# High Performance Computing for Theoretical Physics

## Leonardo Cosmai

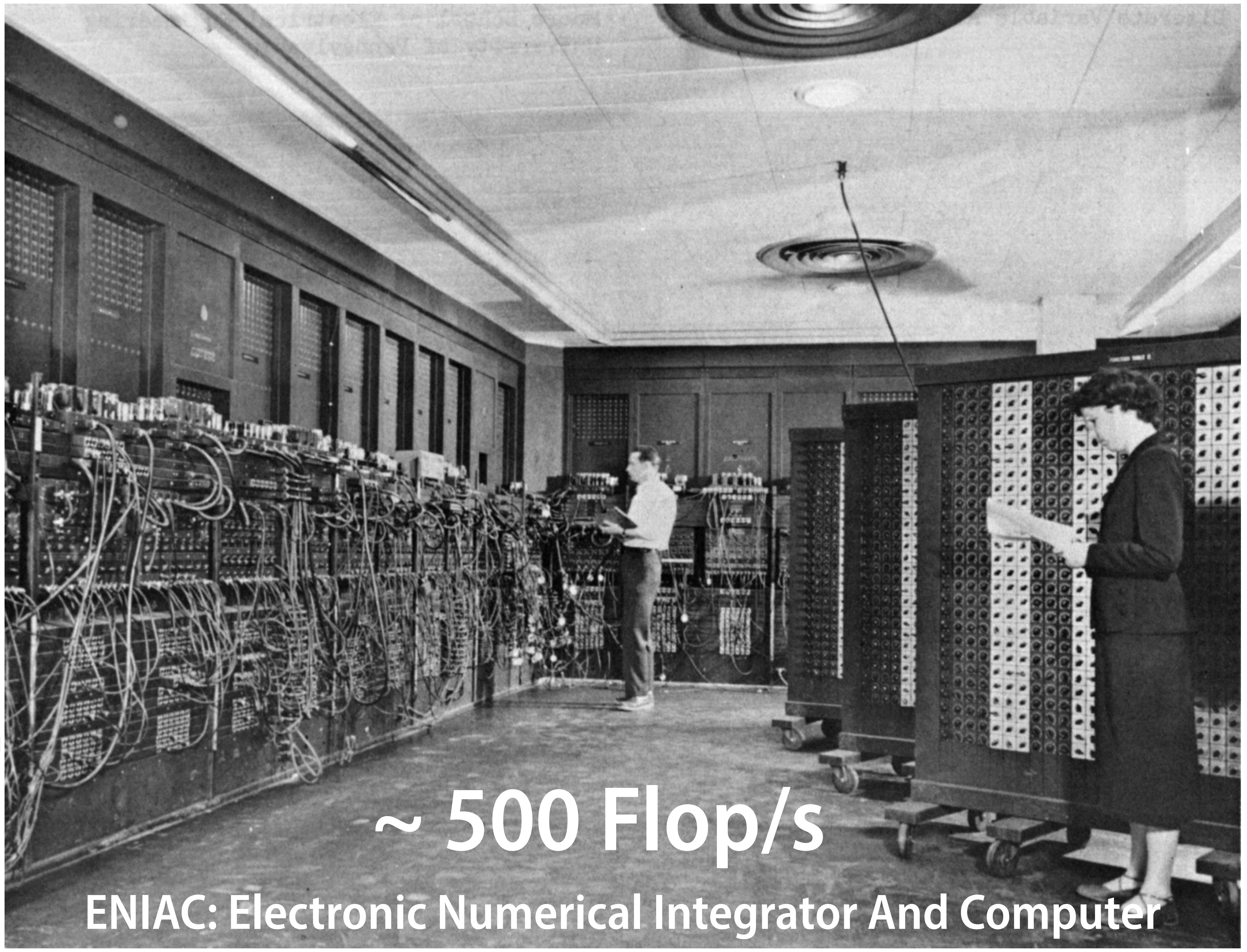
INFN

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

*Bari, 10 Ottobre 2023 - Aula A “Beppe Nardulli” - Dipartimento di Fisica Università di Bari*

# Prolegomena: Computer simulation

- Computer simulation is a widely used method for studying complex systems, with applications in nearly every field of scientific study.
- The history of Computer simulation is as long as that of the digital computer itself, beginning in the United States during World War II.
- The first truly programmable digital computer, the Electrical Numerical Integrator and Computer (ENIAC), was born in 1945.
- Nicholas Metropolis and Stanislaw Ulam (under the encouragement of John Von Neumann and Edward Teller): first computational model of a thermonuclear reaction.
- This model was constructed from a *mixture of well-established theoretical principles, physical insight, and clever mathematical tricks* (as is paradigmatic in the physical sciences). They then transformed the model into a *computable algorithm, which simulated the evolution of the system in question*.

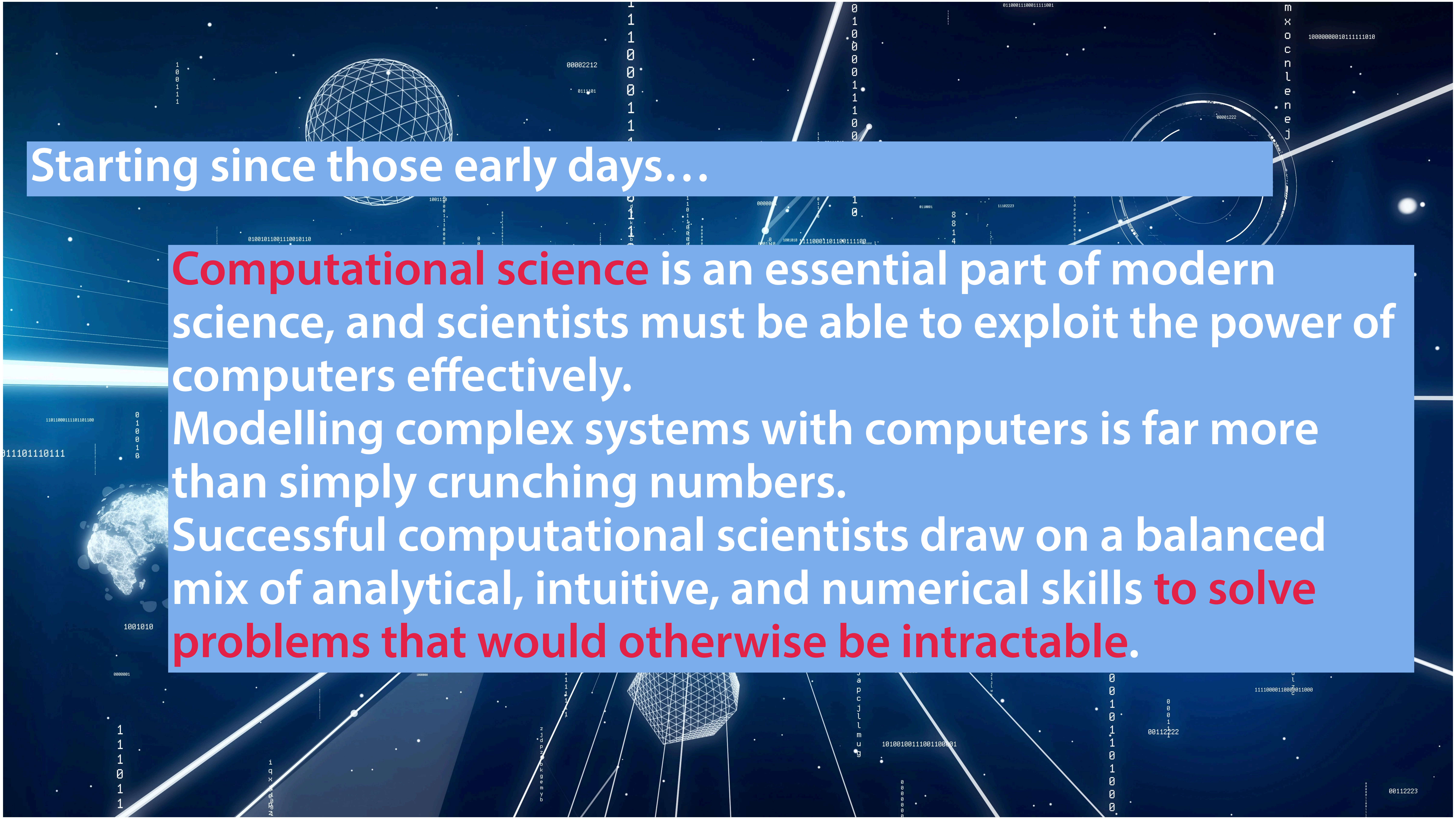


~ 500 Flop/s

ENIAC: Electronic Numerical Integrator And Computer

~100 m² 30 tons 18,000 vacuum tubes

Apple iPhone 12 ~ 11 TFlop/s



# Starting since those early days…

**Computational science** is an essential part of modern science, and scientists must be able to exploit the power of computers effectively.

Modelling complex systems with computers is far more than simply crunching numbers.

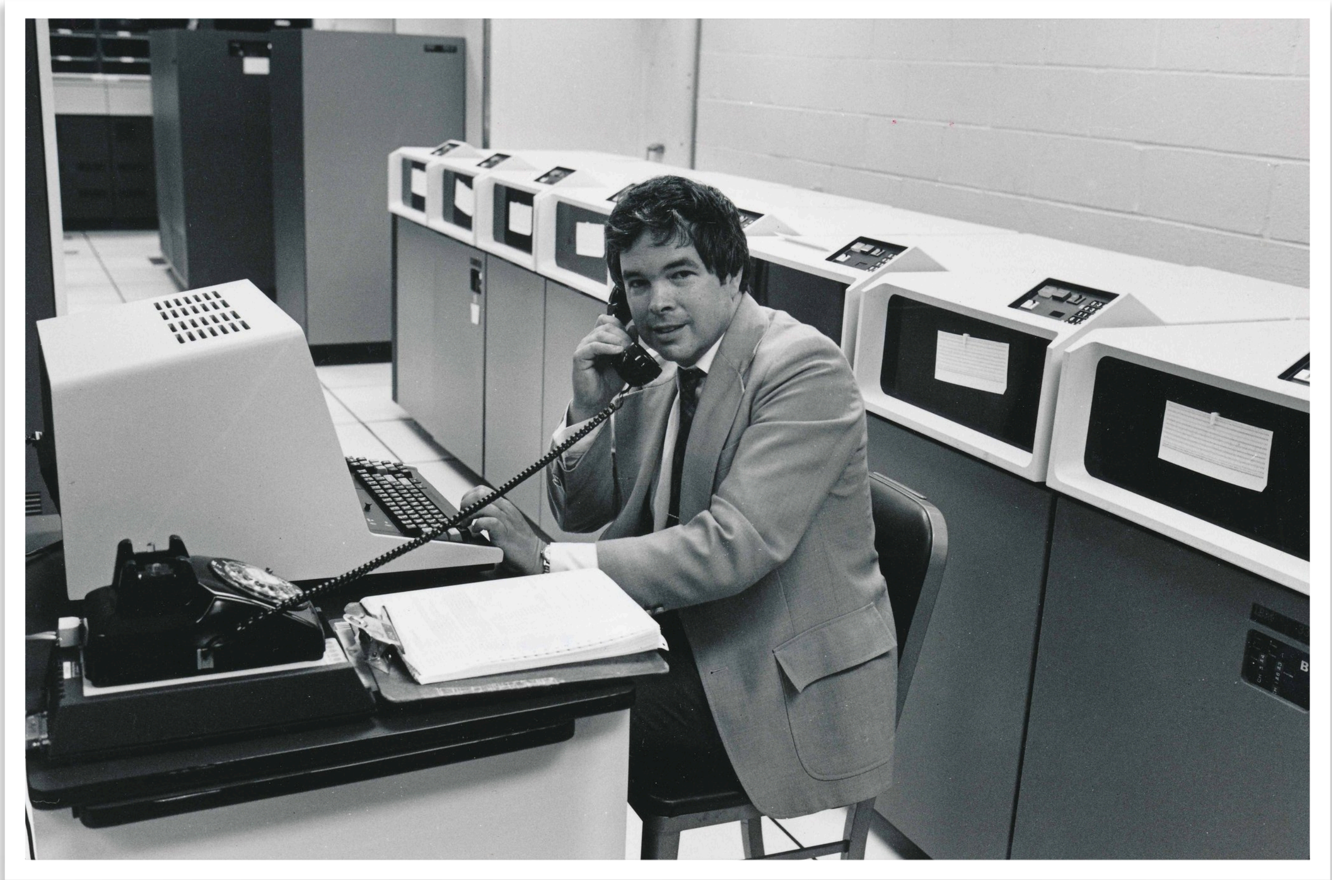
Successful computational scientists draw on a balanced mix of analytical, intuitive, and numerical skills **to solve problems that would otherwise be intractable**.

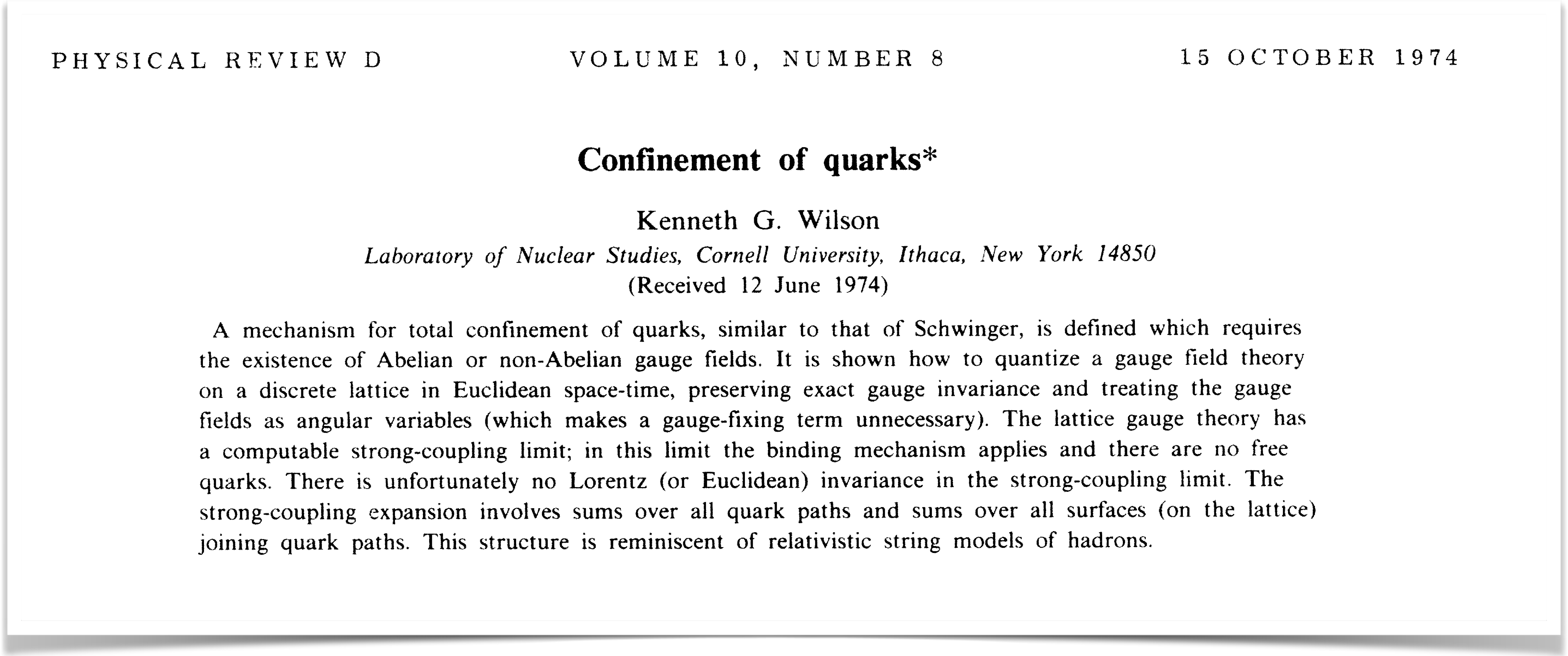
# Outline

- The born of Computational Theoretical Physics
- The evolution of Computational Physics
- Theoretical Computational Physics @ INFN
- Challenges:  ICSC
- Conclusions

# The born of Computational Theoretical Physics

In 1974 the seminal paper by **Ken Wilson** (*1982 Nobel Prize in Physics*) "Confinement of Quarks" paved the way to the study of fundamental interactions from first principles.





