours**

NEUMATT (*R. De Pietri*)

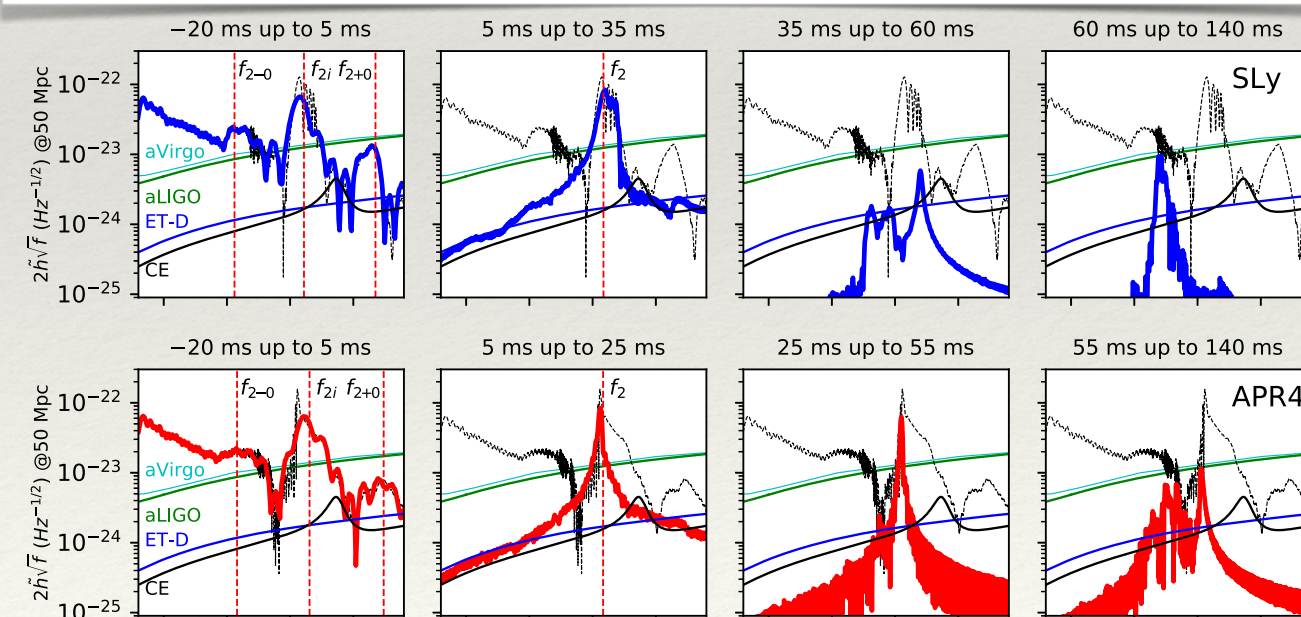
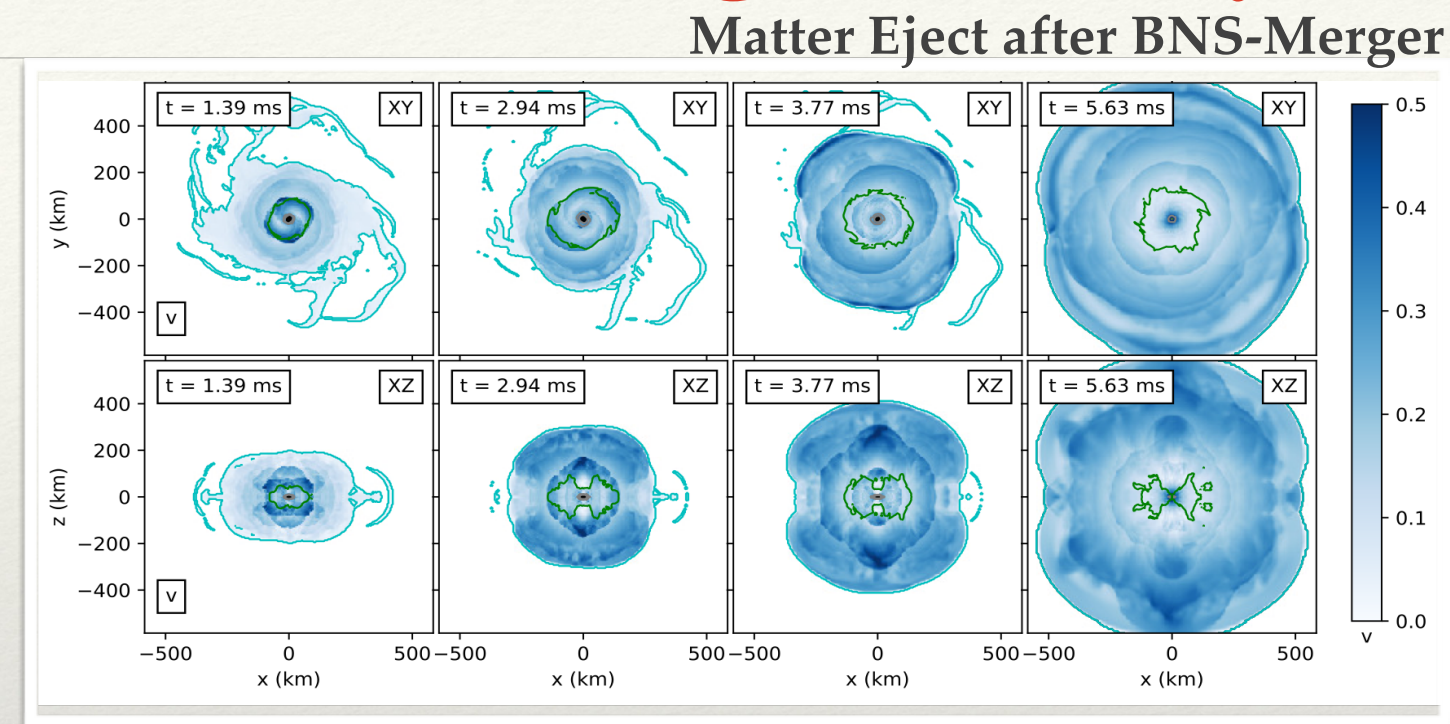
r.n. A. Drago

Gravitational wave signals from the merge of binary neutron stars

Full 3d-simulation of Einstein equation coupled to the matter of the merger

NEUtron star MATTer - Computing Activity

- ❖ National Coordinator : **Alessandro Drago** (Univ. Ferrara)
INFN-CT: Fiorella Burgio, Antonino Del Popolo, Hans-Josef Schulze, Isaac Vidaña INFN-FE: Michal Bejger, Roberto De Pietri, Alessandro Drago, Alessandra Feo, Andrea Lavagno, Giuseppe. INFN-LNGS: Massimo Mannarelli, Francesco Vissani, Giulia Pagliaroli. INFN-MI: Pierre Pizzochero. INFN-PI: Ignazio Bombaci, Domenico Logoteta
- ❖ Main topic: **GRAVITATIONAL WAVE SIGNAL FROM THE MERGE OF BINARY NEUTRON STARS**
- ❖ New research in progress on the R-mode excitation of Neutron Stars as Gravitational Waves-source.
- ❖ Full 3D-simulation of Einstein Equation coupled to matter of the merger. Post-merger signal + study of the the ejected matter. Equation of State effect on the signal.
- ❖ Recent works: ApJ 881 122 (2019), Phys. Rev. D 101, 064052 (2020) + PhD. + MS.Th + work in preparation.



post-merger GWfrequency is changing with time....

COLLIDER PHENOMENOLOGY

QFTATCOLLIDERS (C. Carloni Calame)

r.n. G.P. Vacca

Developing techniques for high-precision computations in Quantum Field Theory and to apply them to particle-physics phenomenology at present and future colliders

QFT@Colliders [BO, CS, FI, MIB, PV]

- ↪ Application of Quantum Field Theory to phenomenology of present and future hadron and lepton colliders
- ↪ Development of Monte Carlo event generators, for meaningful comparison of Theory predictions vs Experimental measurements
- ↪ Simulation of Standard Model and BSM processes, both for backgrounds and signal
- ↪ Steadily increasing complexity in theory predictions: higher-order radiative corrections (NLO, NNLO, ...), both in QCD and EW theory, to processes with more and more external particles
- ↪ CPU intensive computer codes due to multi-loop matrix elements evaluation, Monte Carlo integration and event generation, highly parallelizable
- ✓ QFT@Colliders gets typically 0.4 Mcorehours per year on Marconi under INFN-Cineca HPC agreement
- ✓ MIB won 10 IS CRA C grants (2018-20), for a total of 0.25 Mch on Marconi, 0.22 Mch on Galileo and 23 Kch on Marconi100
- ✓ Furthermore, under a UNIMIB-CINECA agreement, ≈ 2 Mch (effective) on Marconi A3 (2019-22).

