# IL CALCOLO NELLA FISICA TEORICA

Leonardo Cosmai (INFN - Sezione di Bari)

INFN

*Workshop sul Calcolo nell'INFN*, Loano, 22 maggio 2023

Commissione Calcolo Reti

# Computational Theoretical Physics @ INFN

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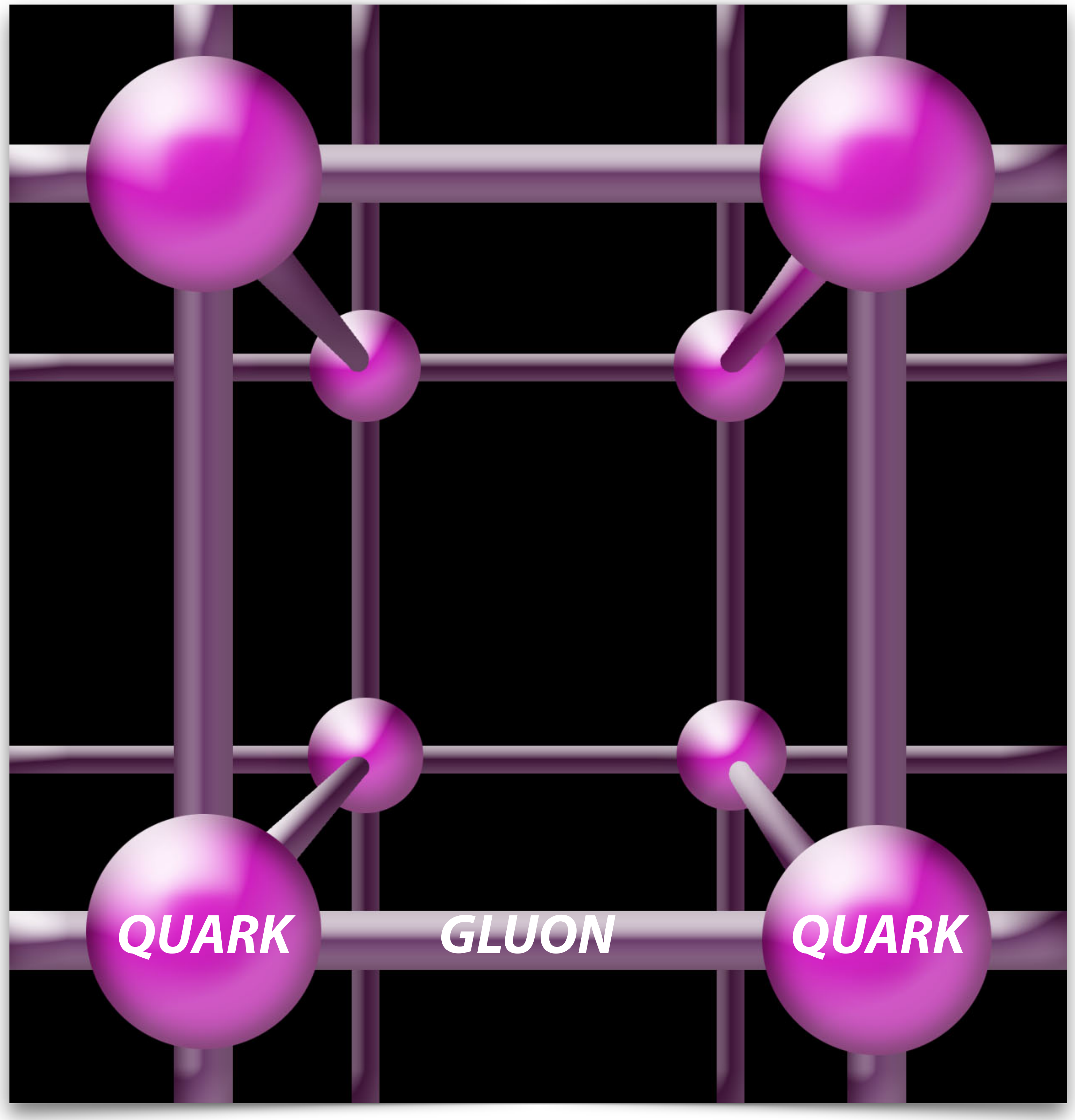
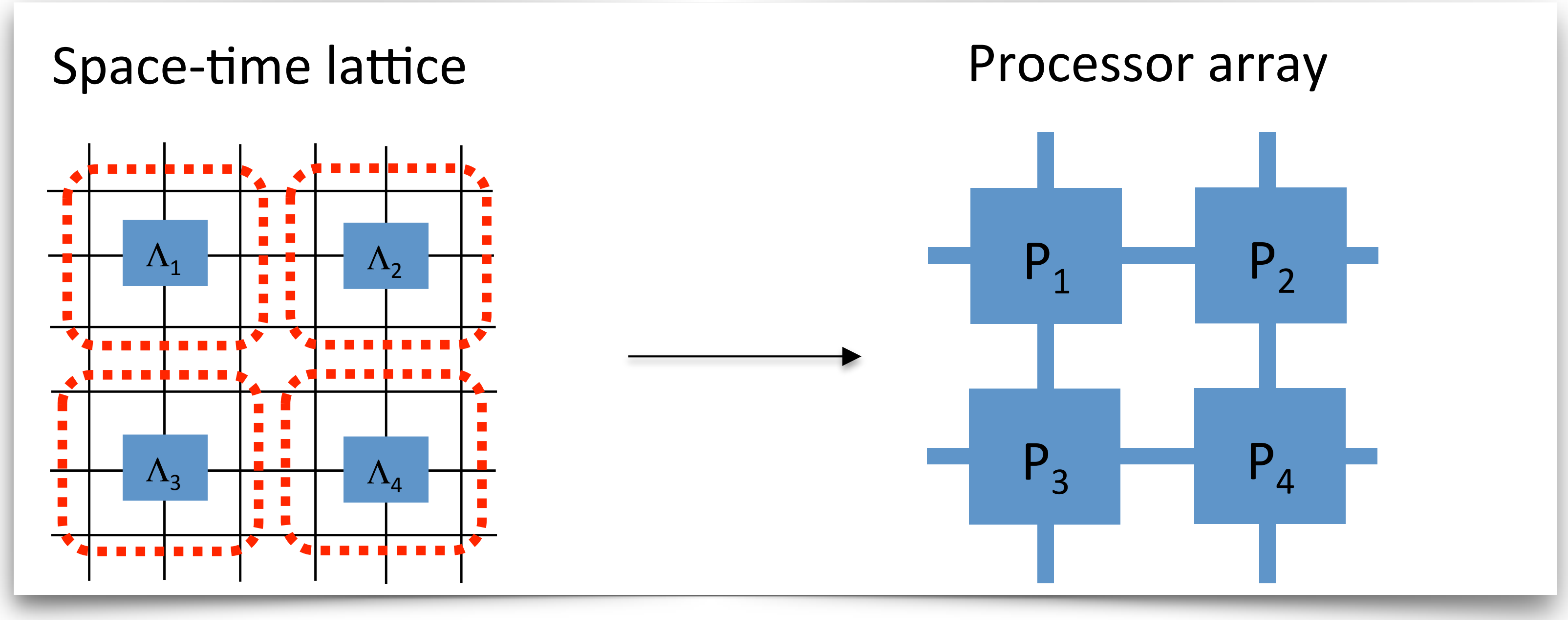