PHYSICAL REVIEW D VOLUME 10, NUMBER 8 15 OCTOBER 1974

**Confinement of quarks***

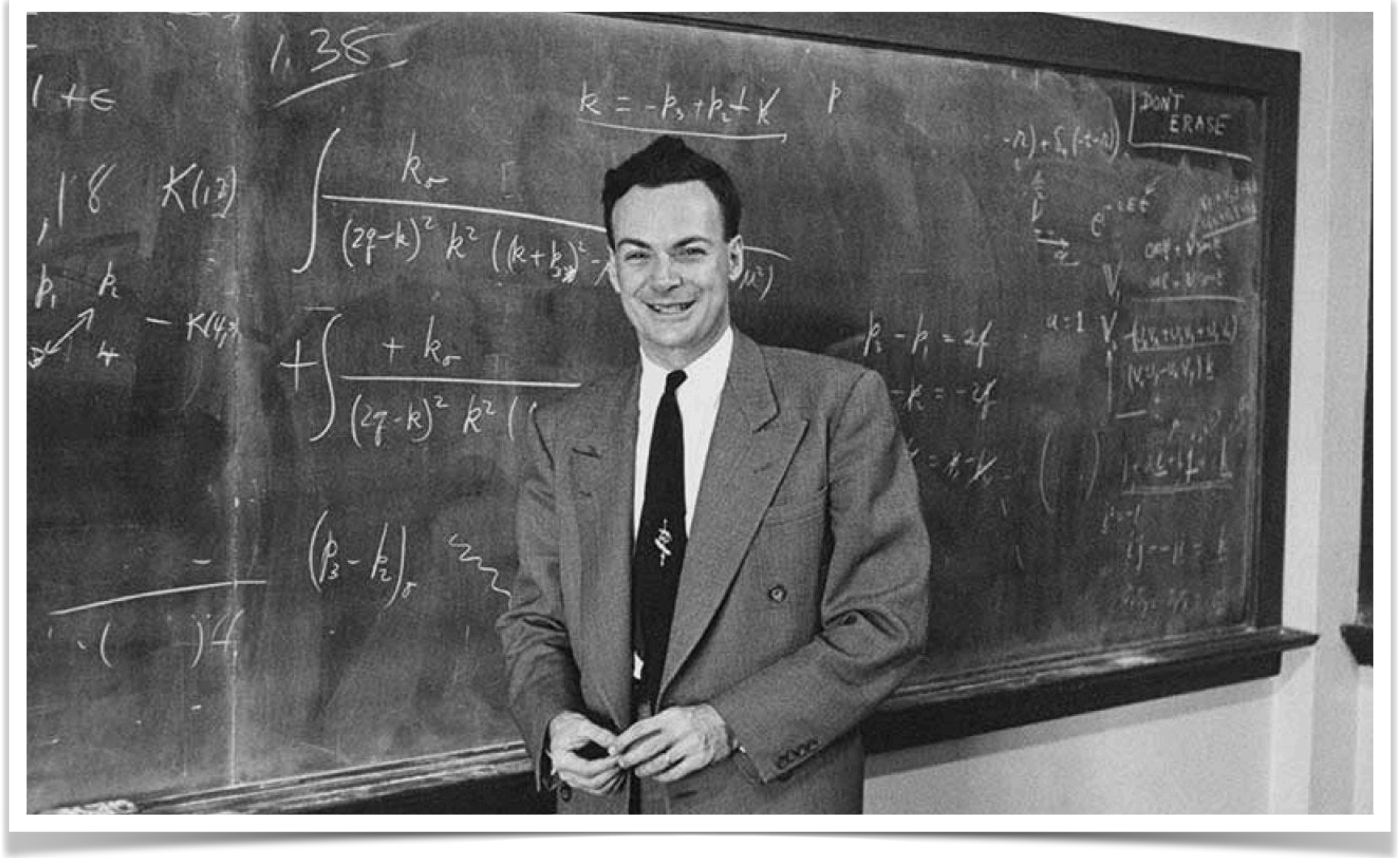
Kenneth G. Wilson

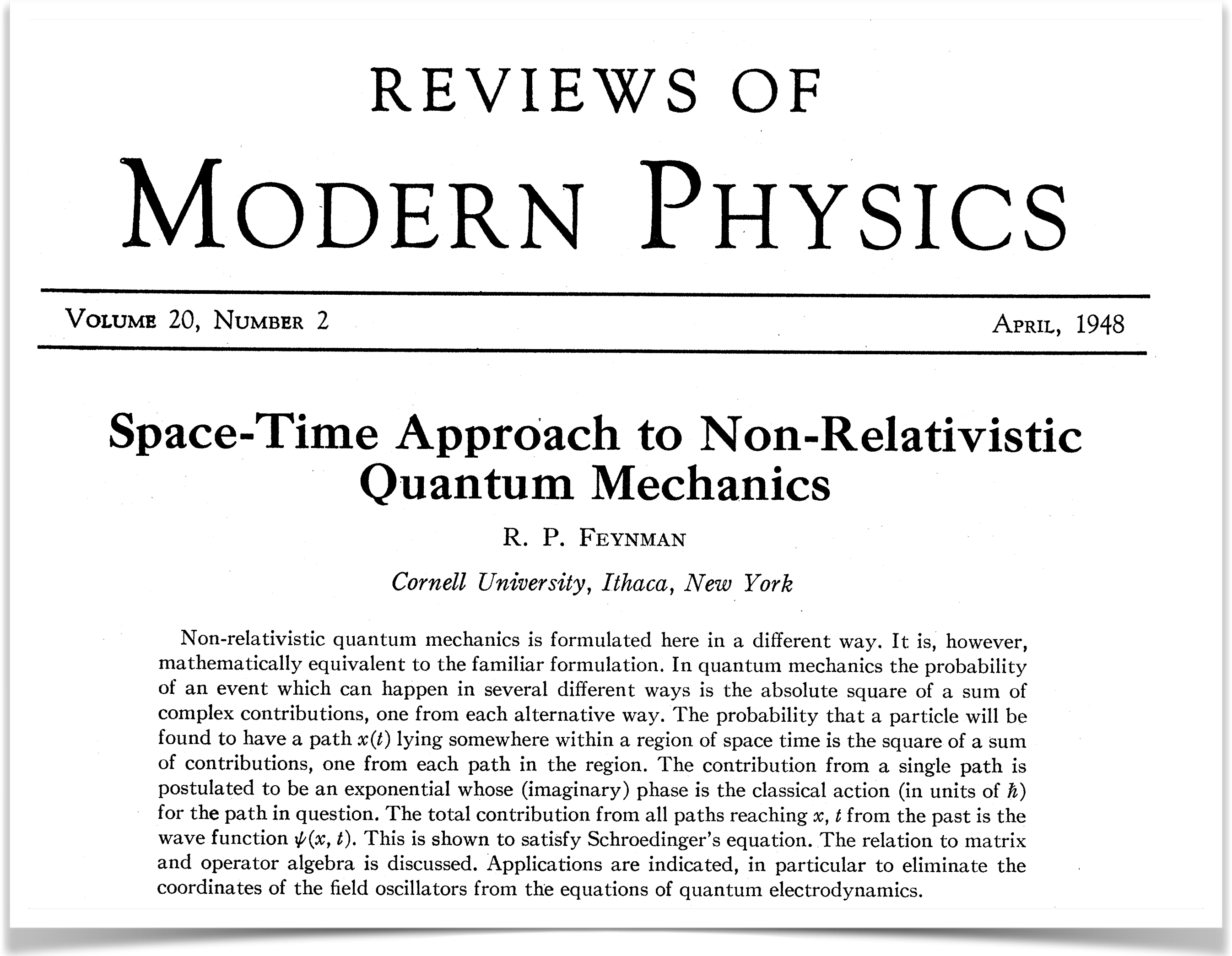
*Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14850*

(Received 12 June 1974)

A mechanism for total confinement of quarks, similar to that of Schwinger, is defined which requires the existence of Abelian or non-Abelian gauge fields. It is shown how to quantize a gauge field theory on a discrete lattice in Euclidean space-time, preserving exact gauge invariance and treating the gauge fields as angular variables (which makes a gauge-fixing term unnecessary). The lattice gauge theory has a computable strong-coupling limit; in this limit the binding mechanism applies and there are no free quarks. There is unfortunately no Lorentz (or Euclidean) invariance in the strong-coupling limit. The strong-coupling expansion involves sums over all quark paths and sums over all surfaces (on the lattice) joining quark paths. This structure is reminiscent of relativistic string models of hadrons.

This paper is fundamentally based on the seminal work of **Richard Feynman**, who introduced the path integral formulation of quantum mechanics and quantum field theory.





REVIEWS OF MODERN PHYSICS

VOLUME 20, NUMBER 2 APRIL, 1948

**Space-Time Approach to Non-Relativistic Quantum Mechanics**

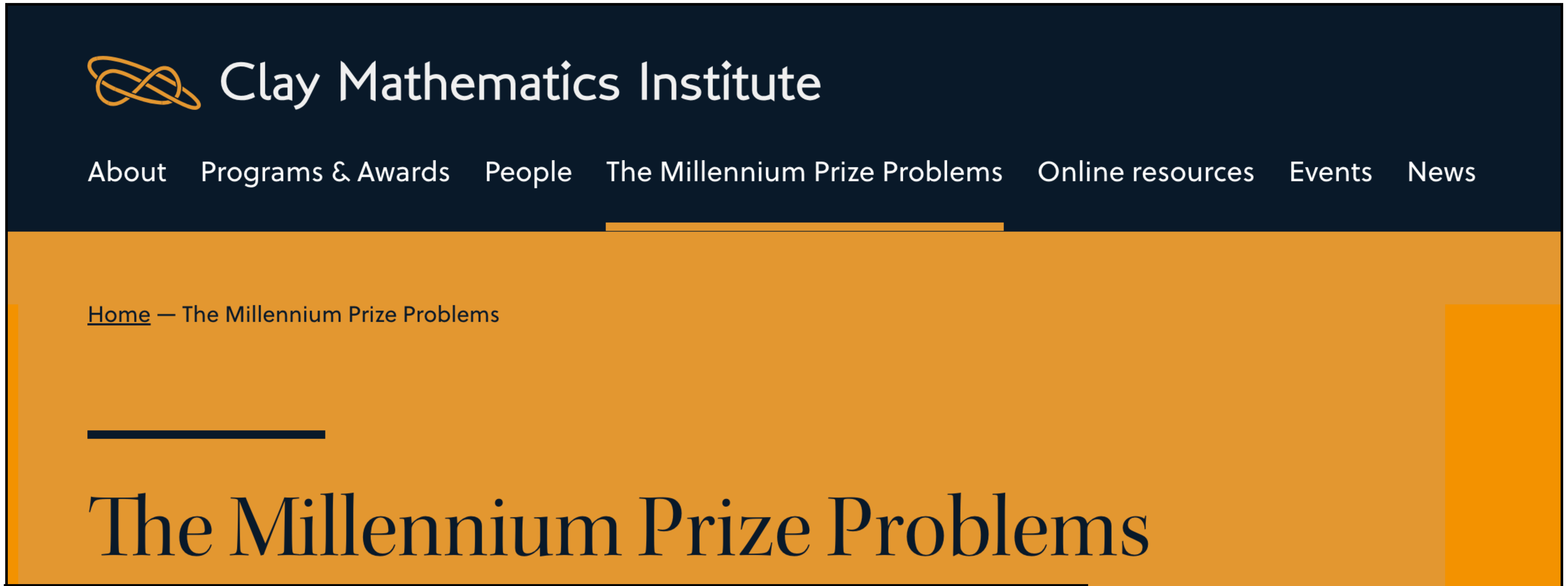
R. P. FEYNMAN

*Cornell University, Ithaca, New York*

Non-relativistic quantum mechanics is formulated here in a different way. It is, however, mathematically equivalent to the familiar formulation. In quantum mechanics the probability of an event which can happen in several different ways is the absolute square of a sum of complex contributions, one from each alternative way. The probability that a particle will be found to have a path $x(t)$ lying somewhere within a region of space time is the square of a sum of contributions, one from each path in the region. The contribution from a single path is postulated to be an exponential whose (imaginary) phase is the classical action (in units of $\hbar$) for the path in question. The total contribution from all paths reaching $x, t$ from the past is the wave function $\psi(x, t)$. This is shown to satisfy Schroedinger's equation. The relation to matrix and operator algebra is discussed. Applications are indicated, in particular to eliminate the coordinates of the field oscillators from the equations of quantum electrodynamics.