HPC for CSN4

1 / 3

QFT@Colliders [BO, CS, FI, MIB, PV]

- A few examples of CPU intensive phenomenological study

S. Catani *et al.*, JHEP 08 (2020) 08, 027 [FI]

“Top-quark pair hadroproduction at NNLO: differential predictions with the \overline{MS} mass”

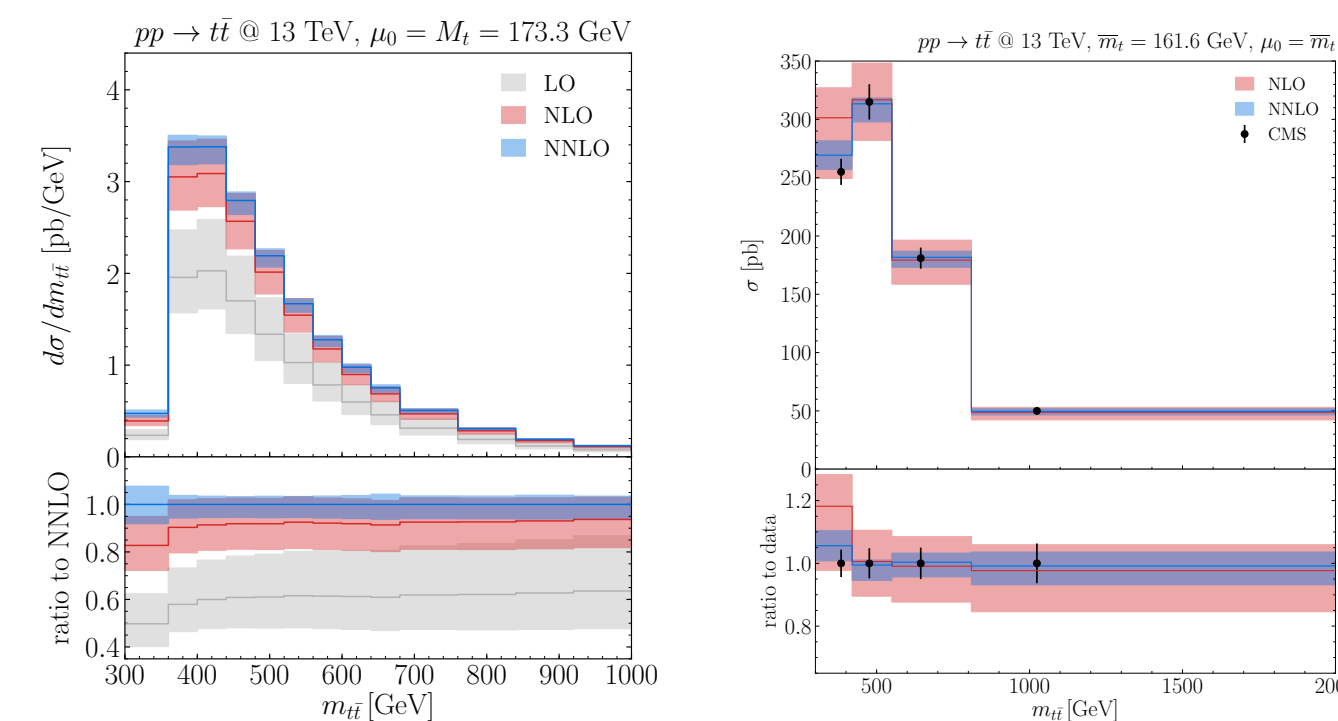


Figure: $m_{t\bar{t}}$ at different accuracies. NNLO greatly improves agreement with CMS data

HPC for CSN4

QFT@Colliders [BO, CS, FI, MIB, PV]

S. Alioli, *et al.*, Phys. Rev. D 104 (2021) no.9, 094020 [MIB]

“Matching NNLO predictions to parton showers using N3LL color-singlet transverse momentum resummation in GENEVA”

S. Alioli, *et al.*, Phys. Lett. B 818 (2021), 136380 [MIB]

“Next-to-next-to-leading order event generation for Z boson pair production matched to parton shower”

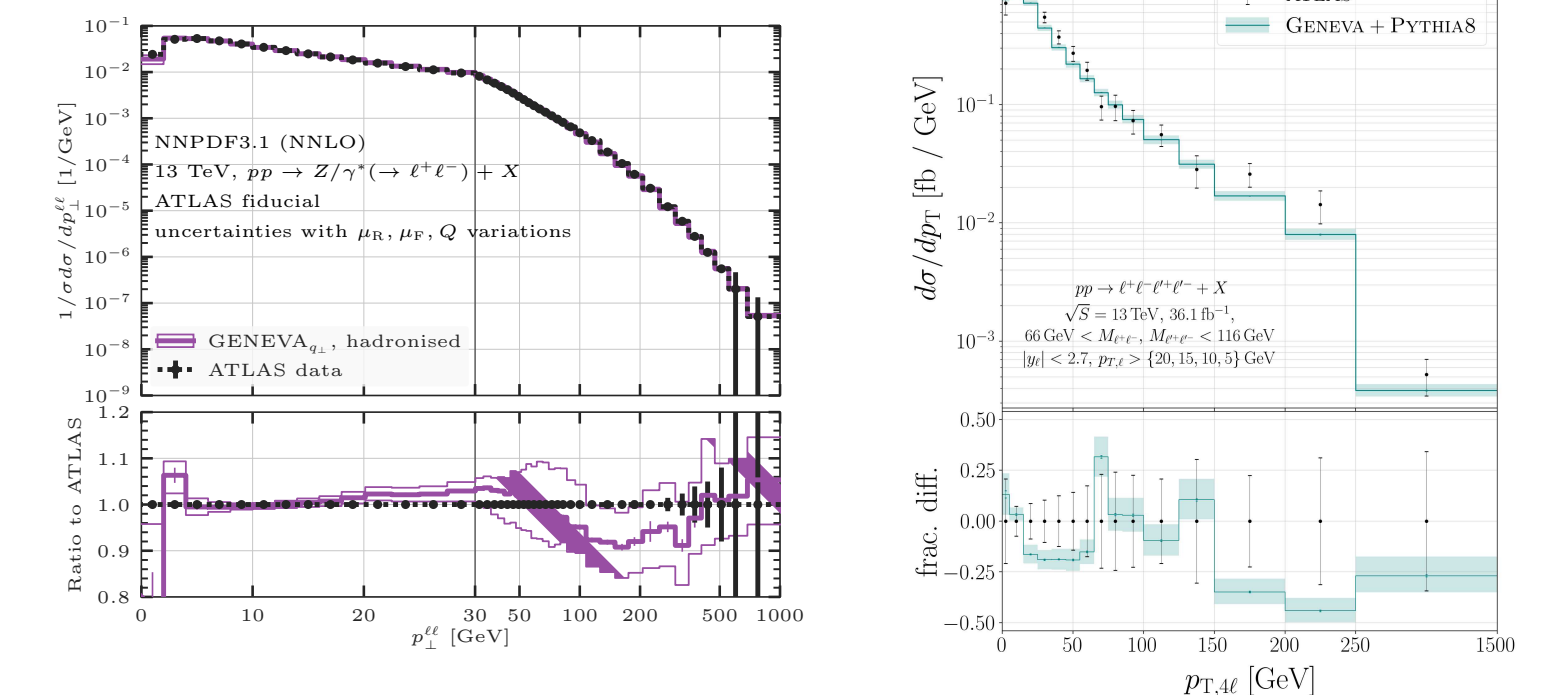


Figure: Matching NNLO to Parton Shower for single and double Z production vs ATLAS data

HPC for CSN4

3 / 3

MONSTRE (N. Itaco)

r.n. E. Vigezzi

Integrated framework for the physics of atomic nuclei, nuclear reactions, and strongly interacting matter.