A. Ukawa, arXiv:1501.04215



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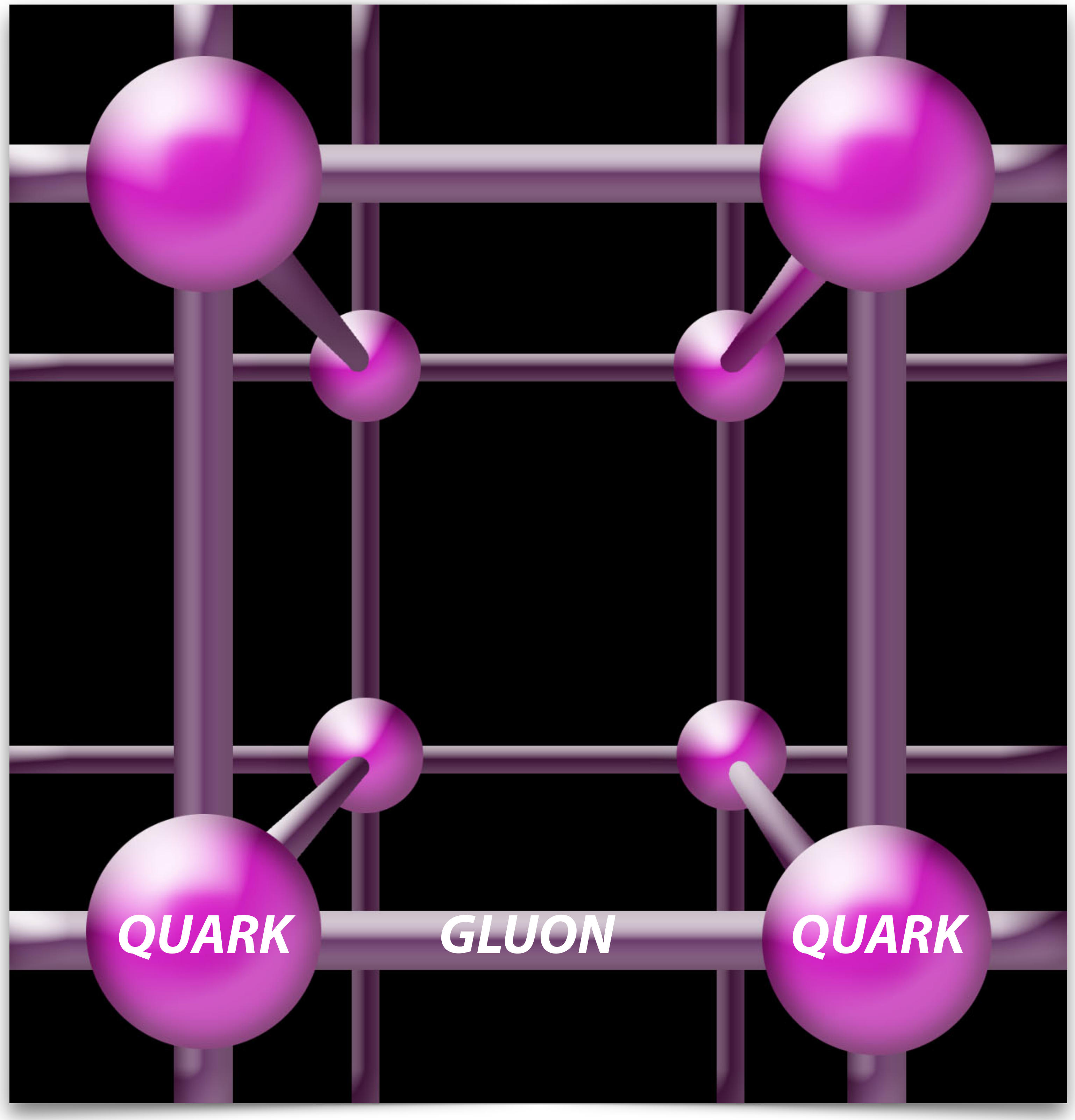
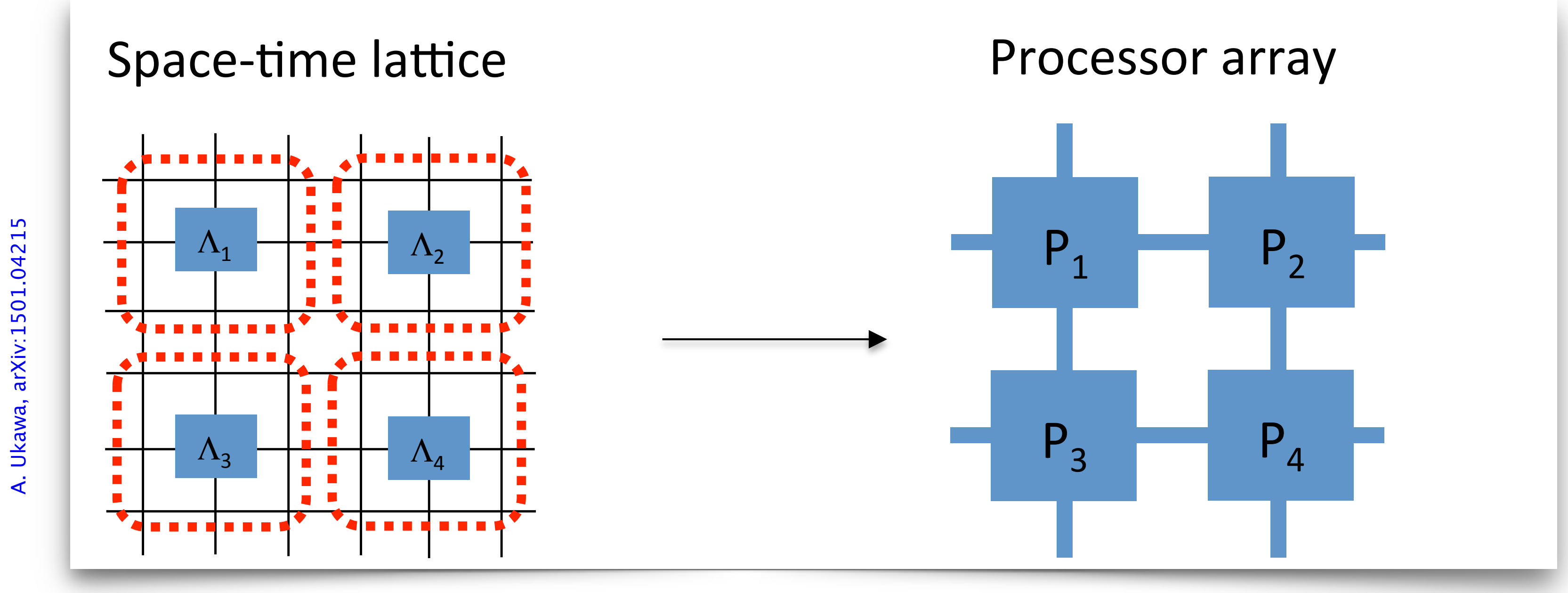
- In 1974 the seminal paper by Ken Wilson “Confinement of Quarks” paved the way to the study of fundamental interactions from first principles.
- The main idea was to discretize the continuous space-time into a finite number of points arranged in a 4-dimensional lattice.
- In this manner, it was demonstrated that it is possible to compute all physically relevant observables of phenomenological interest solely from the fundamental equations of the theory.



# The birth of Lattice QCD

- **To compute physical observables on lattice gauge configurations, one essentially needs to evaluate multidimensional integrals (with a huge number of integration variables).**

- **The path was laid out, but it required the development of algorithms, computational methods, and dedicated hardware.**

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- Apart from contributing to the first seminal papers in LQCD, INFN emerged as a key player on the international stage in the development of dedicated hardware. This significant undertaking, known as the APE project, spanned from 1988 to 2004.

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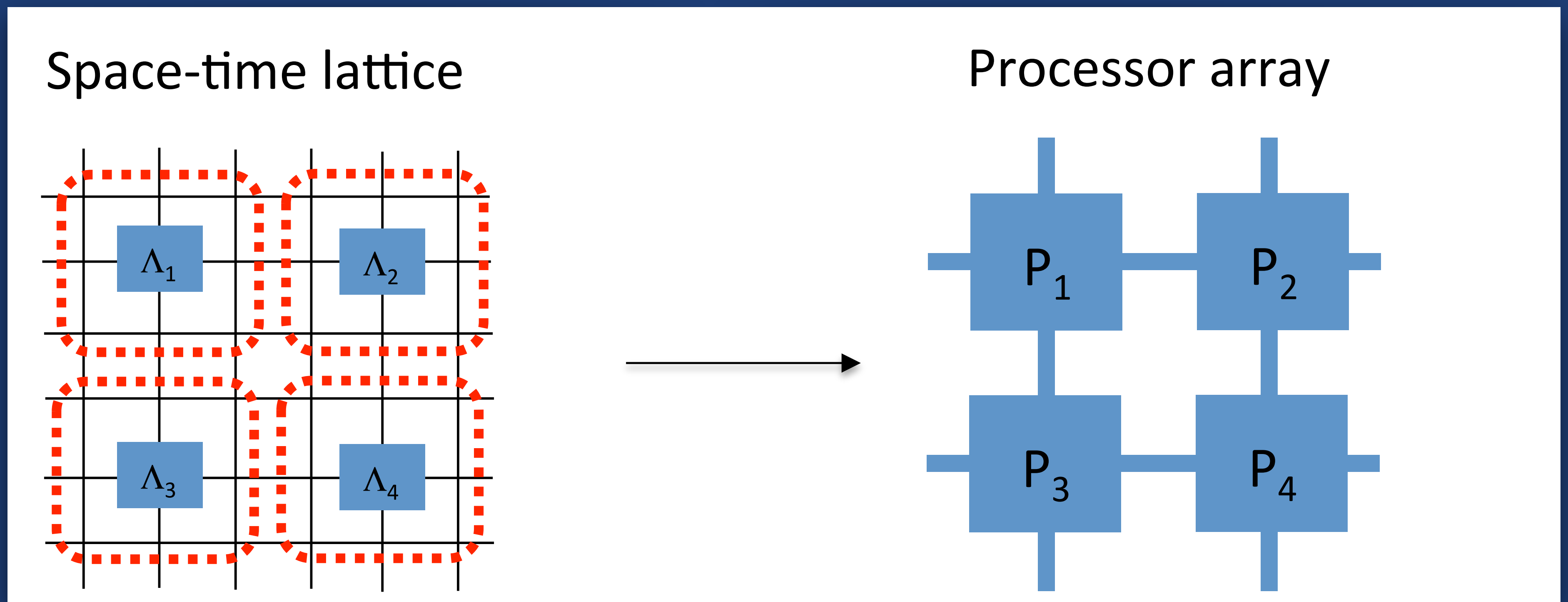
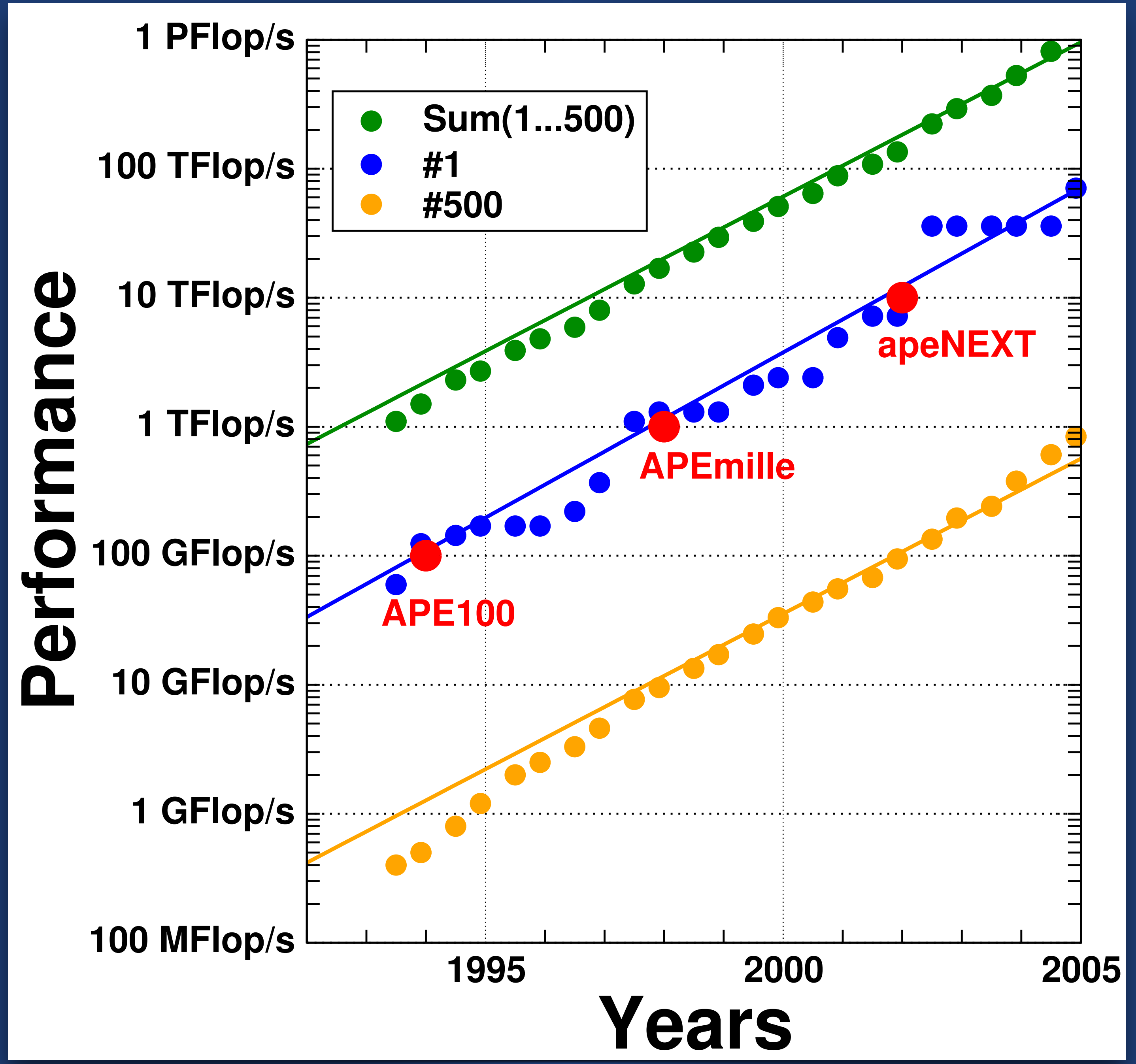