`https://www.claymath.org/millennium-problems/`

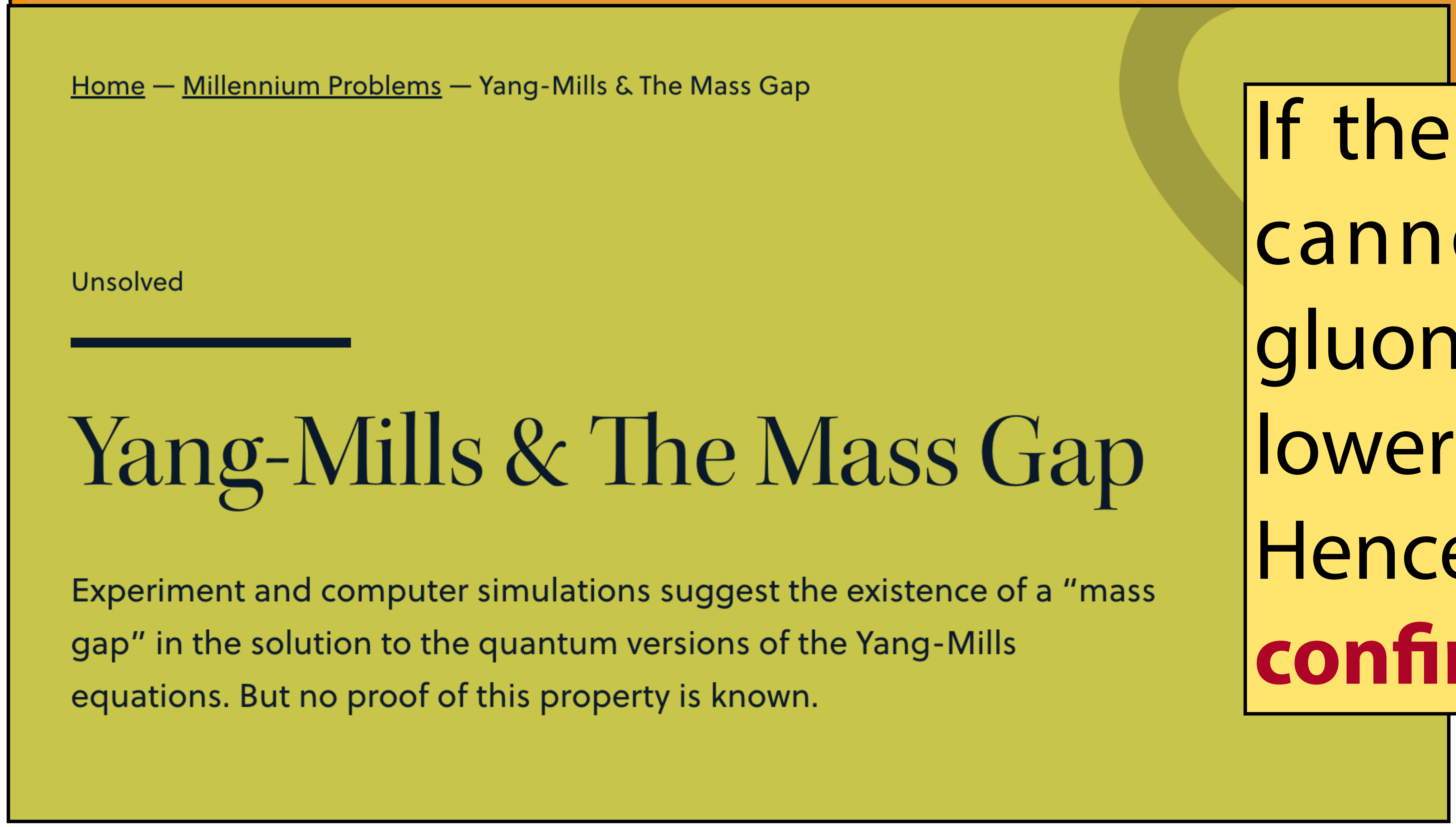
**Color confinement is still an unsolved problem**



Clay Mathematics Institute

Home — The Millennium Prize Problems

The Millennium Prize Problems



Home — Millennium Problems — Yang-Mills & The Mass Gap

Unsolved

Yang-Mills & The Mass Gap

Experiment and computer simulations suggest the existence of a “mass gap” in the solution to the quantum versions of the Yang-Mills equations. But no proof of this property is known.

If there is a **mass gap**, there cannot be free massless gluons which would have no lower bound on their energy. Hence, **a mass gap implies confinement**.

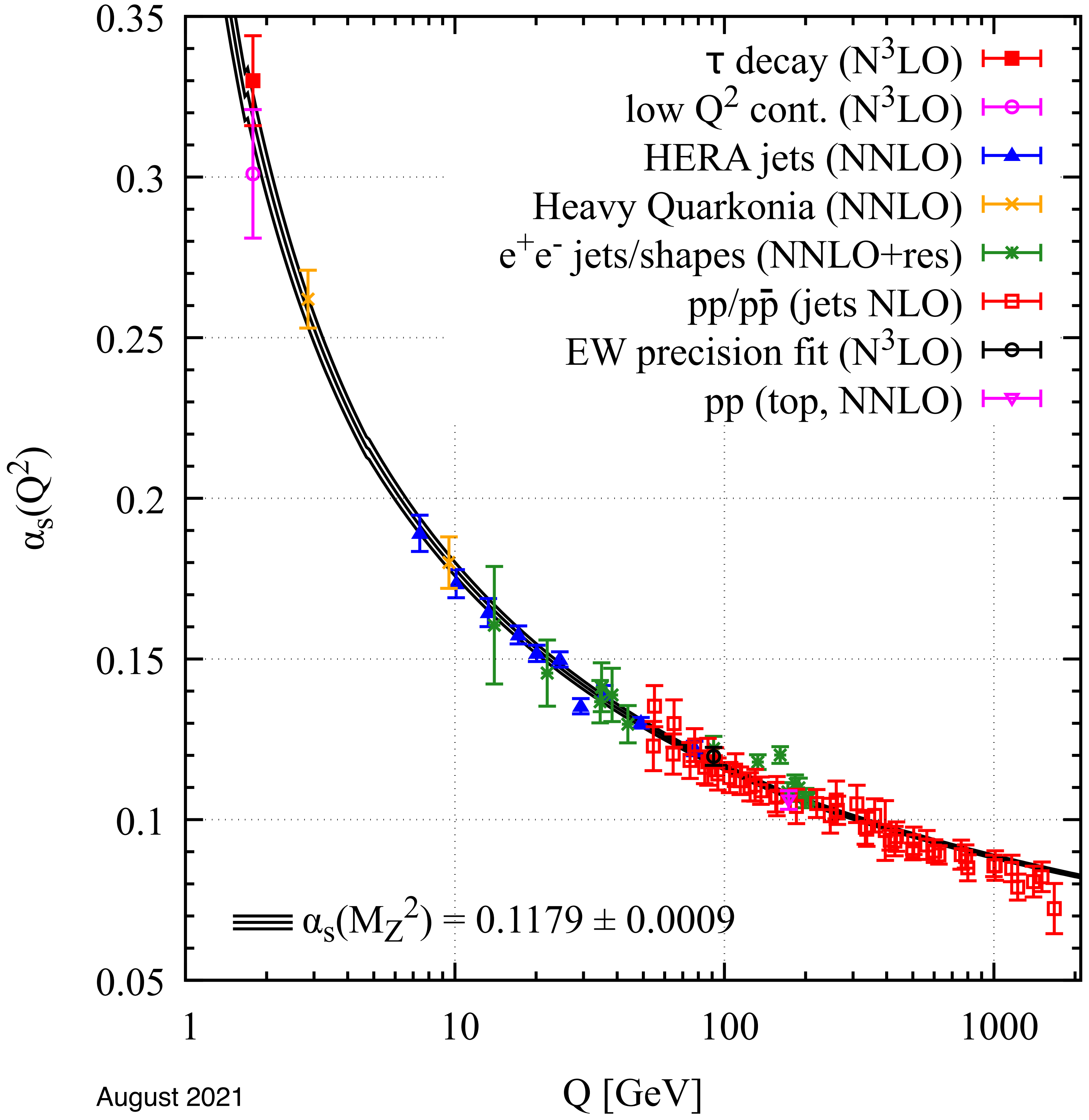
# Lattice QCD and High Performance Computing

**Color confinement** is an unsolved problem, but Ken Wilson's paper opened the possibility of investigating many aspects of the strong interactions *ab initio* (i.e., starting directly from the Lagrangian of the theory).

**Quantum Chromo Dynamics** the theory to describe the strong interactions in the Standard Model of elementary particles, is amenable to a perturbative treatment only at high energies.

The growth of the gauge coupling in the infrared, requires the use of non-perturbative methods to determine the low energy properties of QCD.

**Lattice gauge theory, proposed by K. Wilson in 1974 provides such a method.**



August 2021

**QCD becomes strongly coupled at the hadronic scale 1 GeV or 1 fm ($10^{-13}$ cm)**

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

$$\alpha_s = \frac{g_s^2}{4\pi}$$

**Asymptotic Freedom**

$\gamma_\mu$ Dirac matrices

$g_s$ QCD coupling constant

$\psi_{q,a}$ quark-field spinor for a quark of flavor ***q*** and mass ***$m_q$***
a color index running from ***a=1*** to ***$N_c$=3***

$F^A_{\mu\nu} = \partial_\mu \mathcal{A}^A_\nu - \partial_\nu \mathcal{A}^A_\mu - g_s f_{ABC} \mathcal{A}^B_\mu \mathcal{A}^C_\nu$ field tensor

$\mathcal{A}^C_\mu$ gluon fields $C = 1, \ldots, N_c^2 - 1 = 8$

$[t^A, t^B] = i f_{ABC} t^c$ $\quad t^C_{ab} \equiv \lambda^C_{ab}/2$ generators of the SU(3) group

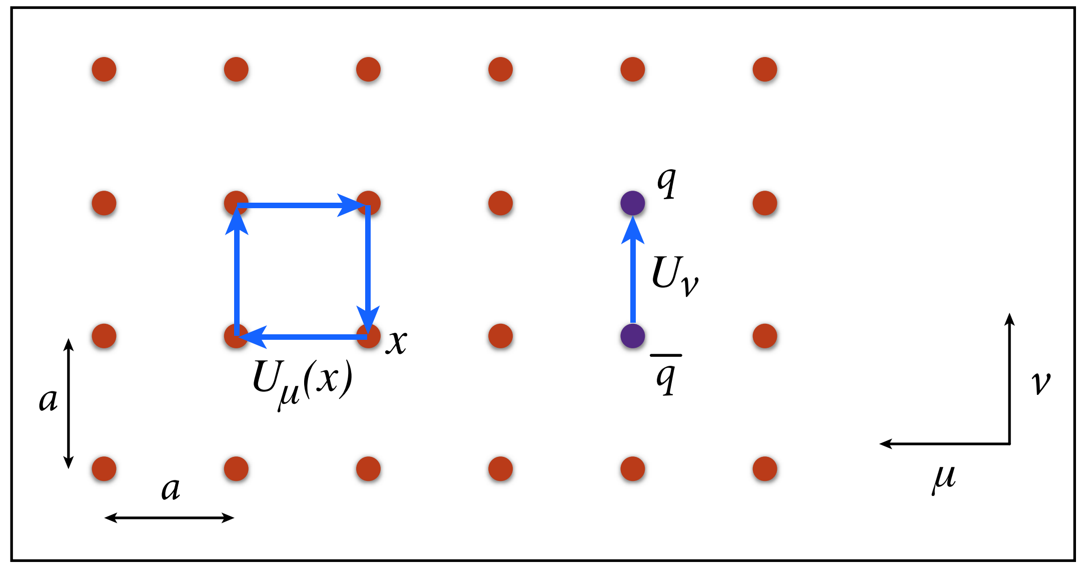
# LATTICE QCD

## (Quantum Chromo Dynamics on a discrete space-time lattice)

Ken Wilson (1974) —> space-time discretisation —> lattice regularization of QCD —>

non-perturbative calculations by numerical evaluation of the Feynman path integral that defines the theory

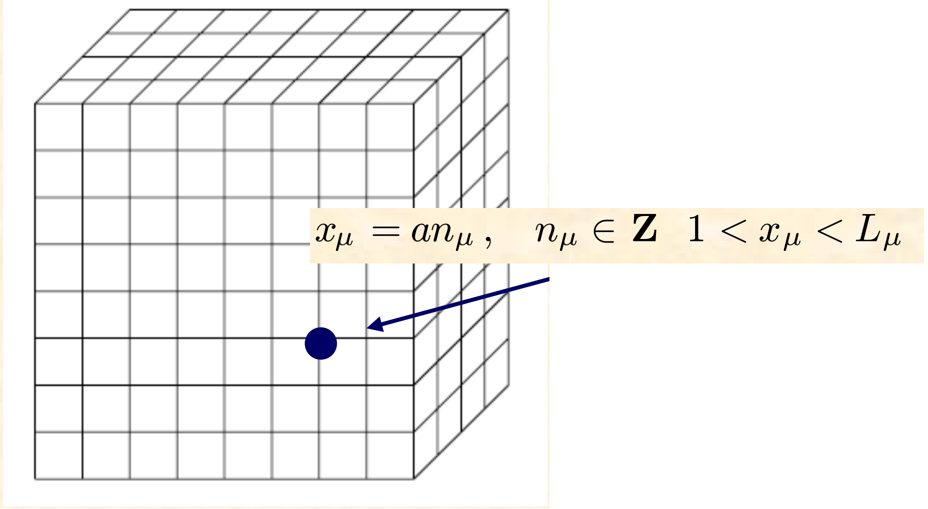
$$\langle \mathcal{O}(U,q,\bar{q})\rangle = (1/Z)\int [dU]\prod_f [dq_f][d\bar{q}_f]\mathcal{O}(U,q,\bar{q})e^{-S_g[U]-\sum_f \bar{q}_f(D[U]+m_f)q_f}$$



$$Z = \int [dU]e^{-S_g[U]}\prod_f \det(D[U]+m_f)$$

**hyper cubic lattice**

$$V_{\text{lat}} = N_s^3 \times N_t$$



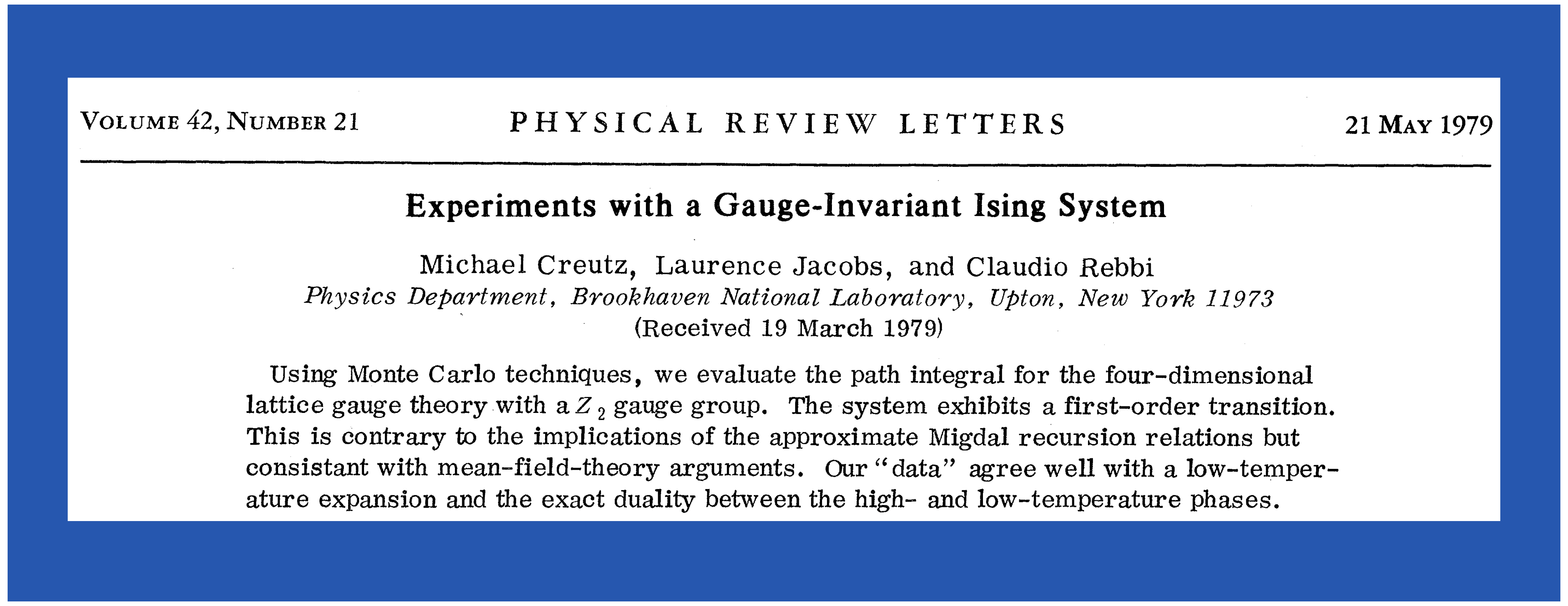
Equivalence with Classical Statistical Mechanics