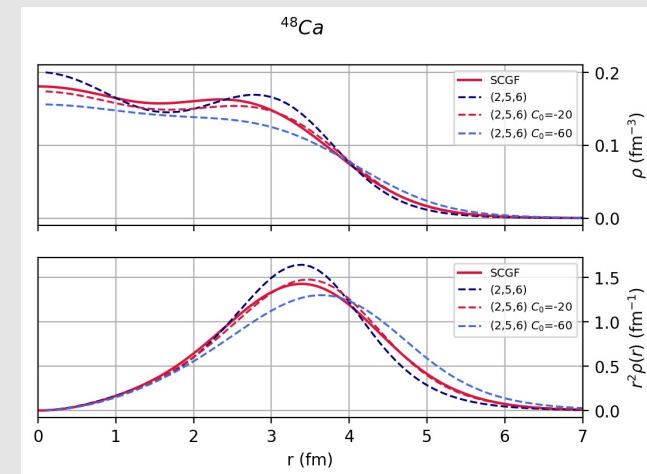
Iniziativa Specifica MONSTRE MOdeling Nuclear SStructure and REactions

- Bologna
- Catania
- Lecce
- LNS
- Milano
- Napoli
- Padova
- TIFPA - Trento

Quadro unificato per lo studio dei nuclei atomici, delle reazioni nucleari e della materia fortemente interagente

Keywords

- Struttura Nucleare
- Reazioni Nucleari
- Metodi a Multi-Corpi
- Funzionali Densità



MONSTRE & HPC

Large Scale Shell-Model Calculations

- **Thick-Restart Lanczos method** - OpenMP-MPI hybrid (dim 10^{11})
- Elementi di matrice di interesse per esperimenti con sonde elettrodeboli (Neutrinoless **double-beta decay**)

Funzionali dell'energia

- Eq. di stato della materia nucleare

Calcoli *ab initio*

- Quantum Monte Carlo
- Machine Learning

“Quantum Computing applied to Artificial Intelligence”
nell'ambito del programma PON R&I 2014-2020

- 1) IscraC:
A three-body chiral interaction for nuclear structure calculations of heavy nuclei
Acronym: Ch3B
Code: HP10C8TBT0
Validity: 6/08/2019-6/12/2020
Budget: 245.000 local hours su Marconi A2 + 8100 local h su Marconi100
- 2) IscraB:
Calculation of the Nuclear matrix element of Neutrinoless double beta decay using realistic shell model approach
Acronym: NLDBD
Code: HP10B51E4M
Validity: 9/10/2019 to 9/03/2021
Budget: 750.000 su Galileo + 45000 su M100+875.000 su Marconi A2
- 3) Prace_icei
Neutrinoless double beta decay of ^{100}Mo
08-10-2020: creazione progetto al 22/10 /2021
Budget: 1.6M local hours su Marconi100
- 4) IscraC:
Quenching effect of two-body currents on the axial vector constant g_a
Acronym: QTbGA
Thursday, 10 March, 2022 to Saturday, 10 December, 2022
Budget 100.000 local hours su G100

NUCSYS (M. Viviani)

r.n. A. Kievsky

Strongly correlated nuclear system

I.S. nucsys: study of dd fusion

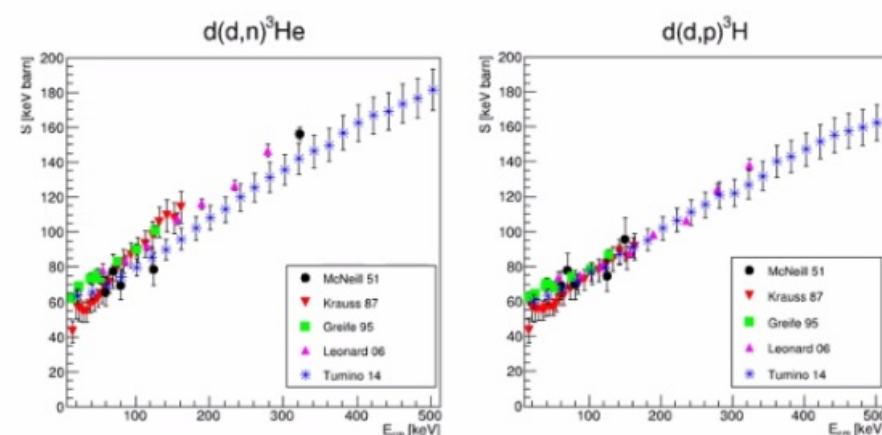
Theoretical study of the $d(d,p)$ H & $d(d,n)$ He reactions

Interest: 1) BBN primordial deuteron abundance 2) fusion reactors

Astrophysical factor for $d(d,p)$ H & $d(d,n)$ He reactions

Problem:

- No ab initio calculations
- Large uncertainties from experiments [Yeh, Olive, & Fields, 2021]
- This uncertainty affects the output of BBN codes



Rates of the reactions $d(d,p)$ H & $d(d,n)$ He with polarized fuel

Interest:

- For $d+$ He reactors, the possibility to suppress the production of neutron from $d(d,n)$ He (**Quintic suppression factor**)
- The possibility to control the direction of emission of neutrons (products emitted preferably in a direction)

→“Lean neutron reactors” reduction of the cost of the walls, more safety, less induced radioactivity, etc.

Quintic suppression factor = σ / σ_0 ratio between the fusion cross section with polarized deuterons and the unpolarized cross section

I.S. nucsys: study of dd fusion

Method of calculation: expansion of the scattering wave functions in a basis

Problem to be solved: linear system $M X = T(E)$

M =matrix $n \times n$ (independent on energy E), T =known vectors, X =solution vector

Calculation of M & T

Typically $n=300,000$

- 5-dimensional integration
- OpenMP code

Solution of the linear system (Lanczos)

- OpenMP code

Memory intensive calculation: work with 1 node only

- run for different J , energies, interactions,...

- a typical calculation takes 5,000 core hours on 1 Marconi & Galileo100 (48 cores)

NEXT: implementation using GPUs, extension up to $A=6$

Theoretical uncertainty

- **Numerical integration, convergence:** well under control
- **Dynamical input:** we start from a given $V=NN+3N$ interaction, but V is not exactly known

Approach used so far

- Perform the calculations using V derived from chiral Perturbation Theory (ChPT) & vary the cutoff Λ used to regularize the high momentum tail [$\Lambda=500 - 600$ MeV] (rough estimate of the theoretical uncertainty coming from the incomplete knowledge of the dynamical input)

NEXT: calculation with V derived from different orders of ChPT & estimation of the theoretical uncertainties using Bayesian method derived for that purpose.

PHYSICS OF THE COMPLEX SYSTEMS

FIELDTURB (G. Boffetta)

- Complex fluids and active matter
- Turbulence and scaling
- Out of equilibrium systems
- Machine learning with applications to complex flows

Alessandra Lanotte, Unita' Lecce
 2019 Project EU-PRACE 19th Call
 SPECTRA Universality of Kolmogorov spectrum in non ideal turbulent flows
 56 M core-hours Marconi KNL (Cineca)

Luca Biferale, Unita' di Roma 2
 2019 PRA17_4374
 TURB-ROT - Inverse and direct cascades in rotating turbulent flows
 60 M core-hours Marconi 2 (Cineca)

Guido Boffetta, Unita' di Torino
 2019 Iscra B
 Pourun - Turbulent convection in porous media
 4 M core-hours su Marconi KNL