| | YEAR | peak speed |
|---|---|---|
| APE1 | 1988 | 1 GFlop/s |
| APE100 | 1994 | 0.1 TFlop/s |
| APEmille | 2000 | 0.8 Tflop/s |
| apeNEXT | 2004 | 10 TFlop/s |



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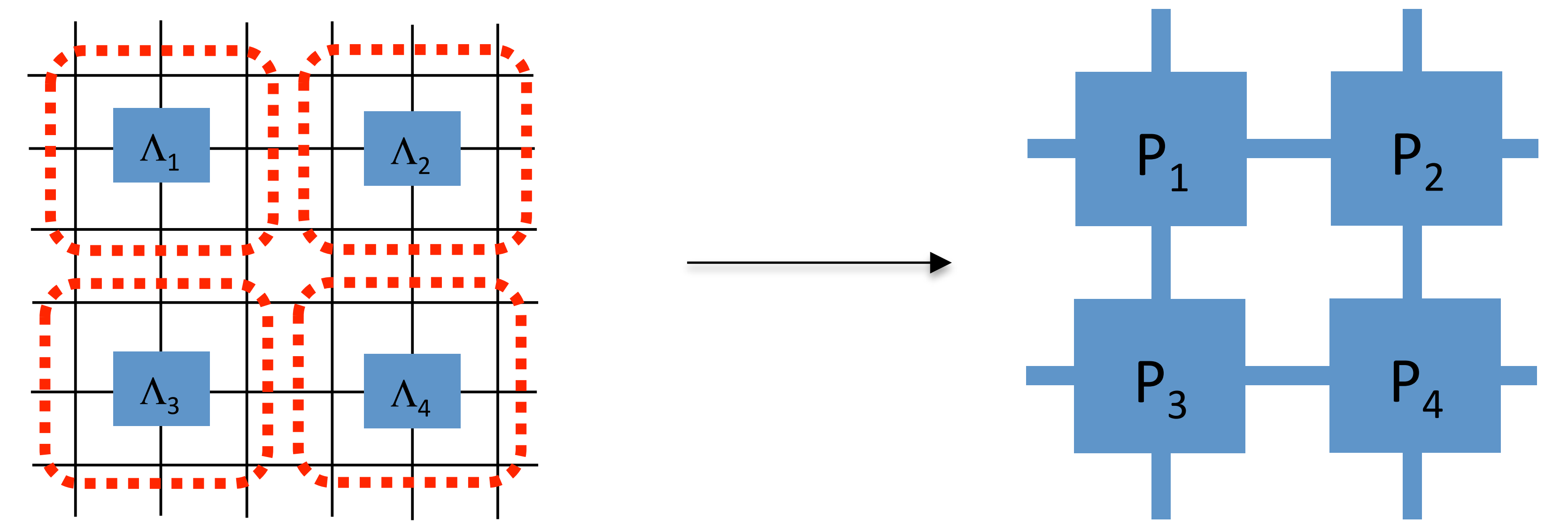


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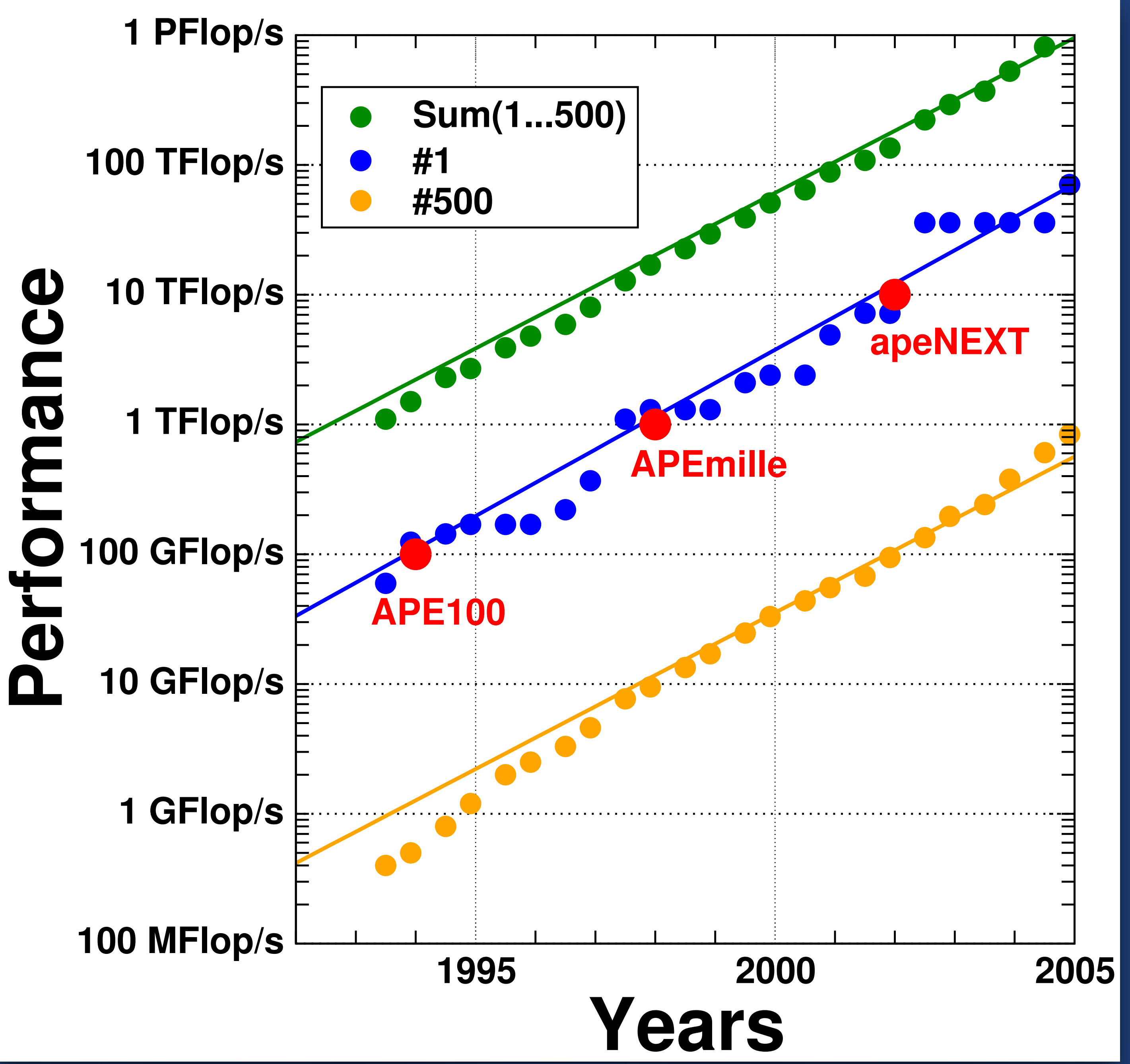


# Exascale frontier

**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 $V \sim (10\,\mathrm{fm})^4$ at a lattice spacing $a = 0.04\,\mathrm{fm}$ ($a^{-1} \sim 5\,\mathrm{GeV}$) (lattice size $256^3 \times 512$)

$\sim$ 12,000 Exaflop hours $= (12{,}000 \times 3{,}600\,\mathrm{s} \times 10^{18}\,\mathrm{Flop/s})$ floating-point operations

$\sim 10^{25}$ floating-point operations

# Lattice QCD as an extraordinary tool for understanding Nature

- Many experimental and theoretical efforts to search for physics in the Standard Model and beyond require supporting QCD calculations that must be carried out to high precision.