**Quantum Field Theory
in d space-time
dimensions**

**Classical Statistical Mechanics
in d spatial dimensions**

# Early days of Lattice QCD

## Soon after the Ken Wilson's seminal paper…

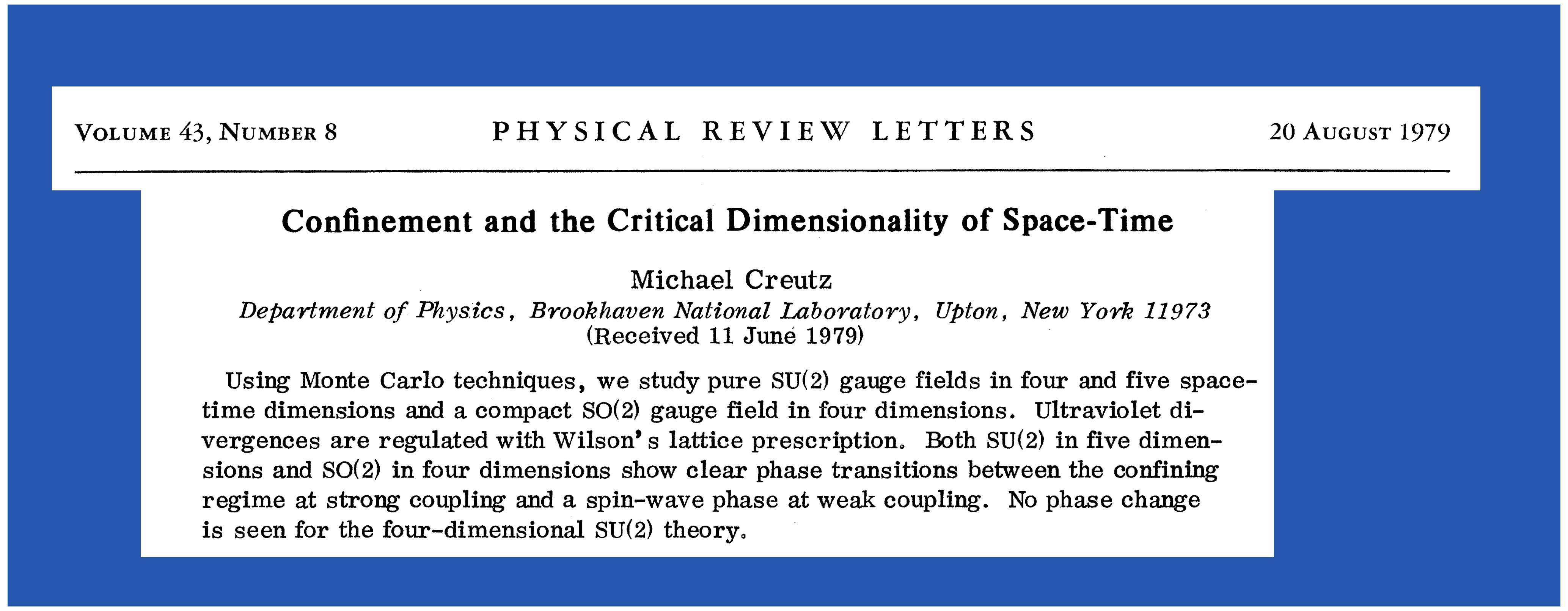


VOLUME 42, NUMBER 21 PHYSICAL REVIEW LETTERS 21 MAY 1979

### Experiments with a Gauge-Invariant Ising System

Michael Creutz, Laurence Jacobs, and Claudio Rebbi
*Physics Department, Brookhaven National Laboratory, Upton, New York 11973*
(Received 19 March 1979)

Using Monte Carlo techniques, we evaluate the path integral for the four-dimensional lattice gauge theory with a $Z_2$ gauge group. The system exhibits a first-order transition. This is contrary to the implications of the approximate Migdal recursion relations but consistant with mean-field-theory arguments. Our "data" agree well with a low-temperature expansion and the exact duality between the high- and low-temperature phases.

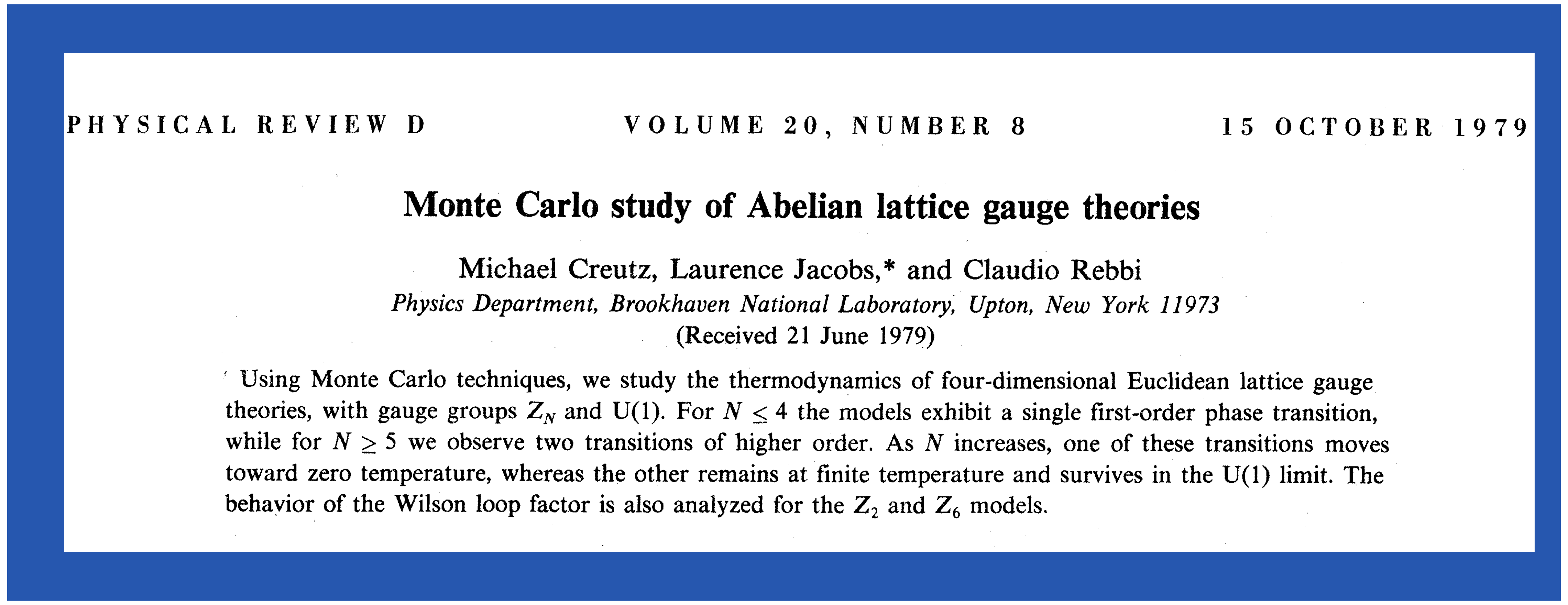


VOLUME 43, NUMBER 8 PHYSICAL REVIEW LETTERS 20 AUGUST 1979

### Confinement and the Critical Dimensionality of Space-Time

Michael Creutz
*Department of Physics, Brookhaven National Laboratory, Upton, New York 11973*
(Received 11 June 1979)

Using Monte Carlo techniques, we study pure SU(2) gauge fields in four and five space-time dimensions and a compact SO(2) gauge field in four dimensions. Ultraviolet divergences are regulated with Wilson's lattice prescription. Both SU(2) in five dimensions and SO(2) in four dimensions show clear phase transitions between the confining regime at strong coupling and a spin-wave phase at weak coupling. No phase change is seen for the four-dimensional SU(2) theory.

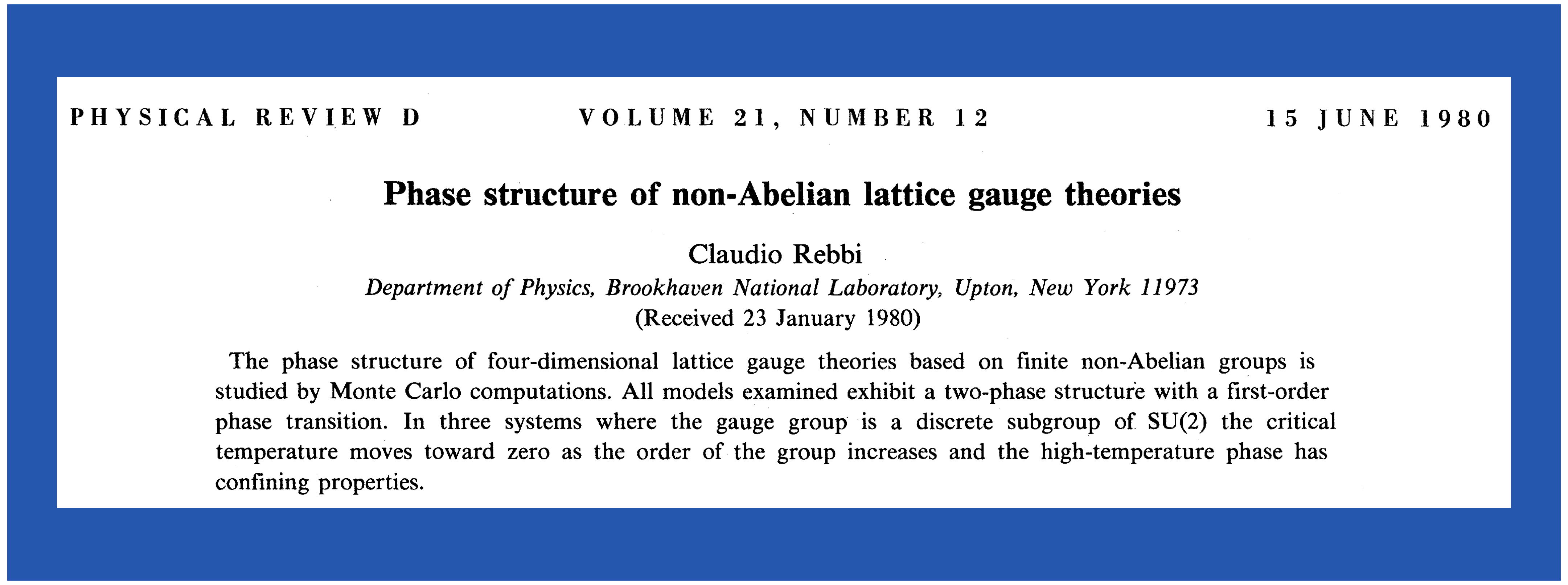


PHYSICAL REVIEW D VOLUME 20, NUMBER 8 15 OCTOBER 1979

### Monte Carlo study of Abelian lattice gauge theories

Michael Creutz, Laurence Jacobs,* and Claudio Rebbi
*Physics Department, Brookhaven National Laboratory, Upton, New York 11973*
(Received 21 June 1979)

Using Monte Carlo techniques, we study the thermodynamics of four-dimensional Euclidean lattice gauge theories, with gauge groups $Z_N$ and U(1). For $N \leq 4$ the models exhibit a single first-order phase transition, while for $N \geq 5$ we observe two transitions of higher order. As $N$ increases, one of these transitions moves toward zero temperature, whereas the other remains at finite temperature and survives in the U(1) limit. The behavior of the Wilson loop factor is also analyzed for the $Z_2$ and $Z_6$ models.

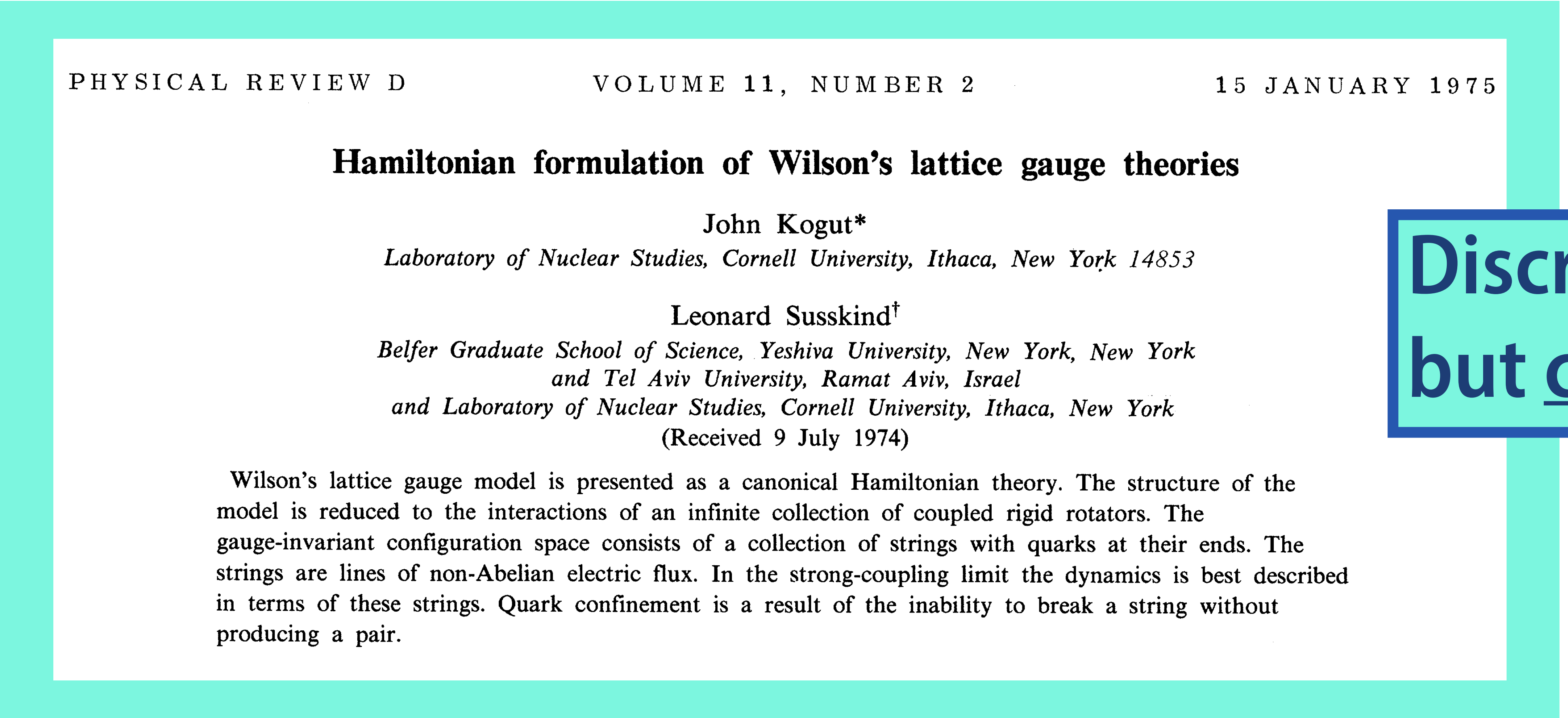


PHYSICAL REVIEW D VOLUME 21, NUMBER 12 15 JUNE 1980

### Phase structure of non-Abelian lattice gauge theories

Claudio Rebbi
*Department of Physics, Brookhaven National Laboratory, Upton, New York 11973*
(Received 23 January 1980)

The phase structure of four-dimensional lattice gauge theories based on finite non-Abelian groups is studied by Monte Carlo computations. All models examined exhibit a two-phase structure with a first-order phase transition. In three systems where the gauge group is a discrete subgroup of SU(2) the critical temperature moves toward zero as the order of the group increases and the high-temperature phase has confining properties.