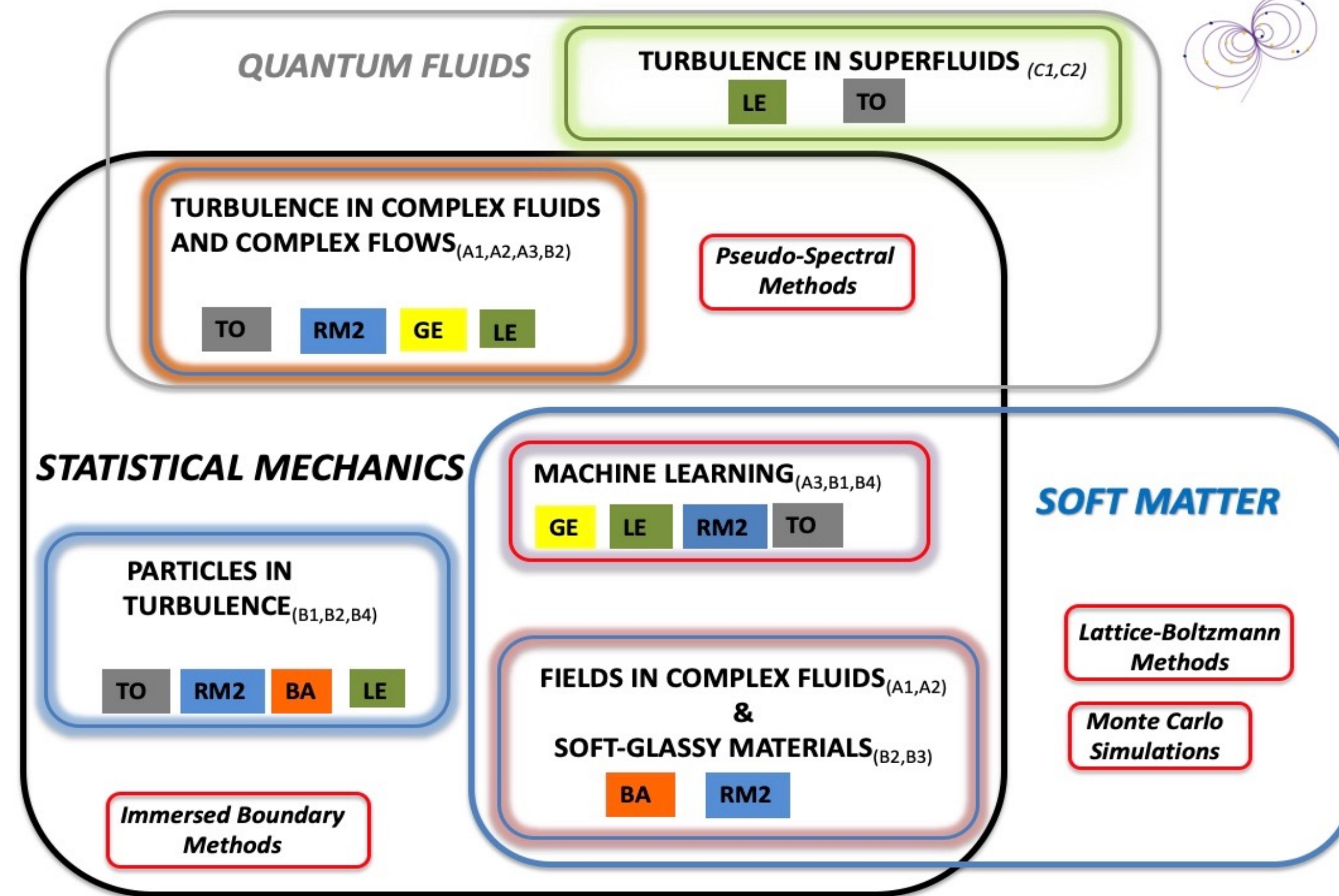
Guido Boffetta, Unita' di Torino
 2020 Iscra Covid
 TurboPuf - Transport of droplets by turbulent multiphase puff
 2 M core-hours su Galileo

Stefano Musacchio, Unita' di Torino
 2022 EuroHPC proposal
 Anisotropy in turbulent emulsions
 richieste 3.58 M core-hours su MeluXina (under revision)

FIELDTURB 2021 - 2024

National Coordinator: Guido Boffetta (Univ. Torino)

PARTICLES and FIELDS in TURBULENCE and in COMPLEX FLUIDS



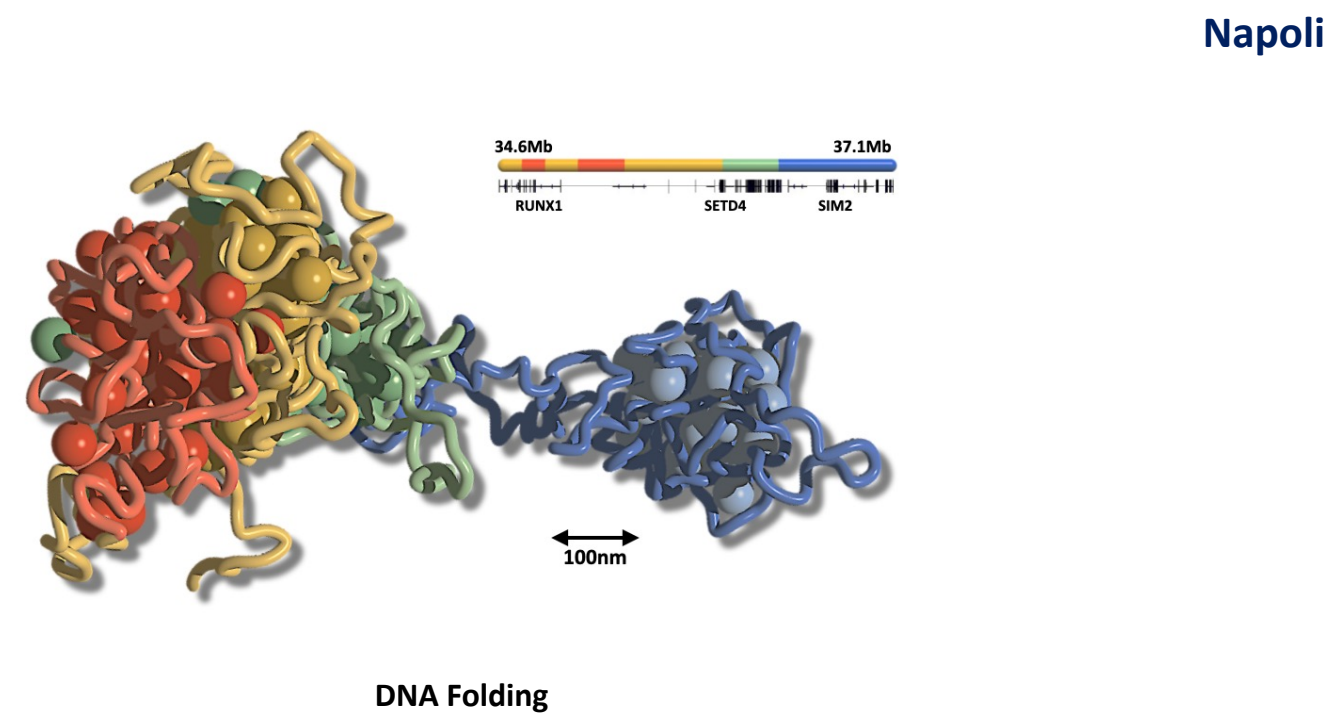
5 Units
 Torino
 Genova
 RM2
 Bari
 Lecce

Keywords : Turbulence, Complex fluids, Active matter, Out-of-equilibrium statistical mechanics, Machine learning

PHYSICS OF THE COMPLEX SYSTEMS

BIOPHYS (*S. Morante*)
r.n. *M. Nicodemi*

Investigation of the three-dimensional structure of the mammalian genome and its links with gene regulation at the single-molecule level by use of extensive **Molecular Dynamics** computer simulations.