- Lattice QCD, which has evolved over four decades, stands as the preferred tool for tackling high precision calculations. With increasingly sophisticated methods and algorithms, it has continually advanced its capabilities, and is now a mature field.

- Similar to experiments (where data are first collected and and later analyzed) the Lattice QCD workflow can be factorized into:
  1) Generation: the so-called *gauge configurations* are generated using the *Markov chain Monte Carlo Method* and then stored to disk.
  2) Measurement of observables (e.g. correlation functions) relevant for the investigation that is carried out are computed on these stored gauge configurations.

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**GENERATION**

Gauge-filed configurations are generated by means of Monte Carlo techniques

A certain number of configurations (each consisting of a fixed number of complex numbers) are stored on disk for subsequent analysis.

↓

**MEASUREMENT**

Measurement of physical observables are computed from the configurations.

↓

**ANALYSIS**

Averaging of the measurements over configurations, extrapolations to certain limits.

Possible comparison of the outcome of these calculations with experimental results.

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*VERY COMPUTE-INTENSIVE —> REQUIRE STATE-OF-THE-ART SUPERCOMPUTERS*

*Typical data size —>* $\mathcal{O}(1)$ **PB** *for configurations and derived data*

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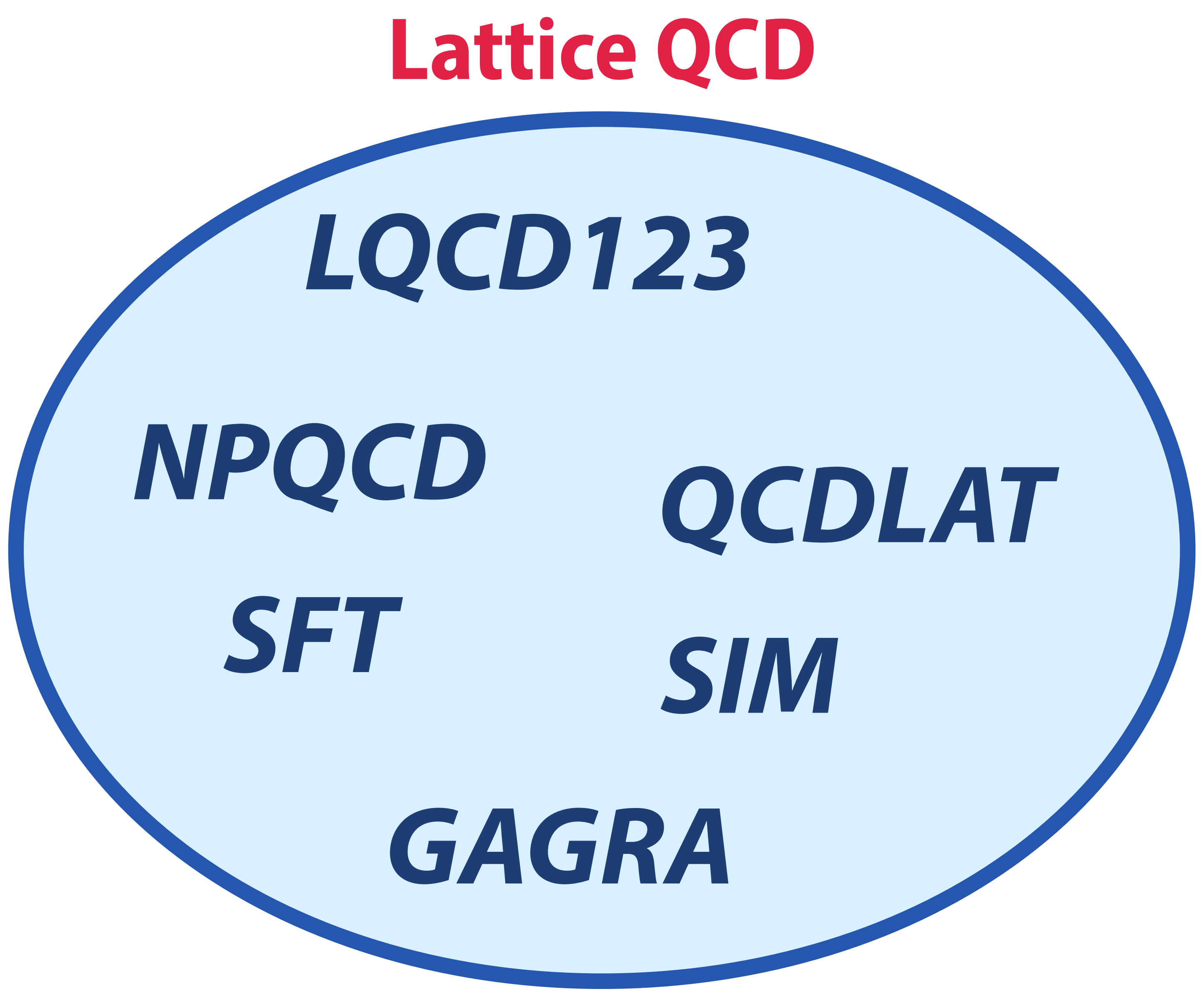

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**Cosmology and Astroparticle Physics**

- *INDARK*
- *NEUMATT*
- *TEONGRAV*

**Lattice QCD**

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

**Physics of Complex Systems**

- *BIOPHYS*
- *ENESMA*
- *FIELDTURB*

**Standard Model Phenomenology**

- *QFTATCOL*

**Quantum Information**

- *QUANTUM*

**Nuclear Physics**

- *MONSTRE*
- *NUCSYS*

**Condensed Matter**

- *NEMESYS*

# Computational Theoretical Physics @ INFN —> *not only Lattice QCD*   ~200 researchers

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Many research groups are involved in the activities of ICSC (Centro Nazionale di ricerca in HPC, Big Data and Quantum Computing)