PHYSICAL REVIEW D VOLUME 11, NUMBER 2 15 JANUARY 1975

### Hamiltonian formulation of Wilson's lattice gauge theories

John Kogut*
*Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14853*

Leonard Susskind†
*Belfer Graduate School of Science, Yeshiva University, New York, New York*
*and Tel Aviv University, Ramat Aviv, Israel*
*and Laboratory of Nuclear Studies, Cornell University, Ithaca, New York*
(Received 9 July 1974)

Wilson's lattice gauge model is presented as a canonical Hamiltonian theory. The structure of the model is reduced to the interactions of an infinite collection of coupled rigid rotators. The gauge-invariant configuration space consists of a collection of strings with quarks at their ends. The strings are lines of non-Abelian electric flux. In the strong-coupling limit the dynamics is best described in terms of these strings. Quark confinement is a result of the inability to break a string without producing a pair.

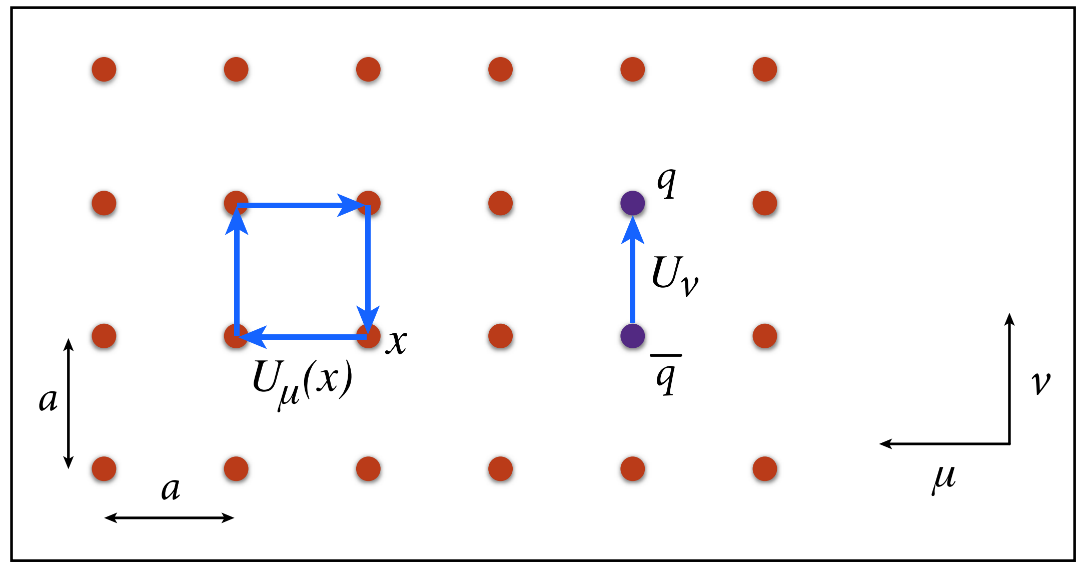
**Discrete space**
**but continuous time**

<u>Problem</u>: numerical evaluation of the path integral expectation value for a given operator $\mathcal{O}(U,q,\bar{q})$

representing a given physical observable (e.g. a hadron mass)

$$\langle \mathcal{O}(U,q,\bar{q})\rangle = (1/Z)\int [dU]\prod_f [dq_f][d\bar{q}_f]\mathcal{O}(U,q,\bar{q})e^{-S_g[U]-\sum_f \bar{q}_f(D[U]+m_f)q_f}$$

$$Z = \int [dU]e^{-S_g[U]}\prod_f \det(D[U]+m_f)$$

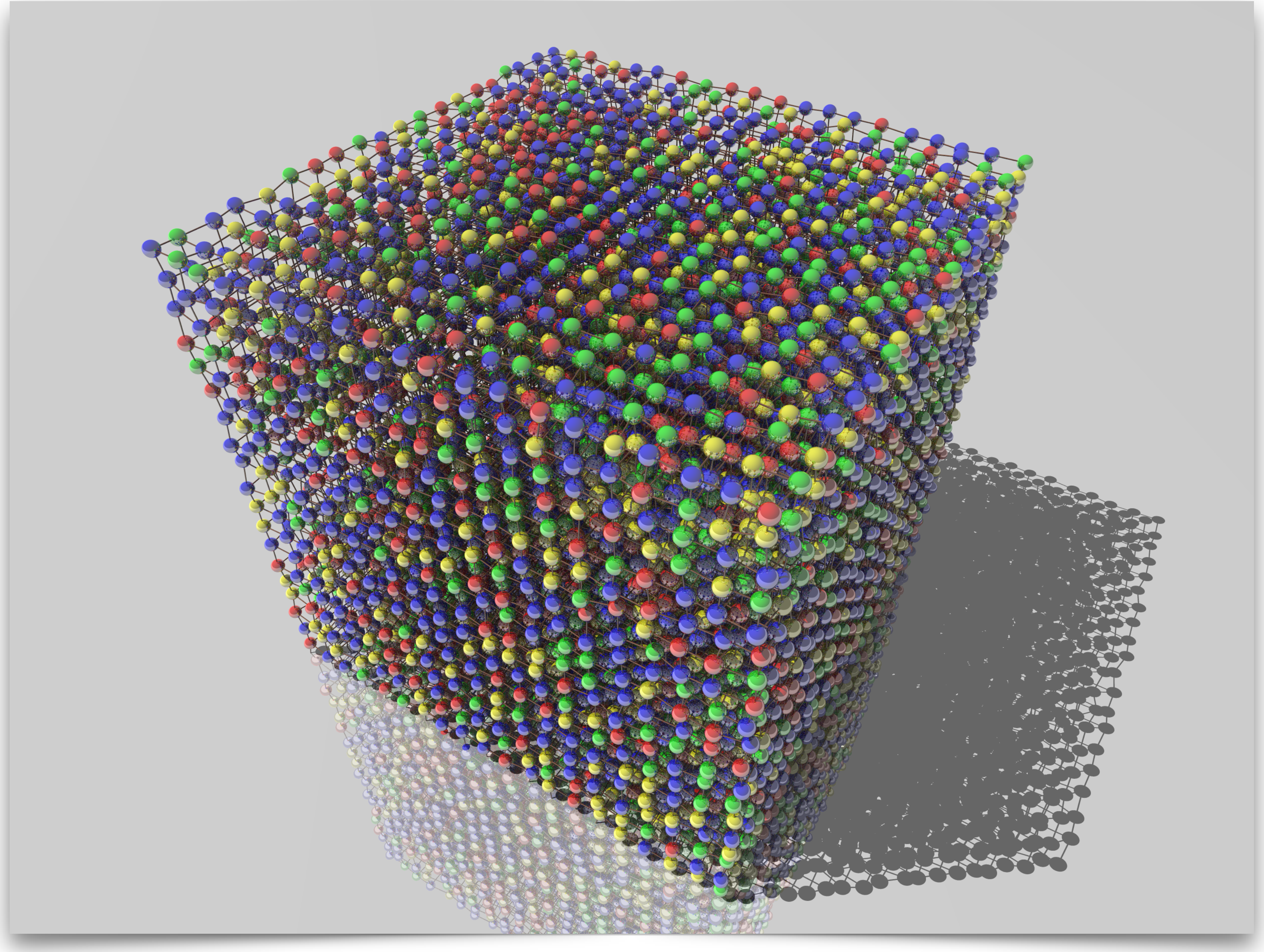


After space-time discretisation the path integral becomes (if we consider only a finite space-time volume)

a multidimensional ordinary integral, <u>but with a huge number of integrations variables</u>

**hyper cubic lattice**

$V_{\text{lat}} = N_s^3 \times N_t$



<u>Example</u>:
SU(3) pure gauge theory (8 real numbers for a SU(3) matrix)
Consider a $40^4$ finite hypercubic lattice: $4 \times 40^4$ links (SU(3) matrices)
The number of integration variables is then: $8 \times 4 \times 40^4 = 81{,}920{,}000$

If we want to evaluate the integral with a standard numerical integration algorithm (e.g. Gauss) and we suppose to consider 10 evaluations for each integration variable:

<u>the number of times the integrand should be evaluated is</u> $10^{8\times4\times40^4} = 10^{81{,}920{,}000}$

## IMPORTANCE SAMPLING

The calculation of the expectation value of a given observable on a lattice is equivalent to averaging the physical observable over a finite subset of all possible field configurations, weighted by the partition function Z of the field theory under consideration.

$$\langle \mathcal{O} \rangle_N = \frac{\sum_{i=1}^{N} \mathcal{O}(C_i)\, p^{-1}(C_i)\, e^{-S(C_i)}}{\sum_{i=1}^{N} p^{-1}(C_i)\, e^{-S(C_i)}}$$

$$p(C_i) = \frac{1}{Z}\, e^{-S(C_i)}$$

statistical weight of a given field configuration $C_i$

## MARKOV CHAIN MONTE CARLO

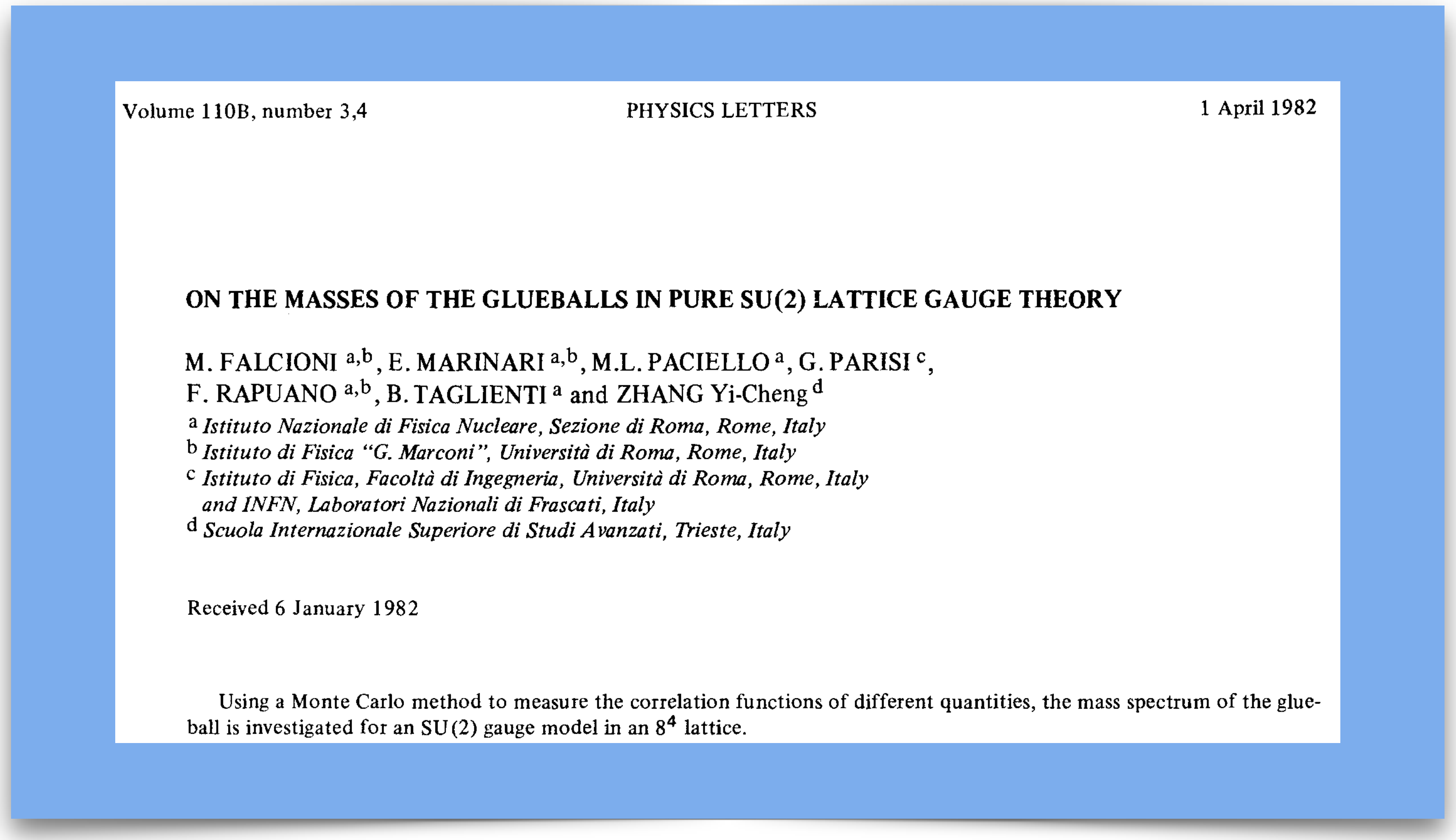
Algorithms for sampling from probability distributions. It works by constructing a Markov chain that has the desired distribution as its equilibrium distribution.

$$C_0 \rightarrow C_1 \rightarrow C_2 \rightarrow \ldots \rightarrow C_N$$

After the chain has reached equilibrium, the samples drawn from the chain will be samples from the desired distribution.

$$\langle \mathcal{O} \rangle_N = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(C_i)$$

# Since the early days of lattice gauge theory, the INFN community has played a leading role in developing and promoting this new computational strategy for fundamental interactions