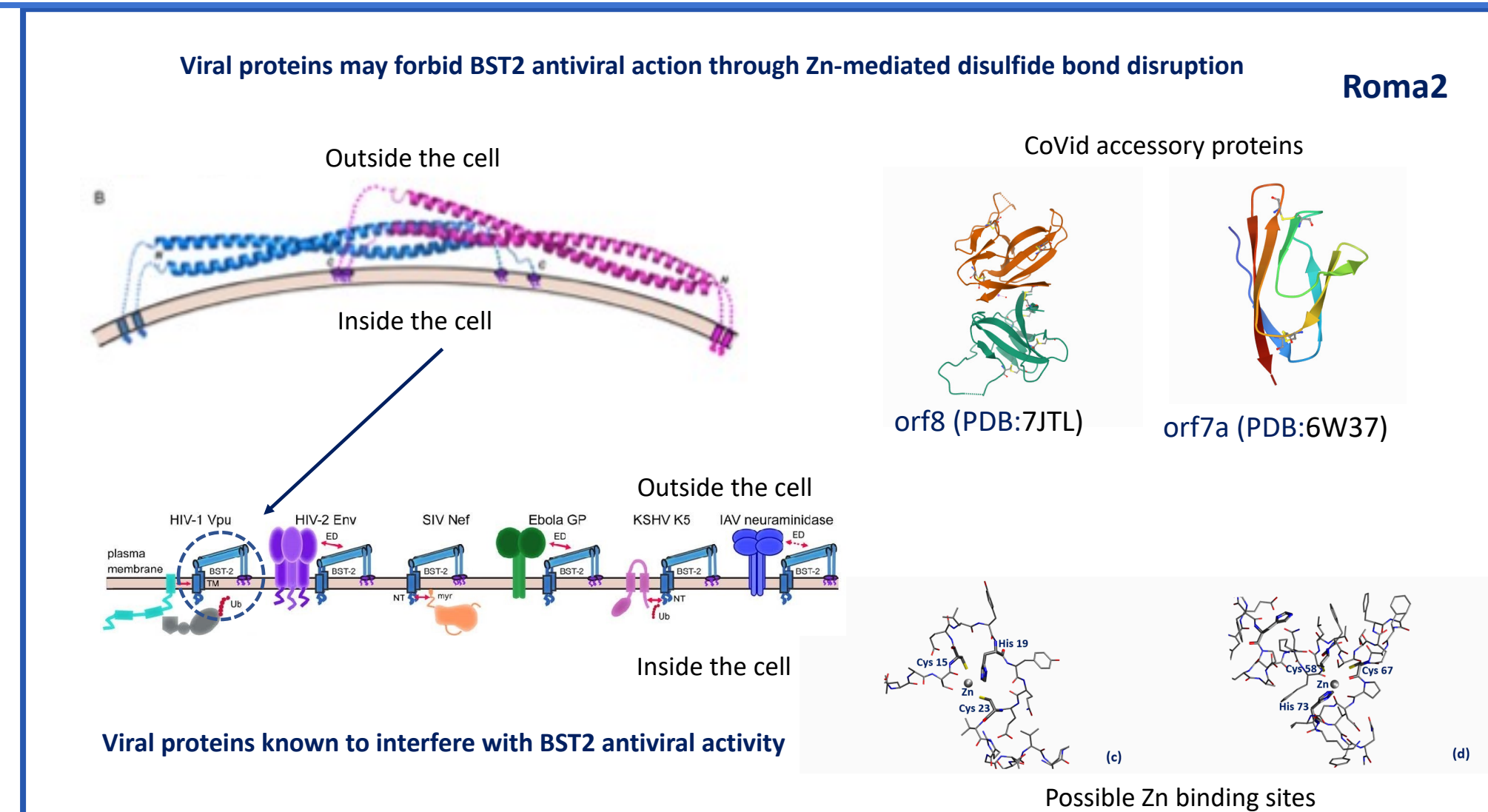
Three-dimensional structure of the mammalian genome and its links with gene regulation at the single-molecule level

ISCRA approved Projects within the IS:

- 4 IscraC projects on Marconi 100 for a total of 128 k core-hours;
- 2 IscraC projects on Marconi 100 for a total of 95 k core-hours
- Iscra B on Marconi 100 of 1.6 M core-hours
- ISCRA-HP10CCZ4KN
- ISCRA-HP10CCZ4KN
- ISCRA C 20' of quantum computing time on the D-WAVE quantum annealer
- ISCRA C project 30,000 hours on CiNECA

Modelling and discovering emergent properties of biological systems by using innovative methods and ideas coming from theoretical physics

Structural properties of proteins and protein assemblies (Fig.2 Covid2-orf7 and orf8, in interaction with BST2)



Study of the structural properties of proteins and protein assemblies in the presence and in the absence of metal ions by using several computational techniques: classical and ab-initio Molecular Dynamics, Monte Carlo and enhanced sampling by molecular dynamics algorithms. The most interesting systems we recently studied are:

- CoVid2 orf7 and orf8 accessory proteins, alone and in interaction with BST2 with the latter being a protein of the human immune system (Fig.2: covid+bst2;)
- Frataxin (FXN), a protein involved in iron transportation, whose malfunctioning is often related to tumor development (Fig.3: FXN)

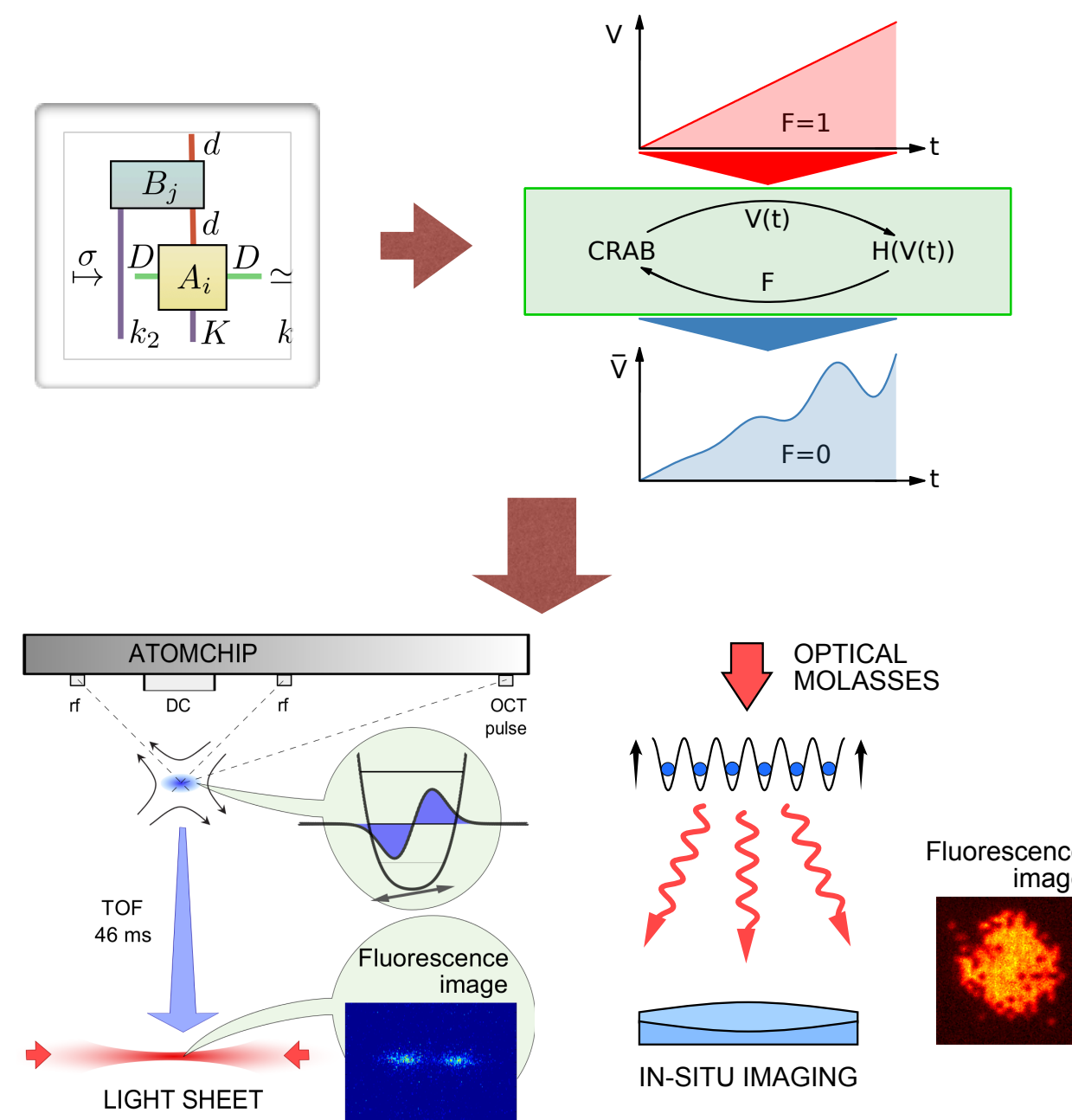
QUANTUM INFORMATION

QUANTUM (S. Montangero)

r.n. P. Facchi

Entanglement and other Quantum Correlations, Quantum Simulation, and Quantum Control

S. MONTANGERO'S GROUP RESEARCH LINES



- Development of efficient (classical and quantum) simulation and control techniques
- Simulation of interesting physics
- Define and probe fundamental limits given by energy, time and information constrains
- Experimental verification of theoretical optimal protocols