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# Nuclear Physics

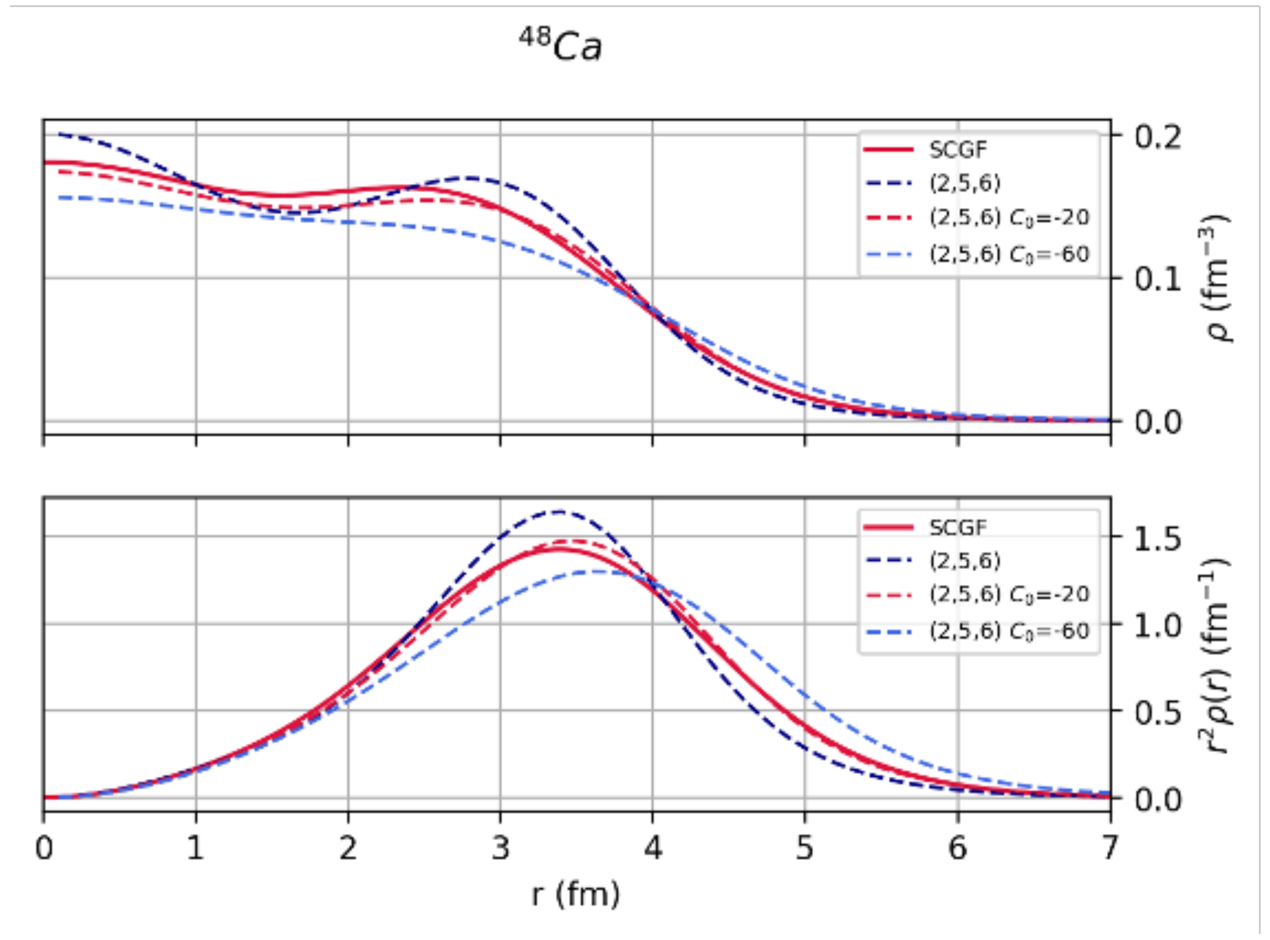
***MONSTRE***
***NUCSYS***

## *MONSTRE*

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

**Keywords**

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




**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

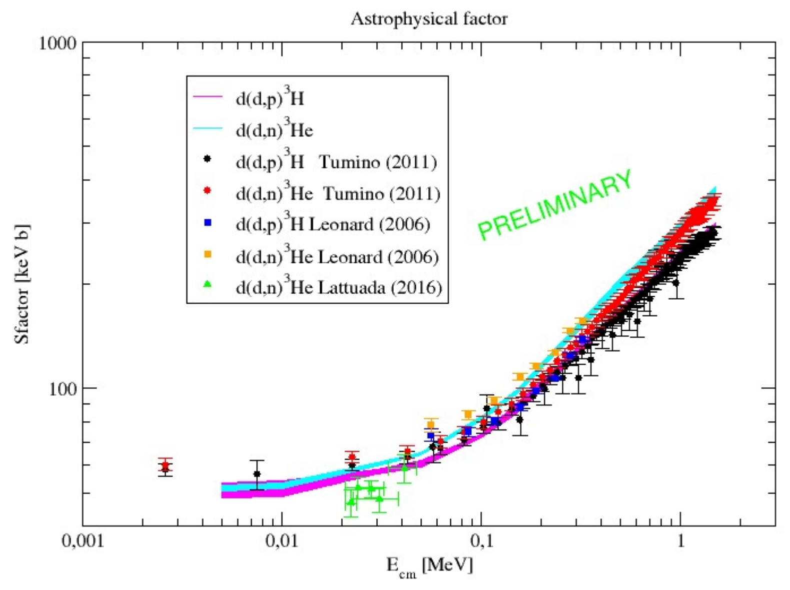
**Calcoli *ab initio***

- Quantum Monte Carlo
- Machine Learning

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

## *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 nxn (independent on energy E), T=known vectors, X=solution vector

**Calculation of M & T**
Tipically 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**

# Standard Model Phenomenology

***QFTATCOL***

## *QFTATCOL*

- Application of Quantum Fiedl 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 [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"

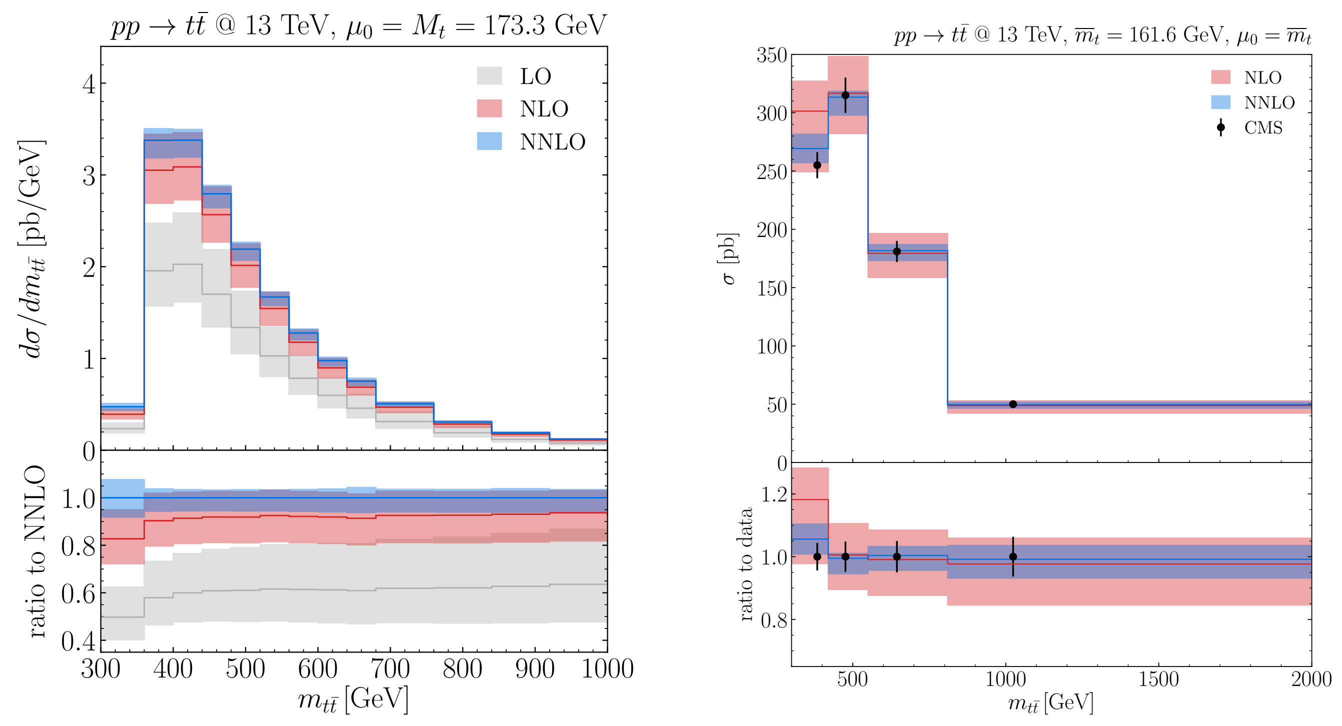



Figure: $m_{t\bar{t}}$ at different accuracies. NNLO greatly improves agreement with CMS data

HPC for CSN4 2 / 3

# Quantum Information

***QUANTUM***

***QUANTUM***

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

The major objectives of the QUANTUM collaboration are the investigation

of typical quantum mechanical effects and phenomena via three major, interrelated avenues:

1. Entanglement and other Quantum Correlations;

2. Quantum Simulation → **quantum-inspired techniques applied to the simulation of**

   **high-energy physics**

   **lattice gauge theories**

   **many-body systems**

3. Quantum Control.

# Cosmology and Astroparticle Physics

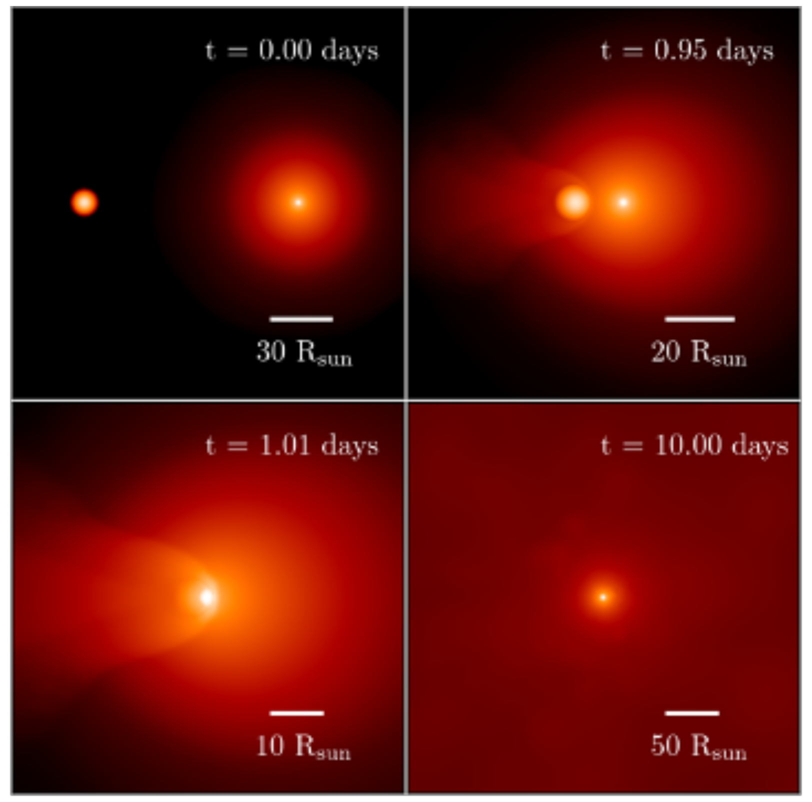
*INDARK* *NEUMATT* *TEONGRAV*

## *TEONGRAV*

- Modelling of **gravitational wave sources** via both semi-analytical and numerical methods;
- Equation of state of matter in the inner core of **neutron stars**;
- Dynamics of **black hole formation**;
- Electromagnetic counterparts of **gravitational wave signals**;
- Study of strong-field phenomena in modified gravity theories.

**Analysis of observational data and numerical simulations of compact objects**
(*e.g. Machine learning techniques to analyze gravitational waves from black hole binaries*)