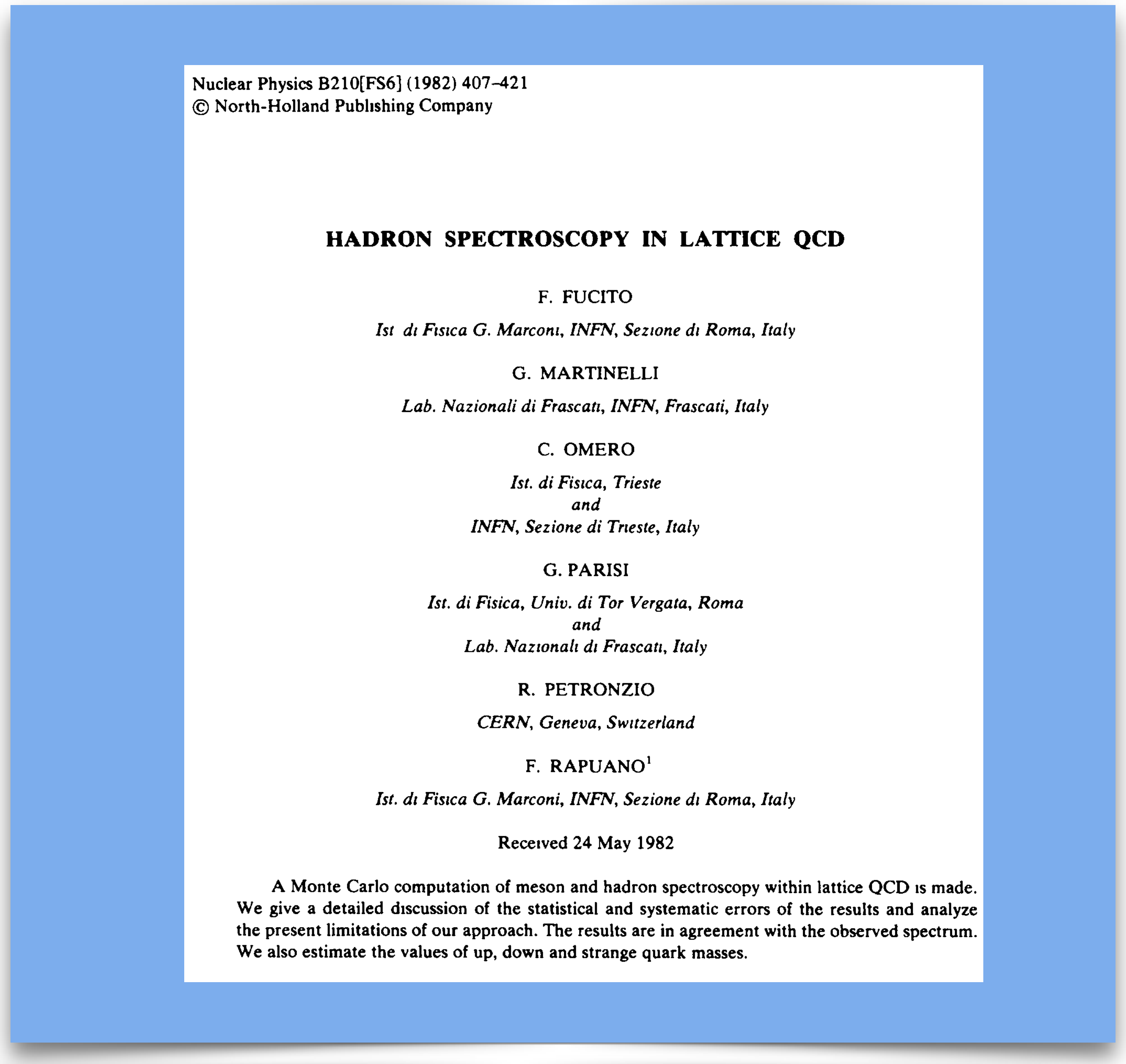

Volume 110B, number 3,4 PHYSICS LETTERS 1 April 1982

### ON THE MASSES OF THE GLUEBALLS IN PURE SU(2) LATTICE GAUGE THEORY

M. FALCIONI [a,b], E. MARINARI [a,b], M.L. PACIELLO [a], G. PARISI [c],
F. RAPUANO [a,b], B. TAGLIENTI [a] and ZHANG Yi-Cheng [d]
[a] *Istituto Nazionale di Fisica Nucleare, Sezione di Roma, Rome, Italy*
[b] *Istituto di Fisica "G. Marconi", Università di Roma, Rome, Italy*
[c] *Istituto di Fisica, Facoltà di Ingegneria, Università di Roma, Rome, Italy and INFN, Laboratori Nazionali di Frascati, Italy*
[d] *Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy*

Received 6 January 1982

Using a Monte Carlo method to measure the correlation functions of different quantities, the mass spectrum of the glueball is investigated for an SU(2) gauge model in an $8^4$ lattice.


Nuclear Physics B210[FS6] (1982) 407–421
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### HADRON SPECTROSCOPY IN LATTICE QCD

F. FUCITO
*Ist. di Fisica G. Marconi, INFN, Sezione di Roma, Italy*

G. MARTINELLI
*Lab. Nazionali di Frascati, INFN, Frascati, Italy*

C. OMERO
*Ist. di Fisica, Trieste*
*and*
*INFN, Sezione di Trieste, Italy*

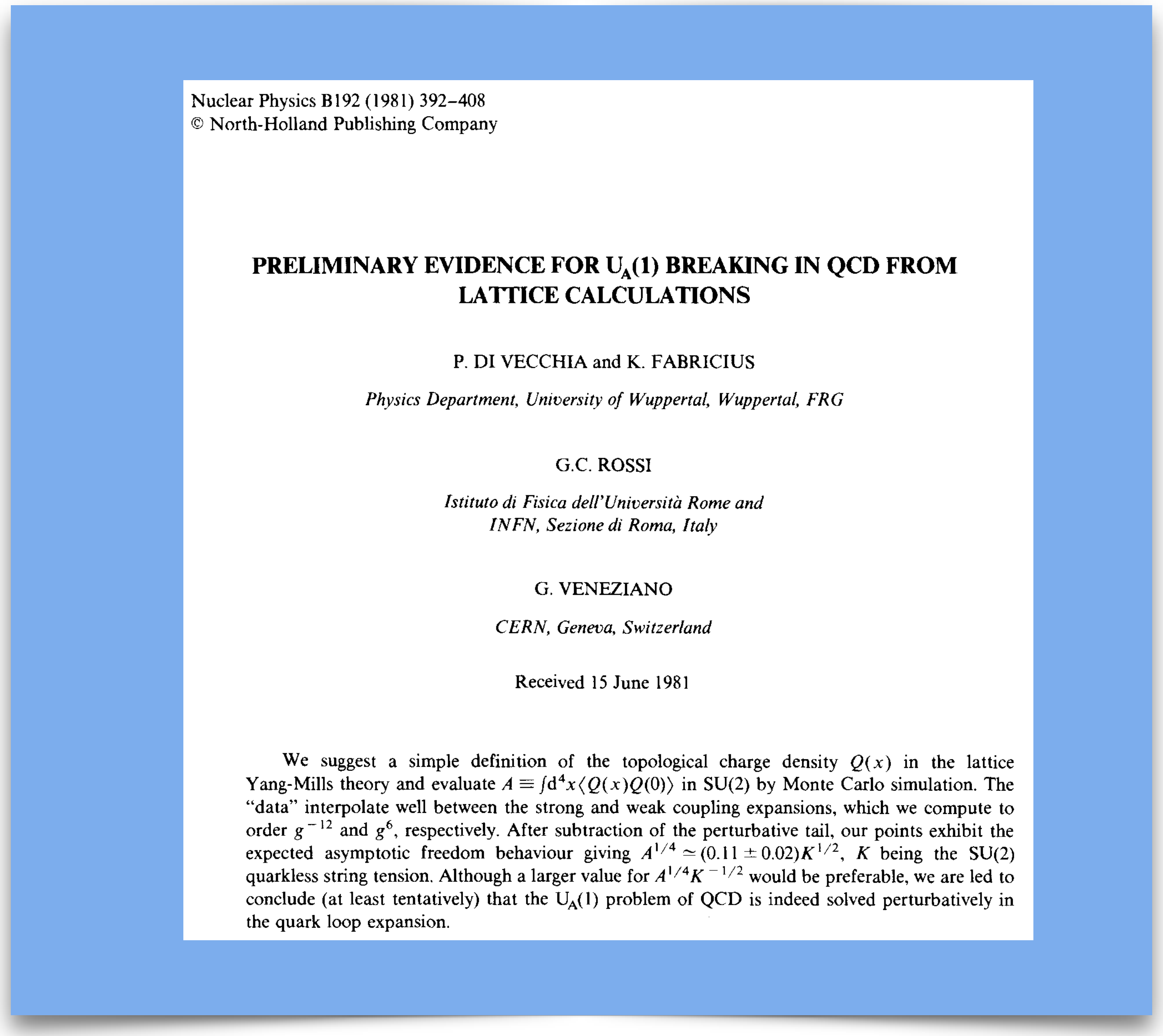
G. PARISI
*Ist. di Fisica, Univ. di Tor Vergata, Roma*
*and*
*Lab. Nazionali di Frascati, Italy*

R. PETRONZIO
*CERN, Geneva, Switzerland*

F. RAPUANO[1]
*Ist. di Fisica G. Marconi, INFN, Sezione di Roma, Italy*

Received 24 May 1982

A Monte Carlo computation of meson and hadron spectroscopy within lattice QCD is made. We give a detailed discussion of the statistical and systematic errors of the results and analyze the present limitations of our approach. The results are in agreement with the observed spectrum. We also estimate the values of up, down and strange quark masses.


Nuclear Physics B192 (1981) 392–408
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### PRELIMINARY EVIDENCE FOR $U_A(1)$ BREAKING IN QCD FROM LATTICE CALCULATIONS

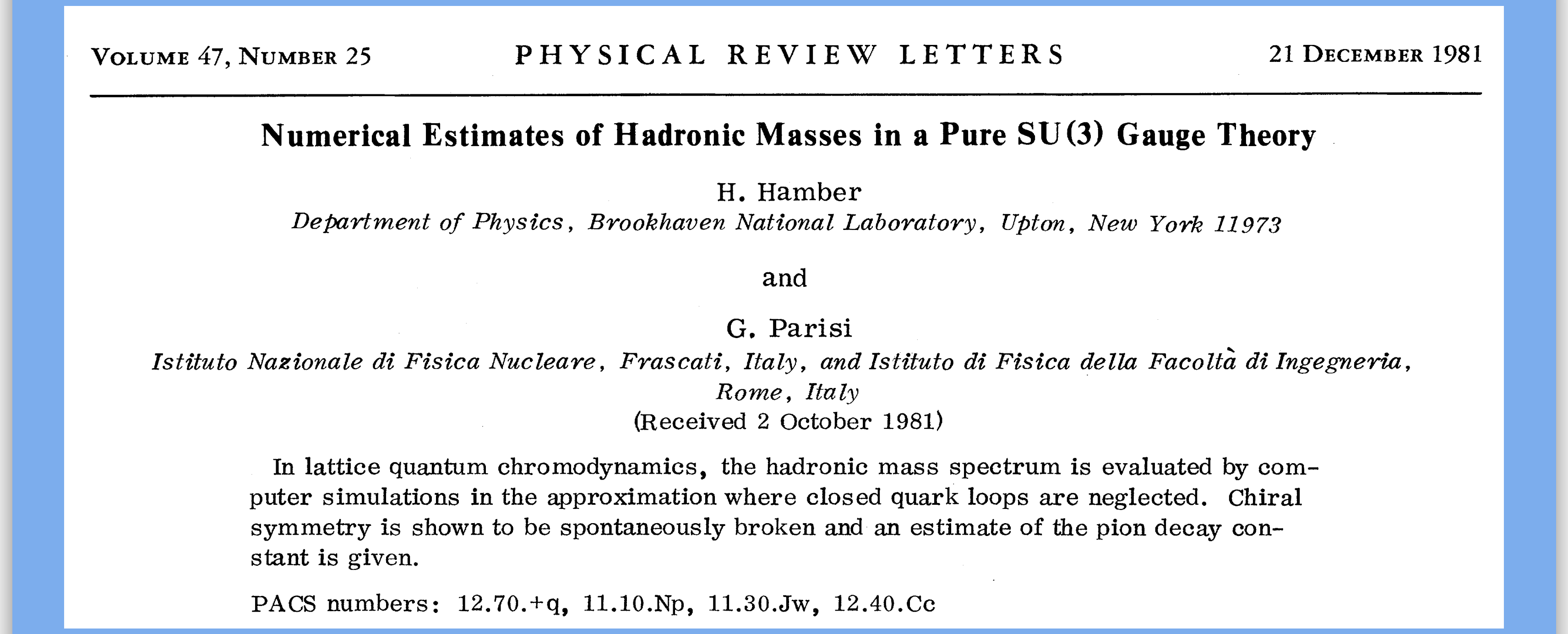
P. DI VECCHIA and K. FABRICIUS
*Physics Department, University of Wuppertal, Wuppertal, FRG*

G.C. ROSSI
*Istituto di Fisica dell'Università Rome and*
*INFN, Sezione di Roma, Italy*

G. VENEZIANO
*CERN, Geneva, Switzerland*

Received 15 June 1981

We suggest a simple definition of the topological charge density $Q(x)$ in the lattice Yang-Mills theory and evaluate $A \equiv \int d^4x \langle Q(x)Q(0)\rangle$ in SU(2) by Monte Carlo simulation. The "data" interpolate well between the strong and weak coupling expansions, which we compute to order $g^{-12}$ and $g^6$, respectively. After subtraction of the perturbative tail, our points exhibit the expected asymptotic freedom behaviour giving $A^{1/4} \simeq (0.11 \pm 0.02)K^{1/2}$, $K$ being the SU(2) quarkless string tension. Although a larger value for $A^{1/4}K^{-1/2}$ would be preferable, we are led to conclude (at least tentatively) that the $U_A(1)$ problem of QCD is indeed solved perturbatively in the quark loop expansion.