HPC COMPUTING RESOURCES 2017-2021

CINECA 2017-2021

EXPERIMENTAL PHYSICS

1.8%

OTHERS

1.4%

COMPLEX SYSTEMS

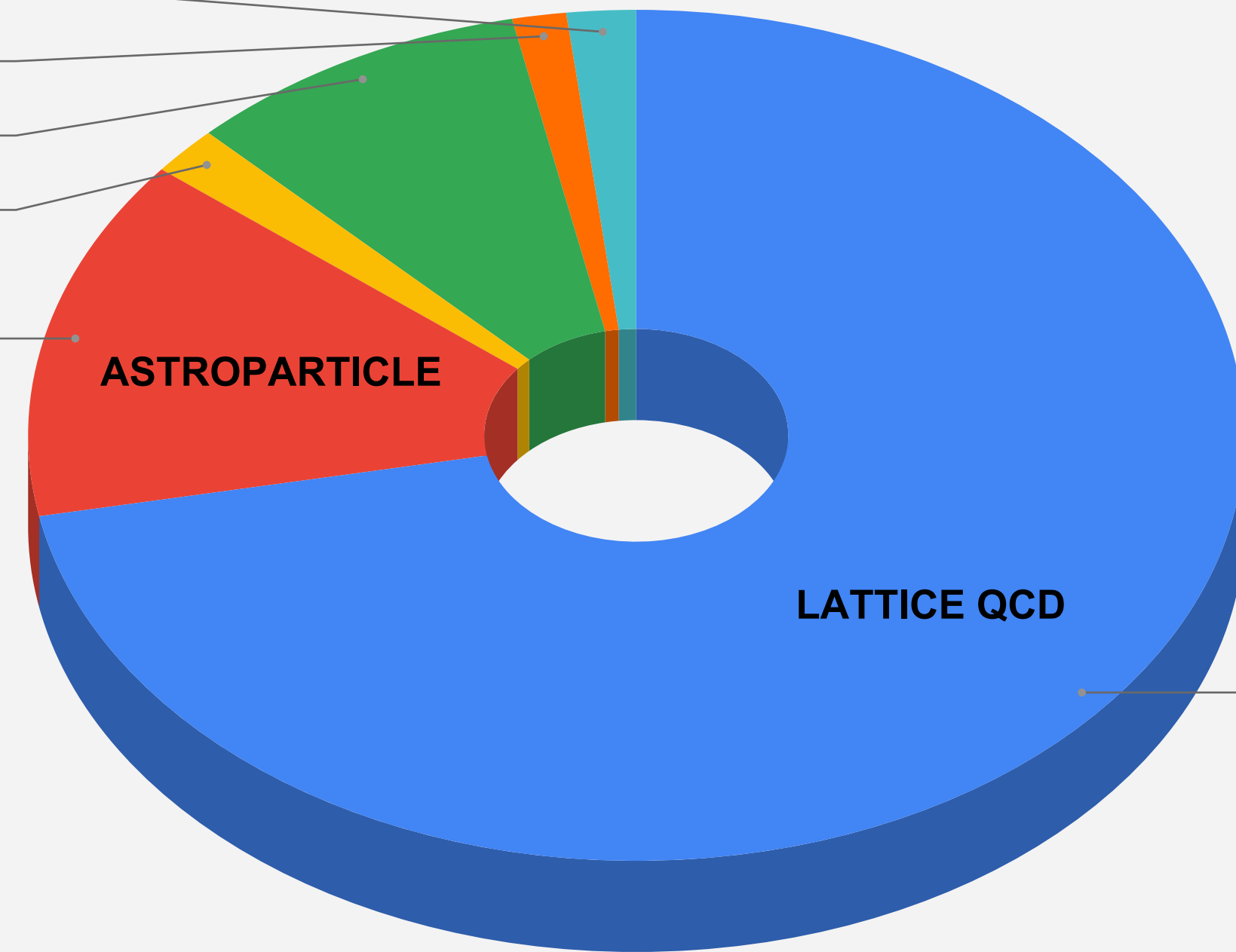
9.1%

NUCLEAR PHYSICS

1.8%

ASTROPARTICLE

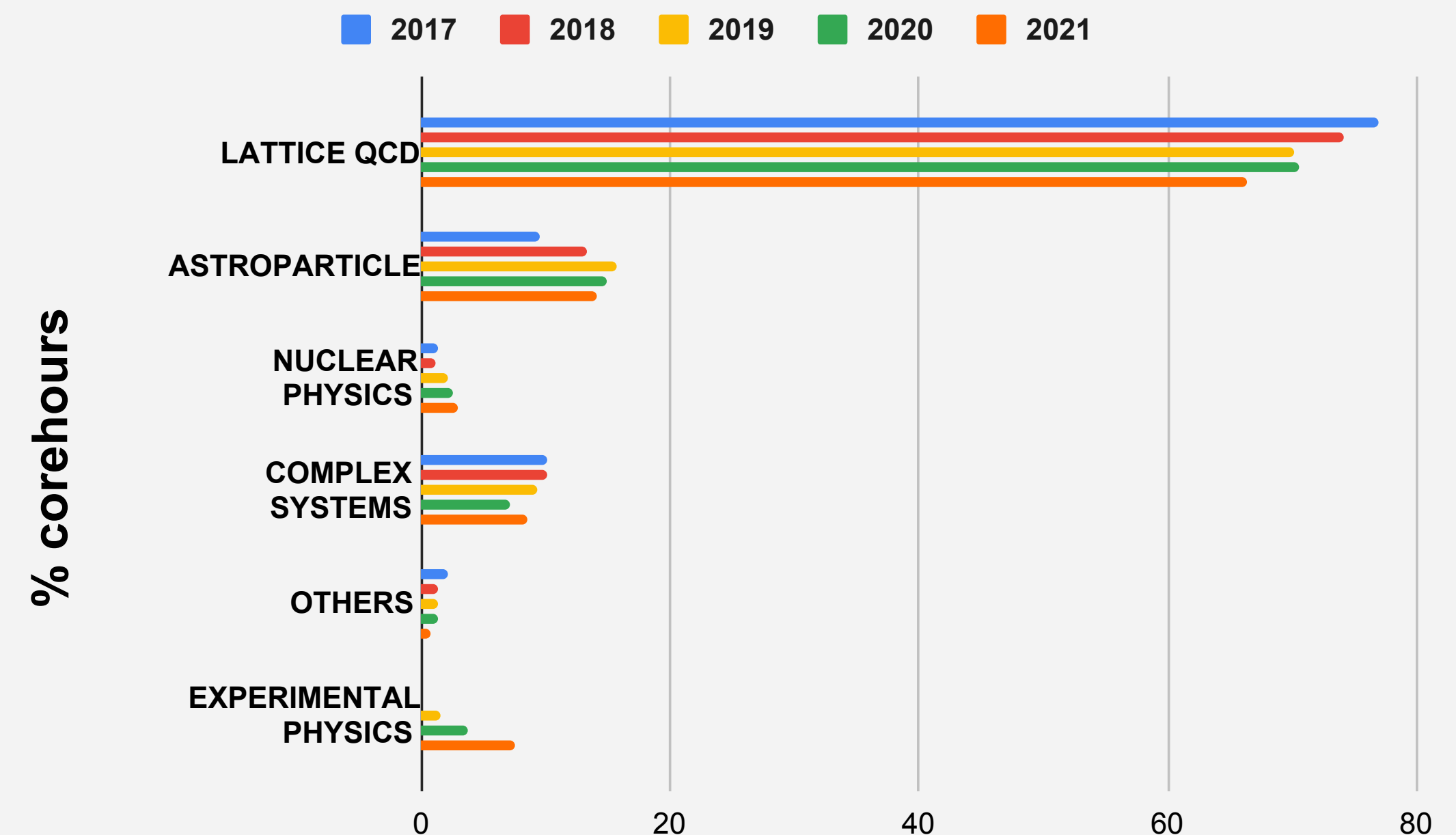
13.8%



LATTICE QCD
72.0%

AREA	corehours	%
LATTICE QCD	687,787,117	72.0
ASTROPARTICLE	131,826,951	13.8
NUCLEAR PHYSICS	17,546,676	1.8
COMPLEX SYSTEMS	87,396,389	9.1
OTHERS	13,724,017	1.4
EXPERIMENTAL PHYSICS	17,596,432	1.8
TOTAL	955,877,582	100