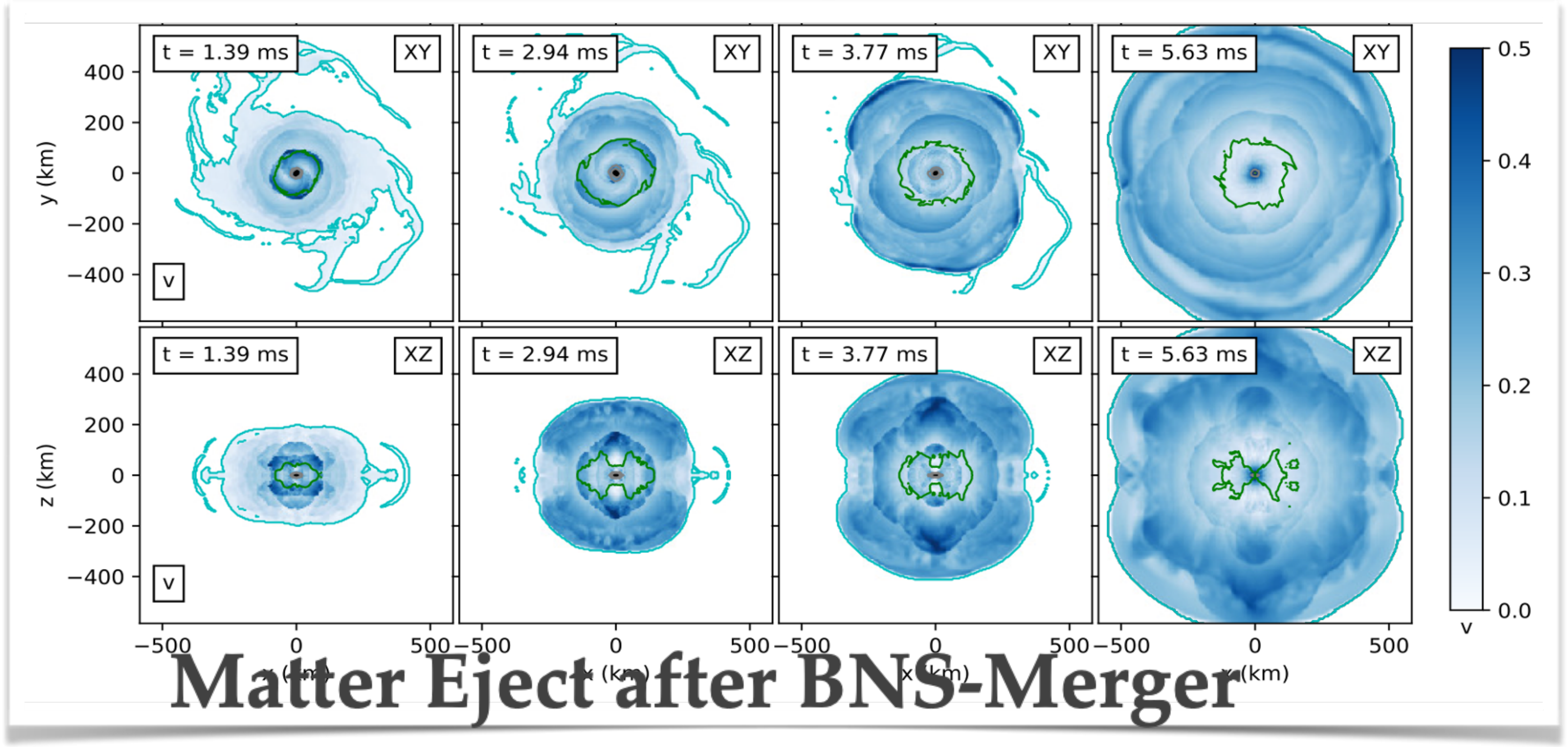
**Hydrodynamics and magnetohydrodynamics simulations using state of the art codes in both the Newtonian and the General Relativistic regime**
(*e.g. Model dynamical evolution and formation of stellar-mass and supermassive black holes via N-body simulations* )




## *NEUMATT*

**GRAVITATIONAL WAVE SIGNAL FROM THE MERGE OF BINARY NEUTRON STARS**

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.




## *INDARK*

dark energy and matter, axions, neutrinos, modified gravity

Markov Chain Monte Carlo codes interfaced with Boltzmann codes

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:

- *Produzione di simulazioni di osservabili cosmologiche*
  - Simulazioni del campo di CMB, ideale o come osservato da diversi esperimenti passati e futuri. Utilizzate per es. per validare estimatori o per studiare il potere vincolante di esperimenti futuri rispetto a nuova fisica.
  - Simulazioni N-body della distribuzione di materia per la costruzione di covarianze ed estimatori di nongaussianità.
  - Simulazioni di calibrazione per la formazione delle strutture cosmologiche per modelli di axion dark matter, gravità modificata, interacting dark energy. Post-processing delle simulazioni prodotte per gli stessi modelli.
  - Calibrazione e ottimizzazione di codici N-body.

# Physics of Complex Systems

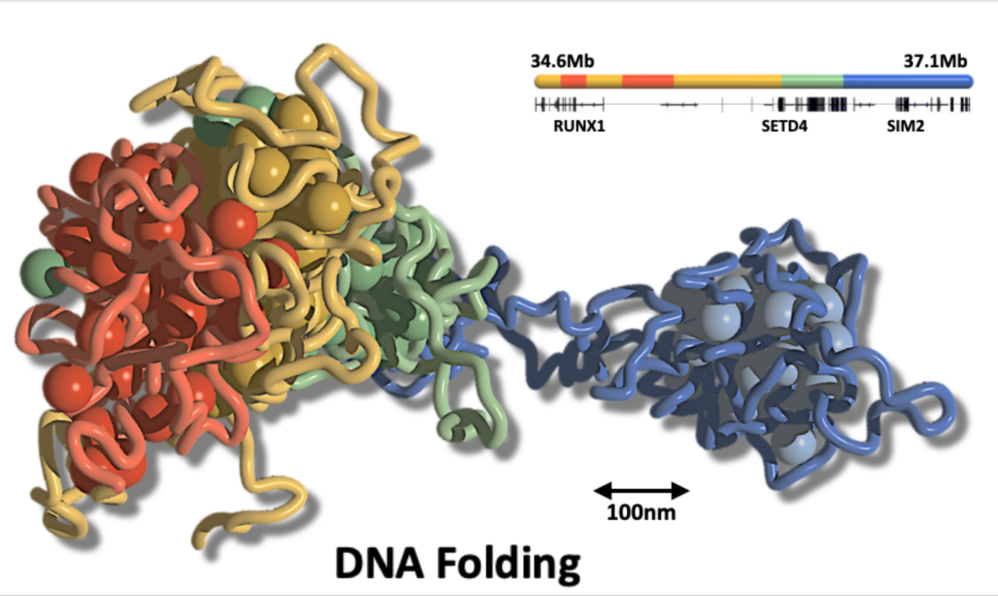
***BIOPHYS*** *(G. La Penna)* ***ENESMA*** *(C. Presilla)*
***FIELDTURB*** *(G. Boffetta)*

## *BIOPHYS*

Investigation of the three-dimensional structure of the mammalian genome

Structural properties of proteins and protein assemblies

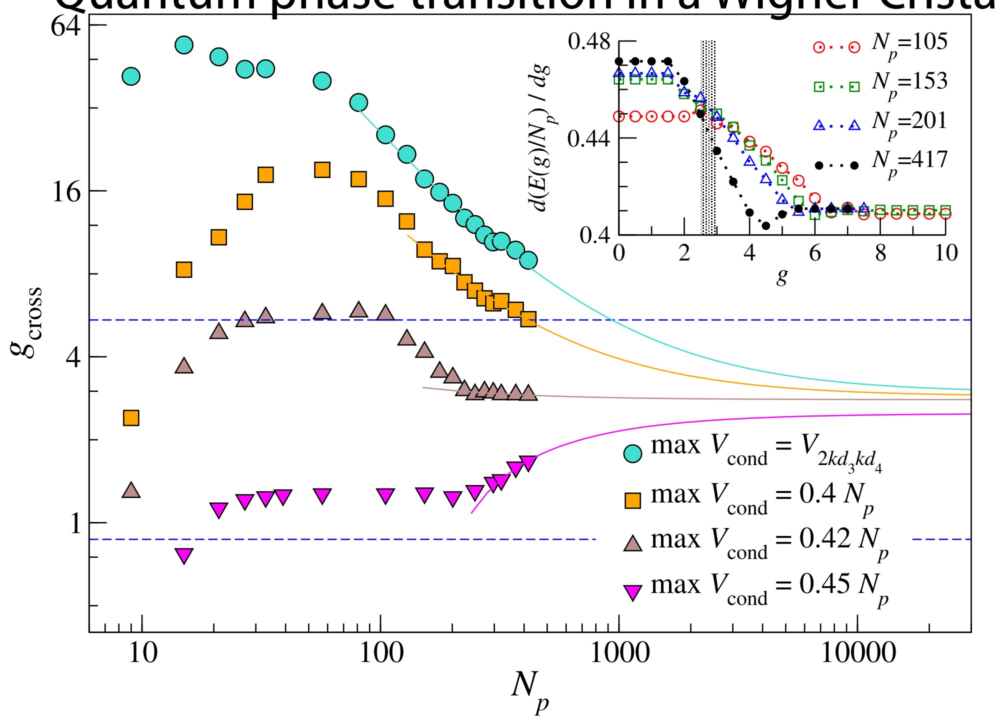
**Computational techniques**: classical and ab-initio Molecular Dynamics, Monte Carlo and enhanced sampling by molecular dynamics algorithms.




## *ENESMA*

**Simulation of disordered systems** (spin glasses, models of structural glasses, hard and soft spheres near the jamming point, optimization and inference problems, models of light propagation in disordered media, ecological models, etc...).