VOLUME 47, NUMBER 25 PHYSICAL REVIEW LETTERS 21 DECEMBER 1981

### Numerical Estimates of Hadronic Masses in a Pure SU(3) Gauge Theory

H. Hamber
*Department of Physics, Brookhaven National Laboratory, Upton, New York 11973*

and

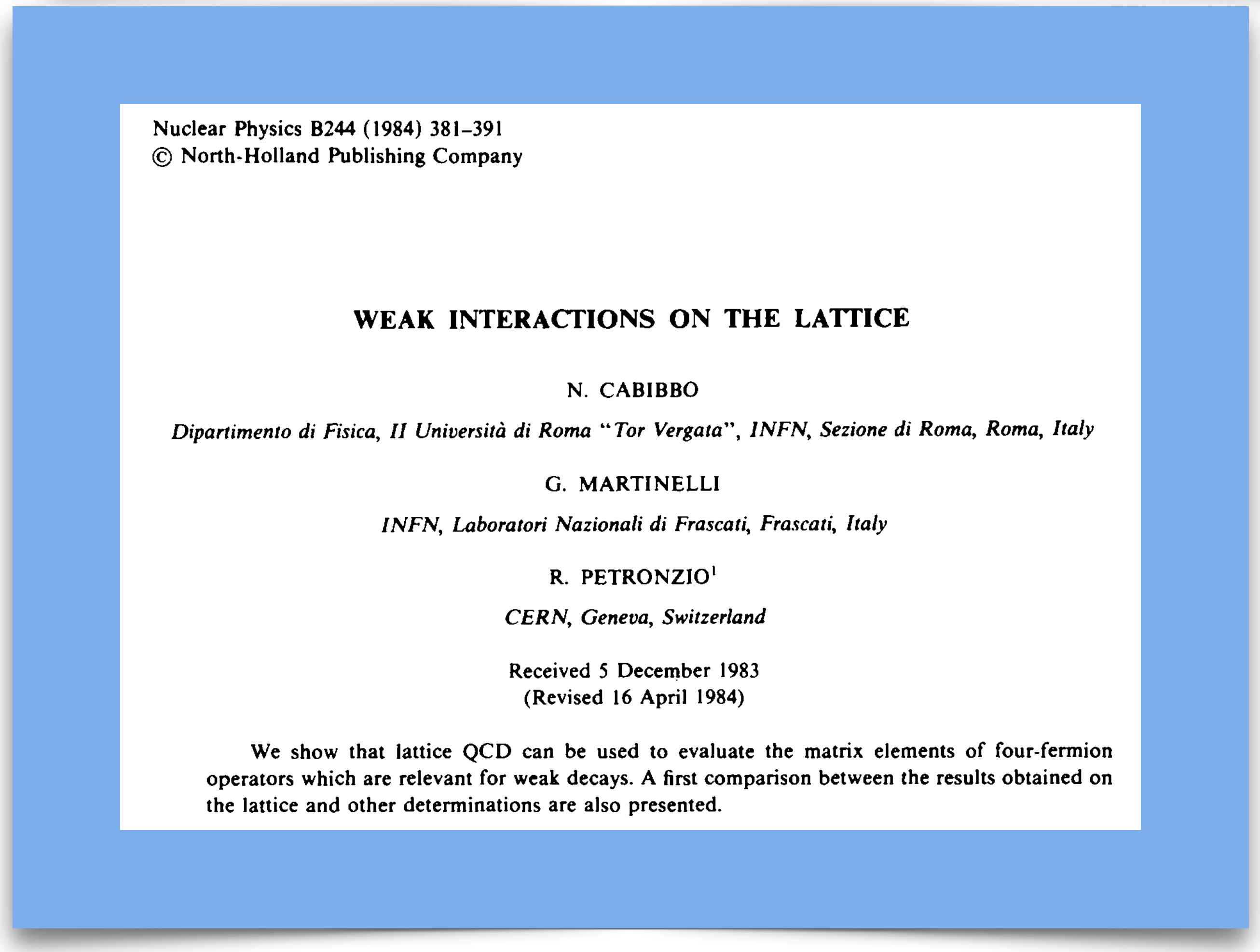
G. Parisi
*Istituto Nazionale di Fisica Nucleare, Frascati, Italy, and Istituto di Fisica della Facoltà di Ingegneria, Rome, Italy*

(Received 2 October 1981)

In lattice quantum chromodynamics, the hadronic mass spectrum is evaluated by computer simulations in the approximation where closed quark loops are neglected. Chiral symmetry is shown to be spontaneously broken and an estimate of the pion decay constant is given.

PACS numbers: 12.70.+q, 11.10.Np, 11.30.Jw, 12.40.Cc

**simulations performed using a VAX 11/780 (8 MB Ram 0.25 MFlop/s)**


Nuclear Physics B244 (1984) 381–391
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### WEAK INTERACTIONS ON THE LATTICE

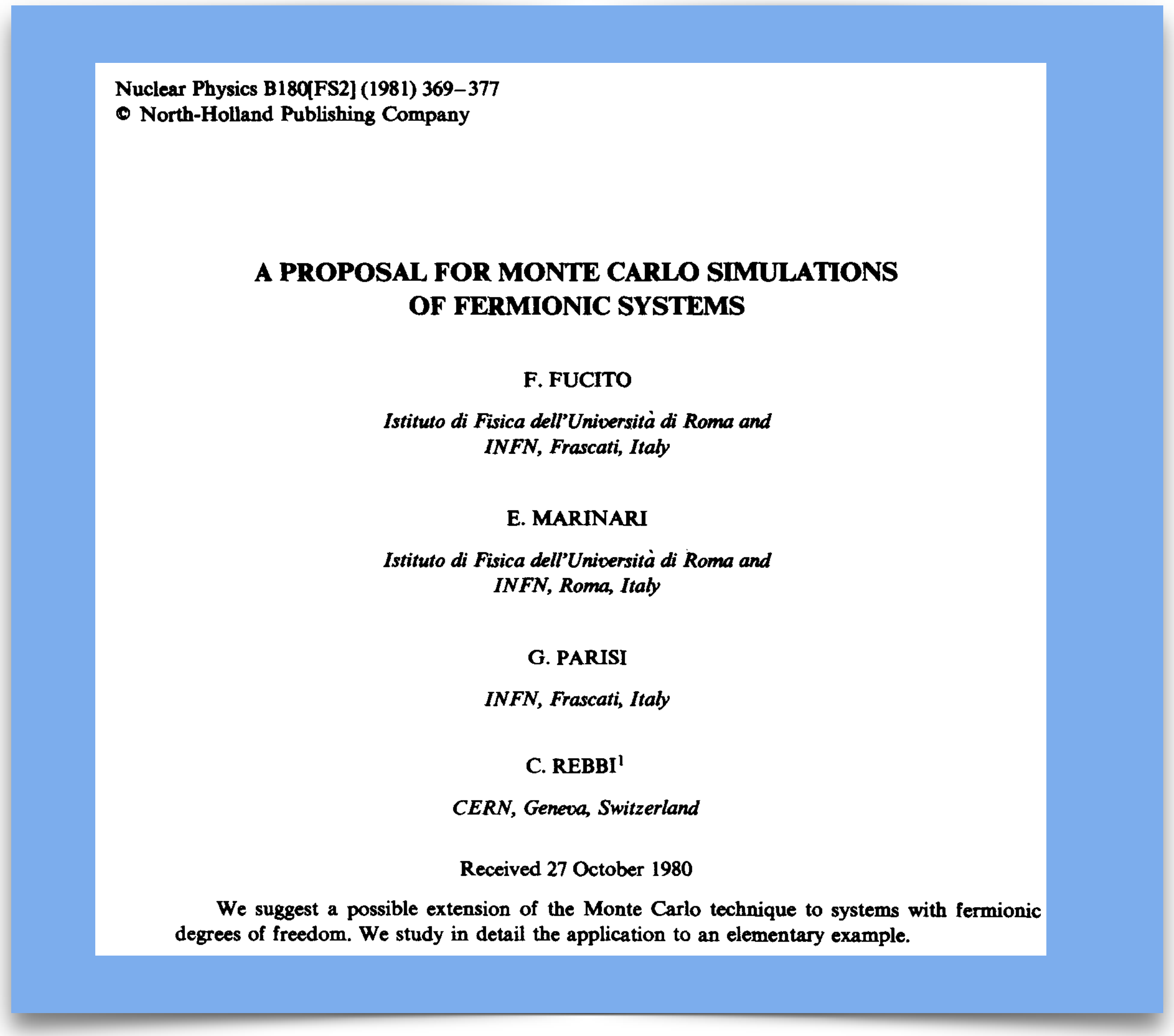
N. CABIBBO
*Dipartimento di Fisica, II Università di Roma "Tor Vergata", INFN, Sezione di Roma, Roma, Italy*

G. MARTINELLI
*INFN, Laboratori Nazionali di Frascati, Frascati, Italy*

R. PETRONZIO[1]
*CERN, Geneva, Switzerland*

Received 5 December 1983
(Revised 16 April 1984)

We show that lattice QCD can be used to evaluate the matrix elements of four-fermion operators which are relevant for weak decays. A first comparison between the results obtained on the lattice and other determinations are also presented.


Nuclear Physics B180[FS2] (1981) 369–377
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### A PROPOSAL FOR MONTE CARLO SIMULATIONS OF FERMIONIC SYSTEMS

F. FUCITO
*Istituto di Fisica dell'Università di Roma and*
*INFN, Frascati, Italy*

E. MARINARI
*Istituto di Fisica dell'Università di Roma and*
*INFN, Roma, Italy*

G. PARISI
*INFN, Frascati, Italy*

C. REBBI[1]
*CERN, Geneva, Switzerland*

Received 27 October 1980

We suggest a possible extension of the Monte Carlo technique to systems with fermionic degrees of freedom. We study in detail the application to an elementary example.

- Parallel to the development of lattice gauge theory (LGT), there have been equally remarkable **advances in computer design** and implementation.
- It soon became clear that **parallel** assemblies of computing nodes offered the most effective route to the **highest computational performance**.

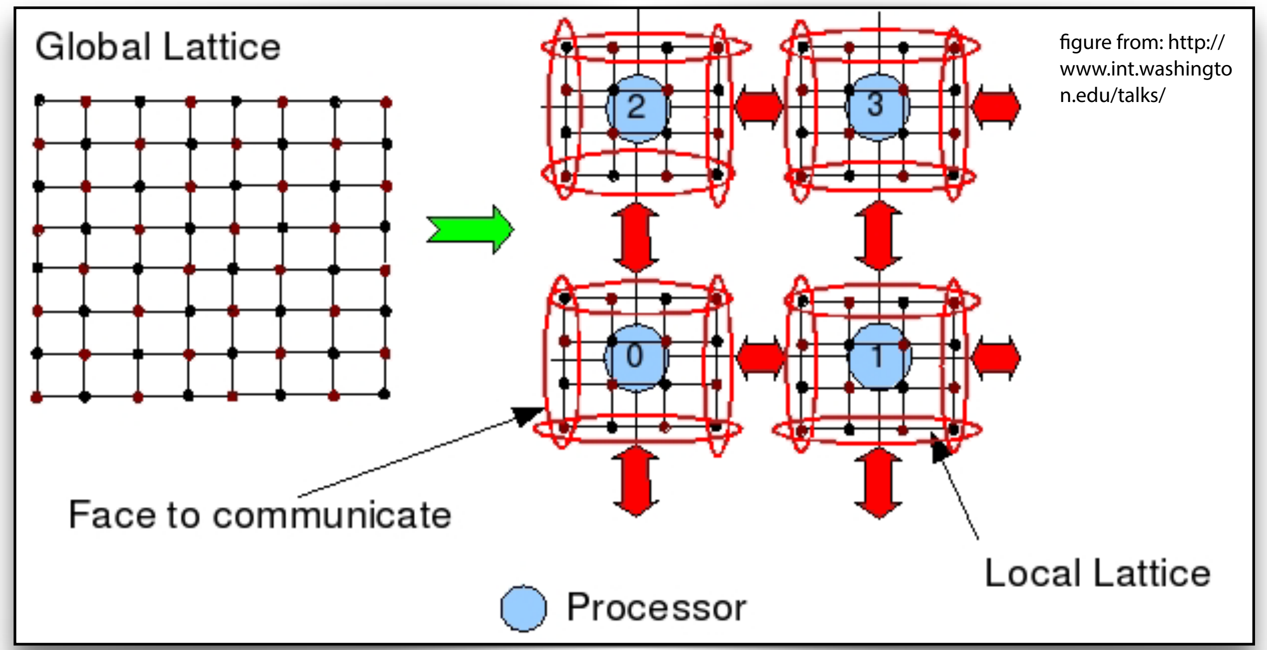
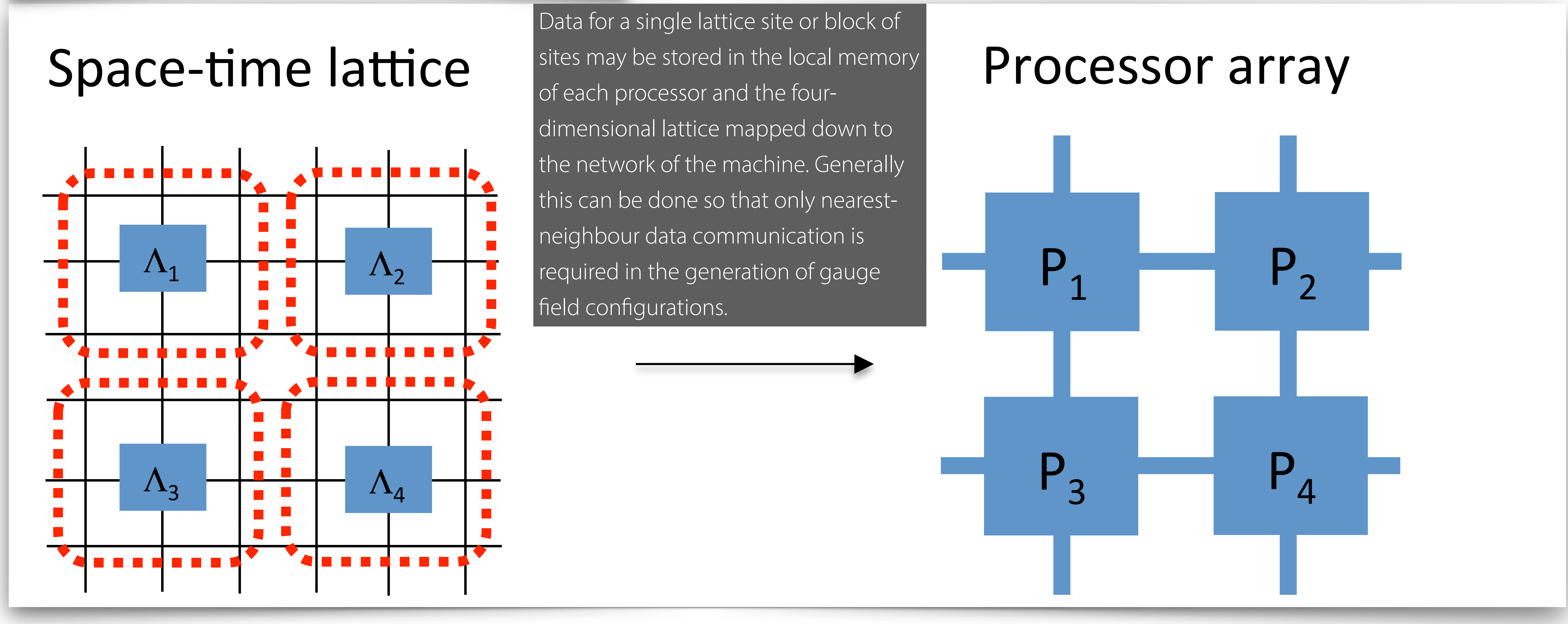


figure from: http://www.int.washington.edu/talks/

**ideal case of the parallel computation paradigm !**



Data for a single lattice site or block of sites may be stored in the local memory of each processor and the four-dimensional lattice mapped down to the network of the machine. Generally this can be done so that only nearest-neighbour data communication is required in the generation of gauge field configurations.