%corehours	2017	2018	2019	2020	2021
LATTICE QCD	76.97	74.09	70.06	70.62	66.31
ASTROPARTICLE	9.49	13.34	15.64	14.80	14.06
NUCLEAR PHYSICS	1.24	1.05	2.17	2.45	2.86
COMPLEX SYSTEMS	10.09	10.10	9.25	7.10	8.51
OTHERS	2.21	1.43	1.35	1.28	0.80
EXPERIMENTAL PHYSICS			1.53	3.75	7.46



OSSERVAZIONI CONCLUSIVE

- **La comunità di Fisica Teorica INFN nel corso degli ultimi 30 anni ha dato contributi fondamentali allo sviluppo del calcolo HPC. Il calcolo HPC é diventato di interesse strategico per tutta la comunità INFN (e anche per la comunità scientifica nazionale: PNRR).**
- **Molti progetti di ricerca in Fisica Teorica Computazionale (Lattice QCD, HEP, Astroparticle, Nuclear Physics, Complex systems) con un grande numero di ricercatori coinvolti.**
- **Il problema della transizione alle GPU** —> modificare e ottimizzare i codici esistenti
Esempio: Lattice QCD
 - I codici per LQCD sono stati scritti per girare su computer basati su CPU: data le notevoli dimensioni dei codici, la transizione alle GPU è onerosa: non esiste una corrispondenza “uno-a-uno” fra un codice CPU e un codice GPU.
 - Scrivere codici LQCD richiede grande “man power”: come tenere conto di possibili evoluzioni delle architetture di calcolo?
- **Il problema della sostenibilità degli sforzi per modernizzare e adeguare i codici alla evoluzione dell’hardware (impegno di considerevoli risorse umane)**
 - Un programma adeguato di formazione e reclutamento è cruciale per creare le competenze necessarie per un utilizzo efficiente delle presenti e future risorse di calcolo (GPUs,...), e anche per la ottimizzazione e lo sviluppo di nuovi algoritmi (—> **Centro di Calcolo Scientifico Nazionale (PNRR)**).

BACKUP SLIDES

Le risorse di calcolo

• Andamento storico (2012-2021)

RISORSE INFN SULLE MACCHINE CINECA A PARTIRE DA SETTEMBRE 2012 (Mcorehours)						
	FERMI	GALILEO	MARCONI (A1)	MARCONI (A2)	MARCONI (A3)	MARCONI100
Set 2012 - Dic 2013	115					
2014	110					
2015	100	15				
2016	100	15				
2017		15	18	120		
2018			9	120	164	
2019				120	164	
2020					164	10
2021					110	21

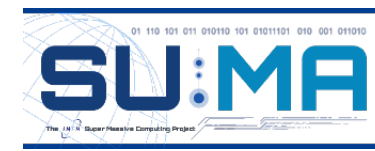
2018	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A1)	9.00	4.90	54.44%
MARCONI (A2)	120.00	119.00	99.17%
MARCONI (A3)	164.00	141.00	85.98%
2019	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A2)	120.00	119.20	99.33%
MARCONI (A3)	166.10	162.80	98.01%
2020	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A3)	169.00	163.00	96.45%
MARCONI100	10.11	11.93	117.98%
2021	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A3)	102.25	73.25	71.64%
MARCONI100	20.70	14.50	70.05%

Le macchine al CINECA (2012-...)

	processor	#cores/node	#accelerators/node	#nodes	#cores	(peak perf)/node [GFlop/s]	(peak perf)/core [GFlop/s]	peak performance [PFlop/s]	start date	end date
FERMI	IBM PowerA2	16		10,240	163,840	204.8	12.8	2.1	01-Sep-2012	18-Jul-2016
GALILEO	Intel Haswell	16		516	8,256	1,170.0	73.1	0.6	01-Feb-0205	20-Nov-2017
MARCONI-A1 (Broadwell)	Broadwell	36		1,512	54,432	1,300.0	36.1	2.0	04-Jul-2016	26-Sep-2018
MARCONI-A2 (KNL)	Knights Landing (KNL)	68		3,600	244,800	3,000.0	44.1	10.8	04-Jan-2017	01-Jan-2020
MARCONI-A3 (SKL)	Skylake	48		3,188	153,024	3,200.0	66.7	10.2	07-Aug-2017	
MARCONI100	IBM Power AC922	32	4 nVidia V100	980	31,360	32,000.0	1,000.0	31.4	04-May-2020	
GALILEO100	Intel Xeon Platinum	48	2 V100 (su 36 nodi)	554	26,592	3,530.0	73.5	2.0	15-Oct-2021	

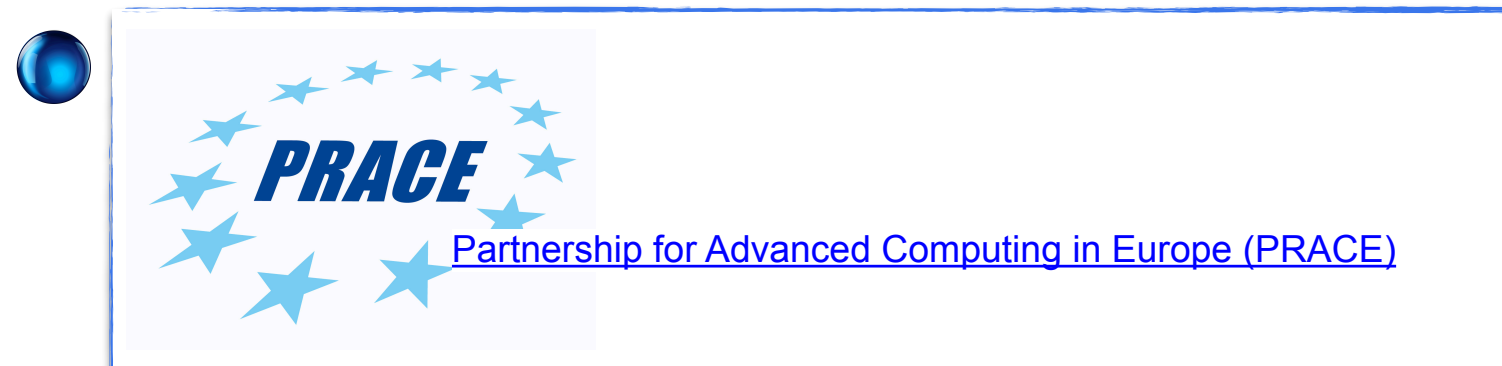
Le risorse di calcolo

Le risorse computazionali oltre l'Accordo CINECA-INFN (e.g. periodo 2017-2019)



agreement CINECA-INFN dal 2012 parzialmente finanziato da:

- progetto premiale SUMA (0.5 Meuro: GALILEO)
- progetto HPC_HTC (CIPE) (1.5 Meuro: MARCONI-SKL)



	# progetti	corehours
CINECA-INFN AGREEMENT (2017-2019)		730,000,000
ISCRA-C	45	20,615,000
ISCRA-B	40	205,440,950
PRACE	30	925,928,640
ALTRE RISORSE INTERNAZIONALI	11	367,000,000
TOTALE		1,518,984,590
GRAN TOTALE		2,248,984,590
Lavori pubblicati (con uso di risorse HPC)	315	

● **Moltiplicatore per accesso a risorse ISCRA e PRACE: $2,250,000,000/730,000,000 = 3$**

Le risorse di calcolo HPC

(in via di approvazione)

- **Accordo Quadro CINECA-INFN 2022-2026**
- **Accordo Attuativo dell'Accordo Quadro CINECA-INFN**

- **MARCONI-A3**
- **MARCONI100**
- **GALILEO100**



	CPU (mhz,core, ...)	Total cores / Total Nodes	Memory per node	Accelerator
MARCONI-A3	Intel SkyLake 2x Intel Xeon 8160 @2.1GHz 24 cores each	48*3216 / 3216	192 GB	-
MARCONI100	IBM Power9 AC922 @3.1GHz 32 cores HT 4 each	32*980 / 980	256 GB	4x NVIDIA Volta V100 GPUs per node, NVlink 2.0 16 GB
GALILEO100	2 x Intel CascadeLake 8260 @2.4 GHz 24 cores each,	48*554 / 554	384 GB 3.0 TB	34 nodes with 2x NVIDIA V100 per node, PCIe3