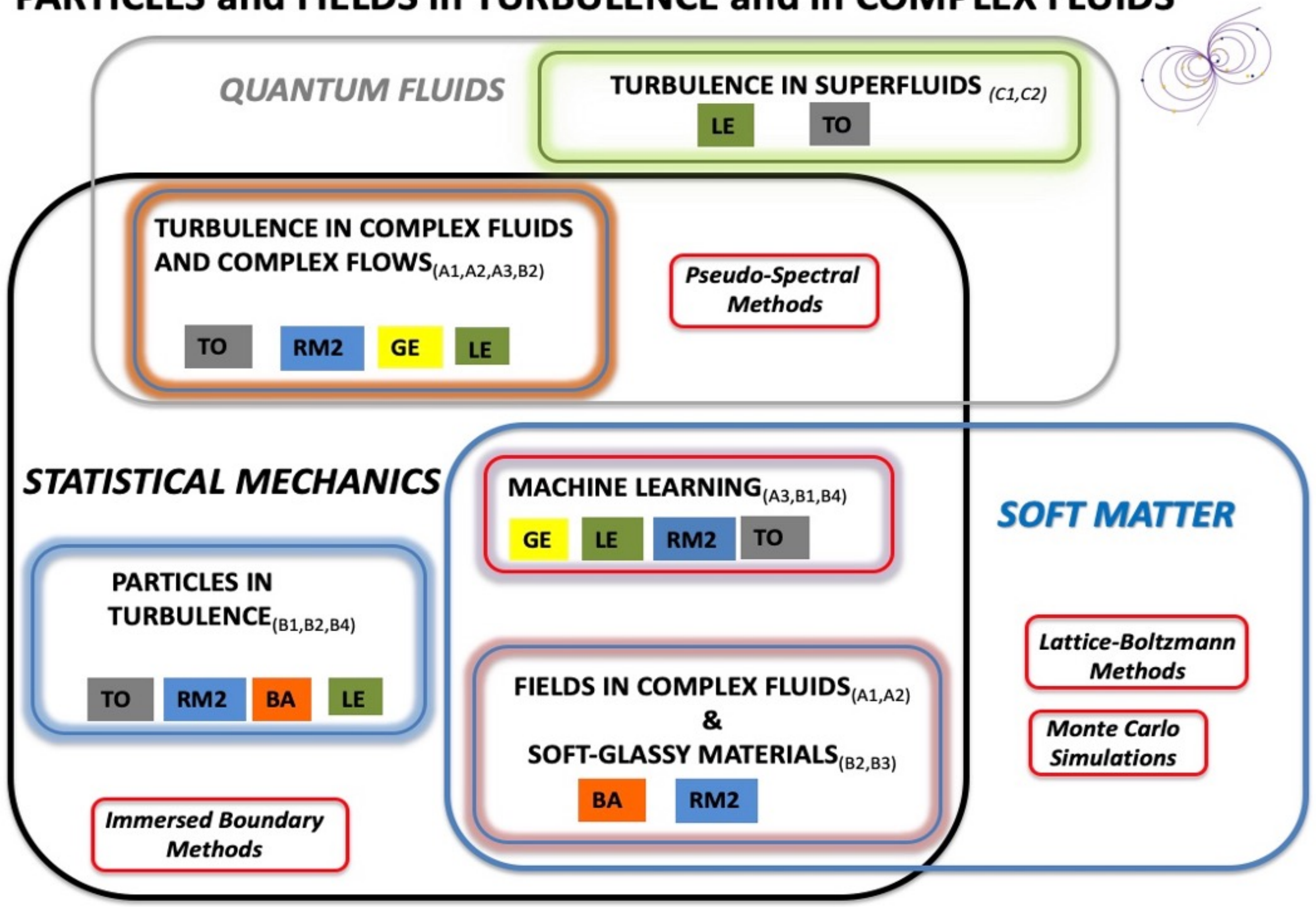
Quantum phase transition in a Wigner Cristal