LEONARDO

Sustained performance: 249.4 PFlop/s
Peak performance: 322.6 PFlop/s



Specifiche tecniche

Il supercomputer Leonardo è costituito da 3 parti:

- La prima, chiamata Booster, è formata da oltre 3.000 nodi basati sui sistemi a raffreddamento diretto a liquido BullSequana XH2000, che integrano una CPU Intel Xeon SP di terza generazione e quattro GPU Nvidia Ampère A100, per un totale di quasi 14.000 acceleratori;
- La seconda, chiamata Data Centric Partition, è formata da oltre 1.500 nodi basati sugli stessi BullSequana XH2000, ma che ospitano processori Intel Xeon di generazione futura.
- L'intero sistema è collegato ad un terzo modulo di servizio e visualizzazione, ed ad un'area di archiviazione multi-tier ad alte performance, con una capienza aggregata di oltre 100 PetaByte, basata sui prodotti DDN. Tutte le parti del sistema comunicano tra di loro grazie un'interconnessione a bassa latenza InfiniBand HDR a 200Gb/s per collegamento, allocata su tecnologia Nvidia Networking.

I processori Intel Xeon di generazione futura sono ottimizzati per eseguire carichi di lavoro computazionalmente intensi in sistemi di calcolo ad alte prestazioni consentendo computing con avanzate capacità di accelerazione AI integrate.

- Più di 136 BullSequana XH2000 rack di raffreddamento diretto a liquido
- 250 PFLOPs HPL Linpack Performance (Rmax) aggregata
- 3+PB RAM
- 10 ExaFLOPs di prestazioni FP16 AI
- 3456 server equipaggiati con Intel Xeon Ice Lake e GPU con architettura Nvidia Ampère
- 1536 server con processori Intel Xeon SP di prossima generazione
- 5PB di storage ad alte prestazioni
- 100PB di storage a grande capacità
- Larghezza di banda di interconnessione minima di 200Gb/s per singolo link InfiniBand HDR
- 9MW di Potenza elettrica aggregate
- Oltre 140 km di cablaggi in fibra ottica

Le risorse di calcolo HPC

● Accordo Quadro CINECA-INFN 2022-2026

ACCORDO QUADRO DI COLLABORAZIONE PER LO SVOLGIMENTO DI ATTIVITÀ DI RICERCA E SVILUPPO NEL SETTORE DEL CALCOLO SCIENTIFICO AD ALTE PRESTAZIONI (HPC) IN AMBITO DI FISICA DELLE ALTE ENERGIE, FISICA ASTROPARTICELLARE, FISICA NUCLEARE

Art. 2 – Oggetto e finalità dell'Accordo

Con il presente Accordo Quadro, le Parti instaurano una collaborazione rivolta allo

- sviluppo e sperimentazione di sistemi di calcolo ad alte prestazioni e ad alta capacità;
- sviluppo di algoritmi e applicazioni relative all'ambito della modellazione e della simulazione numerica e dell'analisi dei dati in aree di interesse della fisica fondamentale, in particolare utilizzando architetture innovative dei processori, delle reti d'interconnessione e delle strutture di input-output;

● Accordo Attuativo dell'Accordo Quadro CINECA-INFN

ACCORDO ATTUATIVO DELL'ACCORDO QUADRO DI COLLABORAZIONE PER LO SVOLGIMENTO DI ATTIVITÀ DI RICERCA E SVILUPPO NEL SETTORE DEL CALCOLO SCIENTIFICO AD ALTE PRESTAZIONI (HPC) IN AMBITO DI FISICA DELLE ALTE ENERGIE, FISICA ASTROPARTICELLARE, FISICA NUCLEARE

- **MARCONI-A3: 60 Mcorehours/anno fino a dismissione**
- **MARCONI100: 60 Mcorehours/anno fino a dismissione**
- **GALILEO100: 6 Mcorehours/anno fino a dismissione**

● **LEONARDO**

PARTIZIONE	2023	2024	2025	2026
General Purpose (CPU)	165 nodi	300 nodi	300 nodi	300 nodi
Booster (GPU)	3 Mnodehours	3 Mnodehours	3 Mnodehours	3 Mnodehours

su 1536 nodi *Intel Sapphire Rapids (48 cores)*

su 3456 nodi *Intel Ice-Lake (32 cores)*

(in via di approvazione)

Le risorse di calcolo HPC

ISCRA: Italian SuperComputing Resource Allocation



CINECA, through the **Italian SuperComputing Resource Allocation - ISCRA**, releases Call for Proposals.

CINECA, the Italian most powerful HPC center, twice a year **will directly award in excess of 100 millions core hours**, to ensure an adequate supply to scientists and engineers for HPC-related research.

CINECA infrastructure offers different HPC resources to its users. The available resources are divided in three categories:

- The TIER-0, top level computing resources, which is the new **MARCONI100** machine and can be accessed through class B and C projects.
- The TIER-1 level, is **GALILEO100** (BROADWELL) and can be accessed through class C and B projects.
The Big Data resources and new state-of-the-art public CLOUD.
The data infrastructure is available for data analysis, visualization, post-processing, bio-informatics applications.
The **CLOUD** infrastructure integrates and completes the HPC ecosystem, providing a tightly-integrated infrastructure that covers both high performance and high flexible computing. The flexibility of the CLOUD will better adapt to the diversity of user workloads, while still providing high-end computing power.
- The DGX resources:
Available through ISCRA-C: these projects aim to support researchers in the domain of Machine Learning and Artificial Intelligence and their applications.
- The Quantum Computing Resources.
Available through ISCRA-C, CINECA makes quantum computing resources of various kinds available to its users. It will be possible to request machine time on our Tier-0 system to emulate complex quantum circuits (both general purpose and special purpose type) and directly request quantum computing resources (currently of quantum annealing type).

Class B projects are received twice a year. They go under peer-review evaluation and a 3 month delay is expected before your project gets access to HPC resources. For each user it is allowed to have only one class B project each 6 months as Project Investigator.

Class C projects are received through continuous submission and reviewed once per month. An average period of about 15 days is required for activating the project. For each user it is allowed to have only one class C project each 6 months as Project Investigator.

Le risorse di calcolo HPC

PRACE, EuroHPC JU (Joint Undertaking)



- International, not-for-profit
- 25 member countries - pan-European supercomputing infrastructure enabled by 5 Hosting Members
 - BSC (Spain), CINECA (Italy), ETH/CSCS (Switzerland), GSC (Germany), GENCI (France)
- Access on basis of peer-reviewed (open) science & industry proposals
- Additionally, schools, workshops, PRACE IP ...



- Based on 2 EU Council Regulations (2018 & 2021)
- Objectives
- Build and operate a world class integrated HPC and data infrastructure
 - Enable member states to improve HPC competency
 - Foster HPC skills, education and training
 - Develop HPC core technology
 - *European Processor Initiative (EPI)*
 - *Energy efficient HPC*
 - *Quantum Computing*

- Enable high-impact scientific & engineering discovery and R&D.
- Tier-0 computing and data management resources and services through **competitive peer review**.
- Training & education via schools, workshops, seminars.
- Enabled by 5 Hosting Centres.
- **No procurement, no technology development.**

In 2021 EuroHPC planned resources and timelines

Infrastructure and Operations

- **5 x petascale machines** @ 15-30 petaflops. In operation by Q1 2021. Bulgaria, Czech Republic, Luxembourg, Portugal, Slovenia.
- **3 x pre-exascale machines**. In operation Q2/3 2021:
 - CSC - Finland *Cray: 375PF sustained, 552PF peak; GPU, x86, data analytics, cloud container partitions*
 - Cineca - Italy *ATOS-Bull Sequana 249PF sustained, CPU-GPU, DDR5 & local NVM for data analysis*
 - BSC - Spain
- 2 x exascale in operation by 2022-2023. In coordination with EPI (European-based technology) for at least one machine?
- Data I/O, management, storage and security federation for impact: GEANT, EOSC etc

Access

There is an access policy at <https://eurohpc-ju.europa.eu/access-our-supercomputers>

Talk S. Ryan @ GGI Mini Workshop "Phase transitions in particle physics"