## *FIELDTURB*

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

**PARTICLES and FIELDS in TURBULENCE and in COMPLEX FLUIDS**

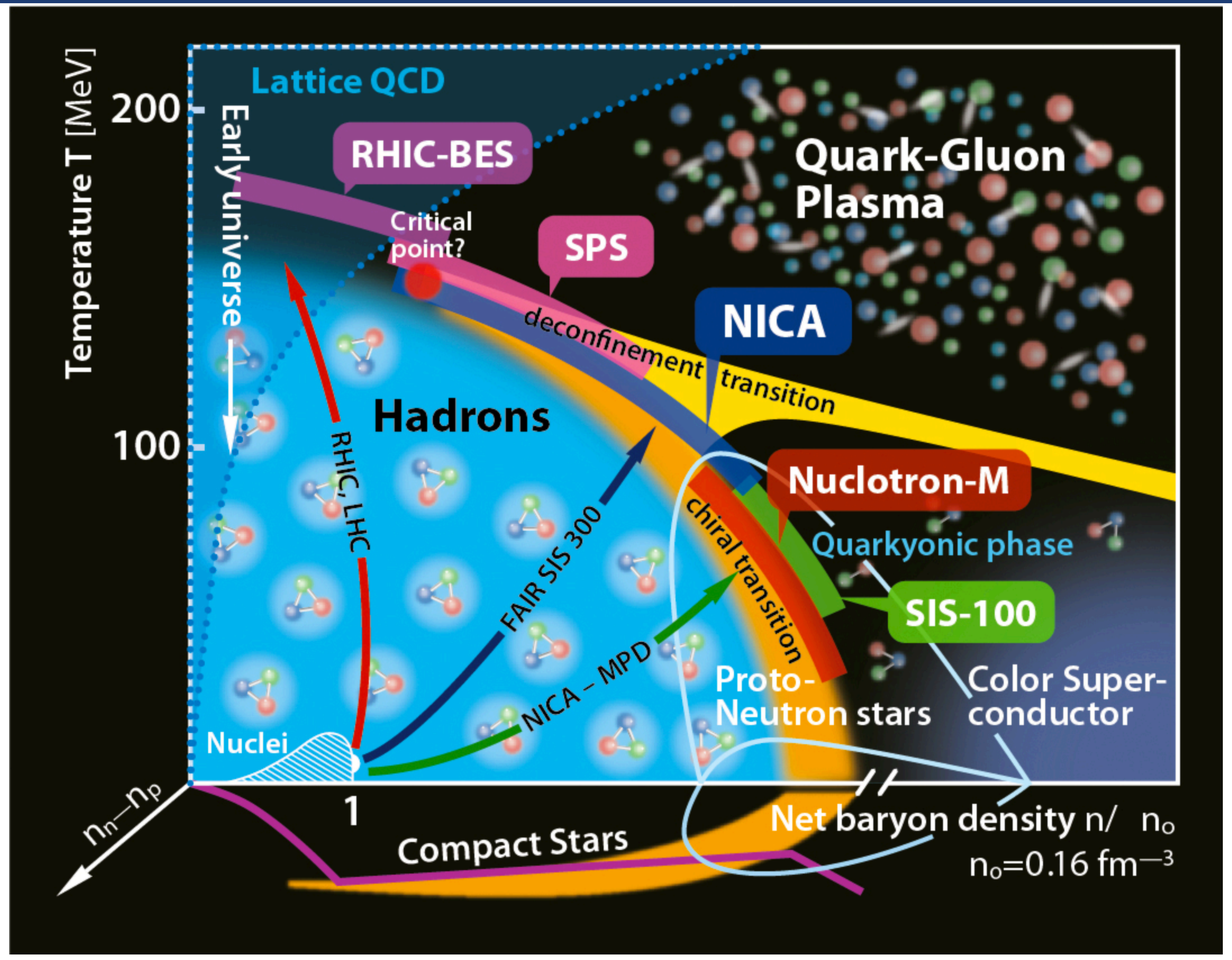



**(—> talk Giuseppe Negro)**

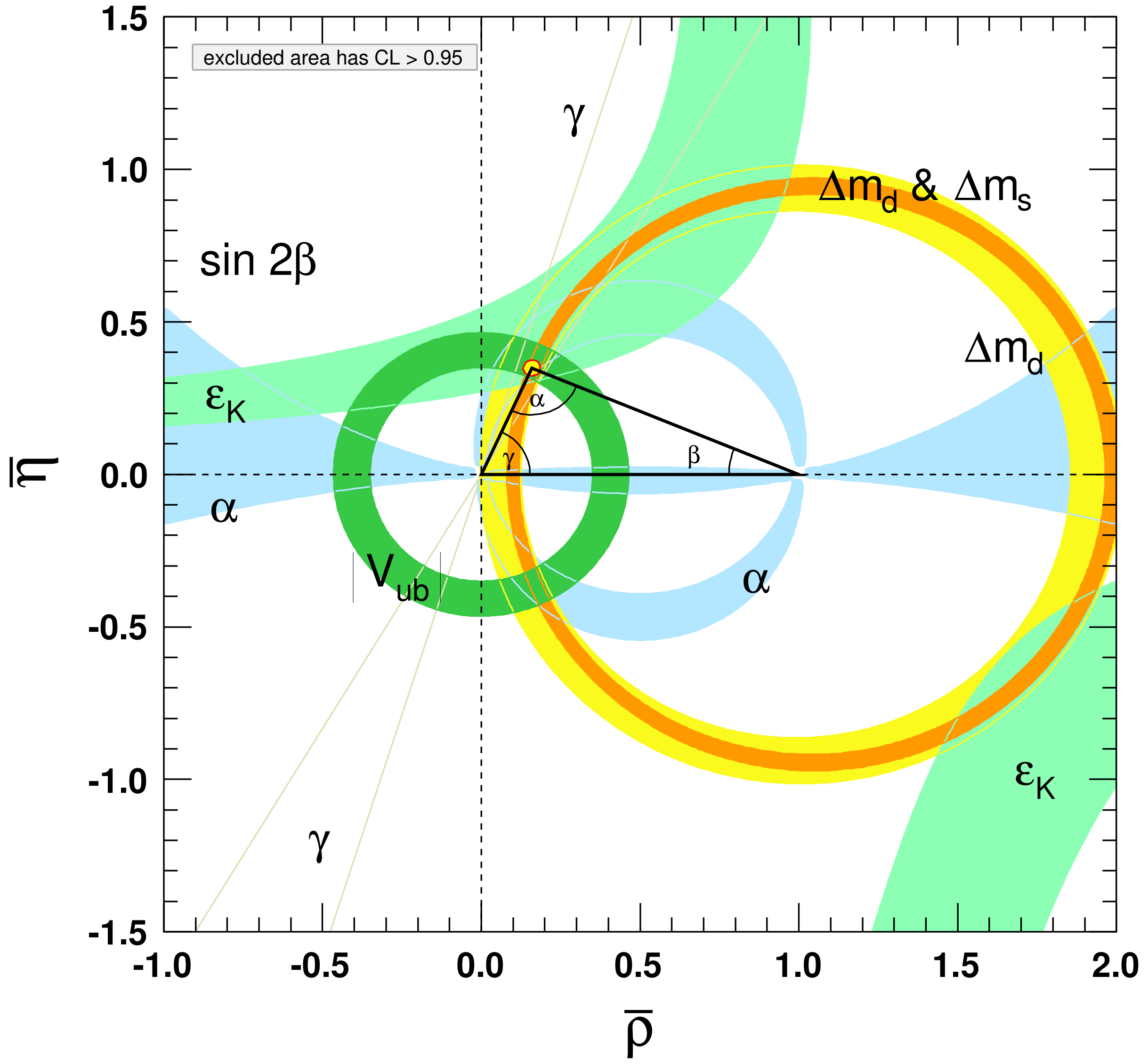
# Lattice QCD

*LQCD123 NPQCD QCDLAT*
*GAGRA SFT SIM*

## Study of QCD in extreme conditions

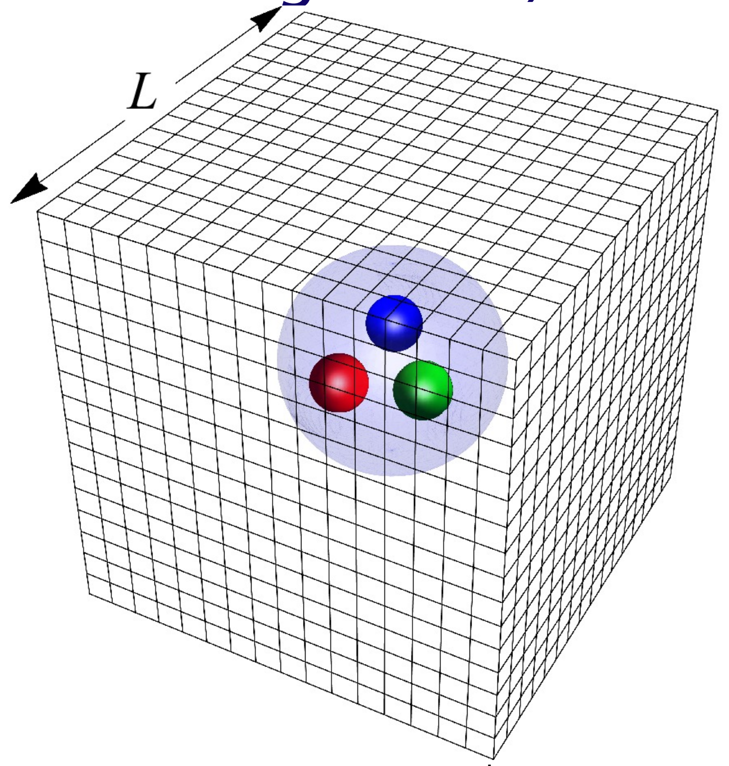


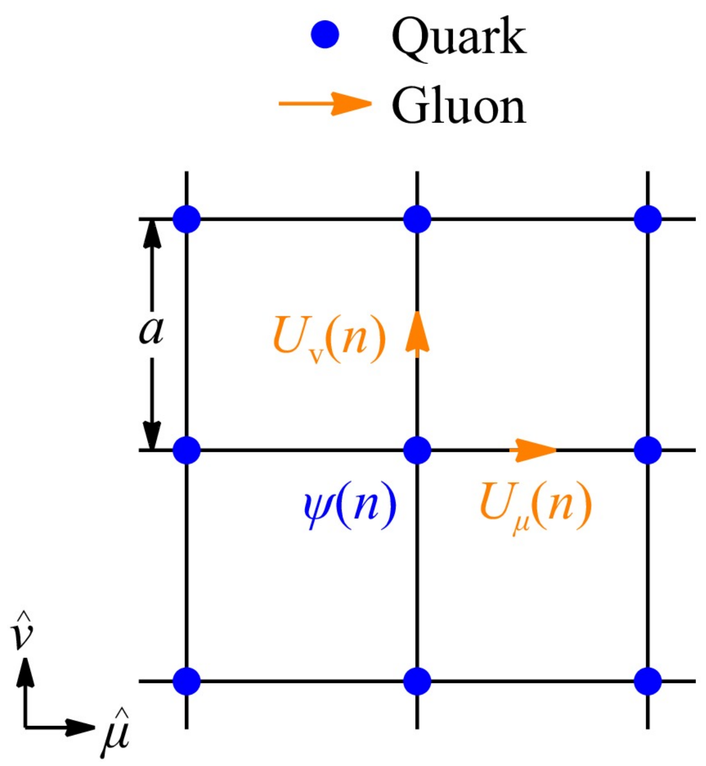

## Precision studies of flavor physics, within and beyond the Standard Model




Generates an ensemble of gluon field configurations $U$ distributed according to the QCD action (using the hybrid Monte Carlo algorithm):

$$\text{Cost} \propto V^{9/8} a^{-2}$$




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.

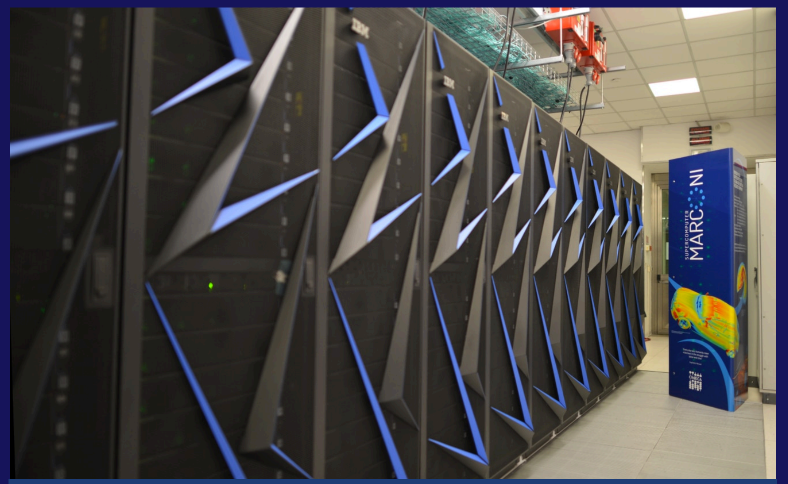
**(—> talk Michele Pepe)**

# HPC resources for Theoretical Computational Physics @ INFN

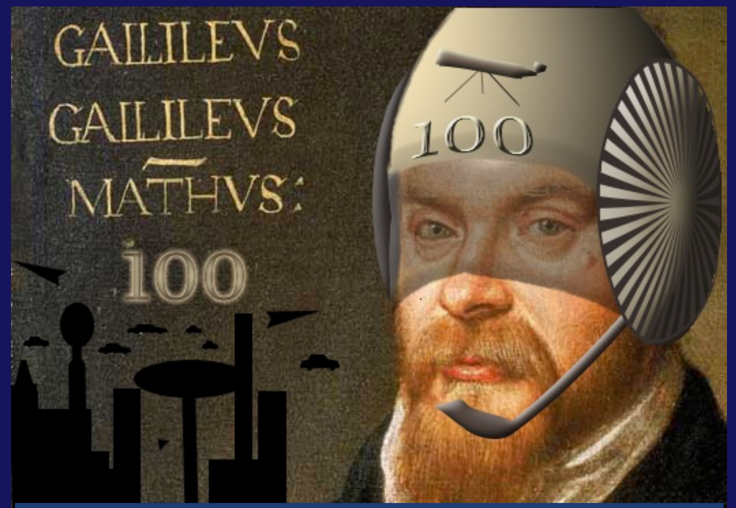
## Domestic resources

### Cineca-INFN agreement

MARCONI-A3
60 Mcorehours



MARCONI100
15 Mcorehours




MARCONI-A3
6 Mcorehours

LEONARDO
Booster: 3 Mnodehours
GP:

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

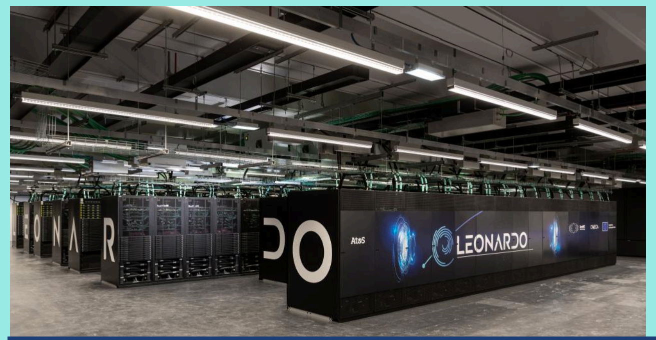
ISCRA
CINECA

## European resources

### EuroHPC JU

EuroHPC
Joint Undertaking

LUMI supercomputer
375 PFlop/s - FINLAND



LEONARDO supercomputer
295 PFlop/s - ITALY


MARENOSTRUM 5
205 PFlop/s - SPAIN


HPC Vega IZUM
6.92 PFlop/s - SLOVENIA

MELUXINA supercomputer
12.81 PFlop/s - LUXEMBOURG

DEUCALION supercomputer
7.22 PFlop/s - PORTUGAL

DISCOVERER supercomputer
4.51 PFlop/s - BULGARIA

KAROLINA supercomputer
9.59 PFlop/s - CZECH Republic

# Computational Theoretical Physics @ INFN - some final remarks

- Computational Theoretical Physics @ INFN:   a rich and enduring tradition, fundamental contributions to the advancement of High Performance Computing (HPC) endeavors.

- Numerous research projects spanning various fields, including Lattice QCD, High-Energy Physics (HEP), Astroparticle Physics, Nuclear Physics, and Complex Systems, involve a substantial number of researchers.

- Challenge: Ensuring the long-term sustainability of efforts to maintain and enhance codes and algorithms, which necessitates a considerable amount of human resources.

- The availability of cutting-edge computing resources is vital for maintaining competitiveness on an international scale.

**This work is (partially) supported by**

**ICSC – Centro Nazionale di Ricerca in High Performance Computing, Big Data and Quantum Computing, funded by European Union – NextGenerationEU.**

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Big Data and Quantum Computing