**Locality:** *(property of the field theoretic description of fundamental interactions)*

- the numerical operations at a site n can be carried out independently of those at a site m unless the pair is within the limited neighborhood of each other;
- calculations by a given processor can be carried out independently of those by the other processors, except that the processors with overlapping boundaries have to exchange values of fields in the boundaries before and/or after the calculations in each sub lattice;
- for a fixed lattice size, the computation time can be reduced by a factor $N_P$, and for a fixed sub-lattice size, one can enlarge the total lattice size proportionately to the number of processors $N_P$ without increasing the computation time.

# Lattice QCD and parallel computers building

| name | year | authors | peak speed |
|---|---|---|---|
| Columbia | 1984 | Christ-Terrano | – |
| Columbia-16 | 1985 | Christ et al | 0.25 GFlop/s |
| **APE1** | **1988** | **Cabibbo-Parisi** | **1 GFlop/s** |
| Columbia-64 | 1987 | Christ et al | 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 |

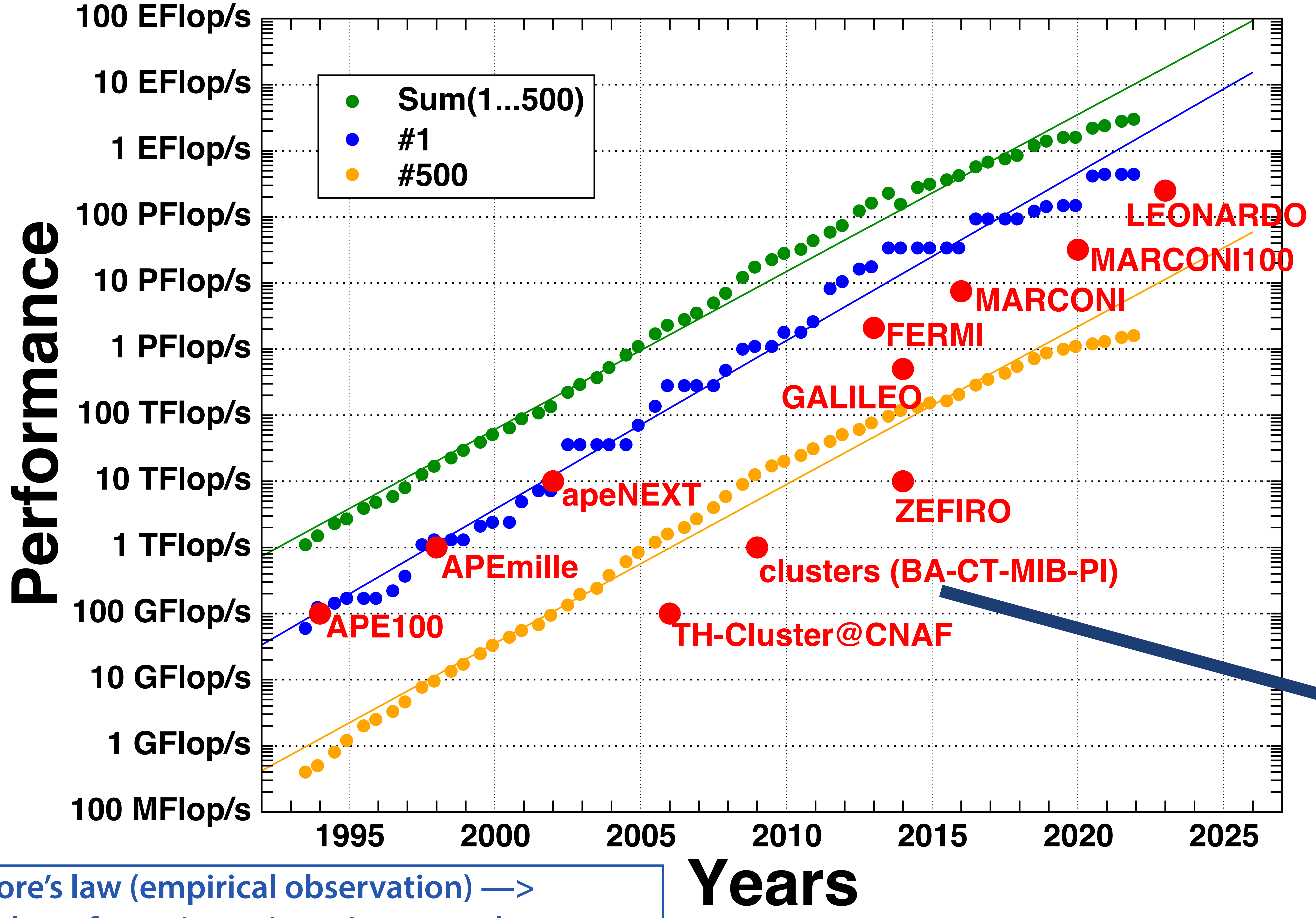
Apart from contributing to the first seminal papers in LQCD, INFN emerged as a key player on the international stage in the development of dedicated hardware. This significant undertaking, known as the APE project, spanned from 1988 to 2004.

APE100

APE computers were also installed at INFN - Bari

APEmille

# A look at computing resources for INFN-TH over the last 30 years



—> Moore's law (empirical observation) —> the number of transistors in an integrated circuit doubles about every two years.

BC²S was as a precursor to ReCaS Bari

# Example: timeline of the computing power @Cineca

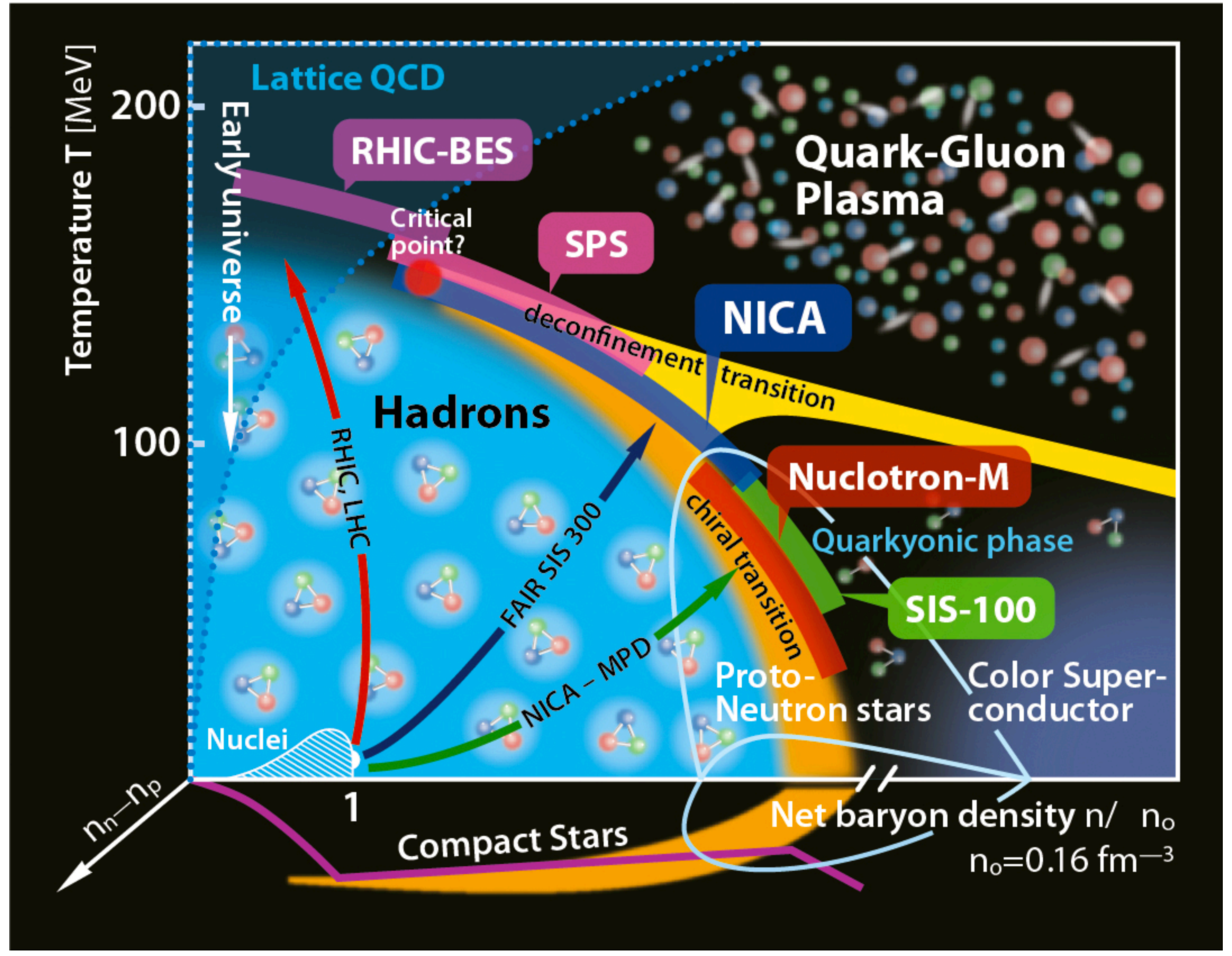
| | | | | | |
|---|---|---|---|---|---|
| 3 MFlops | 800 MFlops | 9.6 GFlops | 2 PFlops | 20 PFlops | Towards ExaFlops |
| CDC 6600<br>1 core | CRAY-XMP<br>2 core | CRAY-T3D<br>64 core | FERMI<br>160000 core | Marconi<br>400000 core | Leonardo |
| **1969** | **1985** | **1995** | **2012** | **2019** | **future** |
| | 400 MFlops/ core | | 12,500 MFlops/ core | 50,000 MFlops/ core | |

## *Not only brute force…*

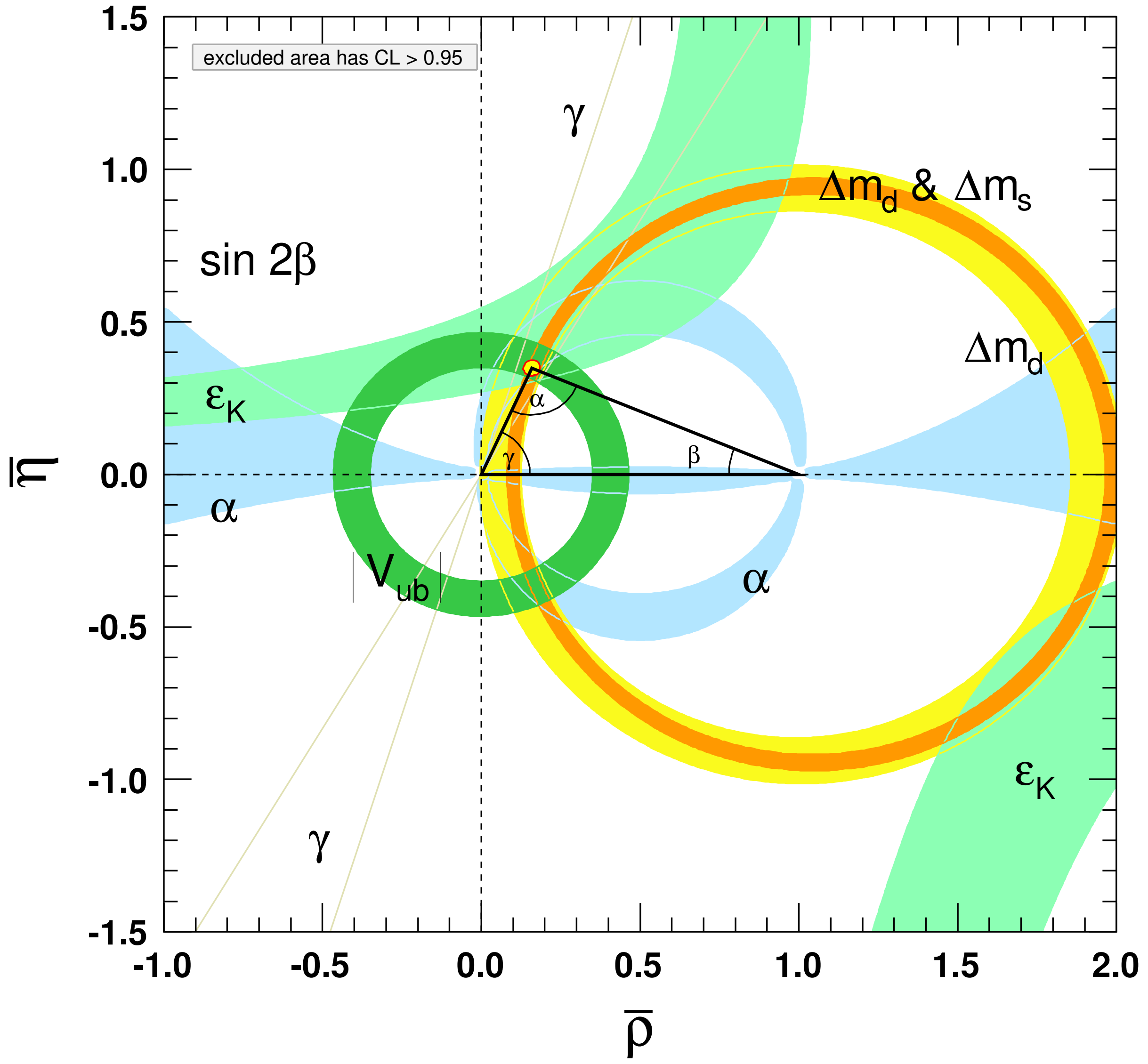
**Developing computational strategies requires combining physical insight with an understanding of modern numerical mathematics and the capabilities of massively parallel computers.**

# Lattice QCD

## Study of QCD in extreme conditions



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



- Lattice QCD is an essential tool for obtaining precise model-free 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 $\mathcal{O}(\mathbf{10^5})$ 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.

# Lattice QCD as an extraordinary tool for understanding Nature

**Similar to experiments** (where data are first collected and and later analyzed) the Lattice QCD workflow can be factorized into:

**Lattice simulations on upcoming exascale computers**

arXiv:2204.00039

| Lattice volume | $a^{-1}$ GeV | Exaflop hours |
|---|---|---|
| $32^3 \times 64$ | 1.4 | 1.5 |
| $40^3 \times 96$ | 1.7 | 3.5 |
| $48^3 \times 64$ | 2.1 | 7.5 |
| $48^3 \times 96$ | 1.8 | 7.54 |
| $64^3 \times 128$ | 2.4 | 25 |
| $96^3 \times 192$ | 2.8 | 120 |
| $64^3 \times 256$ | 2.4 | 50 |
| $96^3 \times 384$ | 2.8 | 250 |
| $128^3 \times 512$ | | 1500 |
| $128^3 \times 512$ | 5.0 | 12000 |

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

lattice size $L = 10$ fm, $m_\pi L = 7$

lattice spacing $a = 0.04$ fm

lattice spacing —> continuum limit

physical volumes large enough to ensure that finite-volume effects are under control.

## GENERATION

Gauge-field configurations are generated by means of Markov chain 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.

# NOT ONLY LATTICE QCD…

~200 researchers

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

## Computational Theoretical Physics @ INFN

**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

- *BIOPHYS (PI S. Stramaglia)*
- *FIELDTURB (PI G. Gonnella)*
- *QUANTUM (PI P. Facchi)*
- *NPQCD*

# Cosmology and Astroparticle Physics

**INDARK** **NEUMATT**

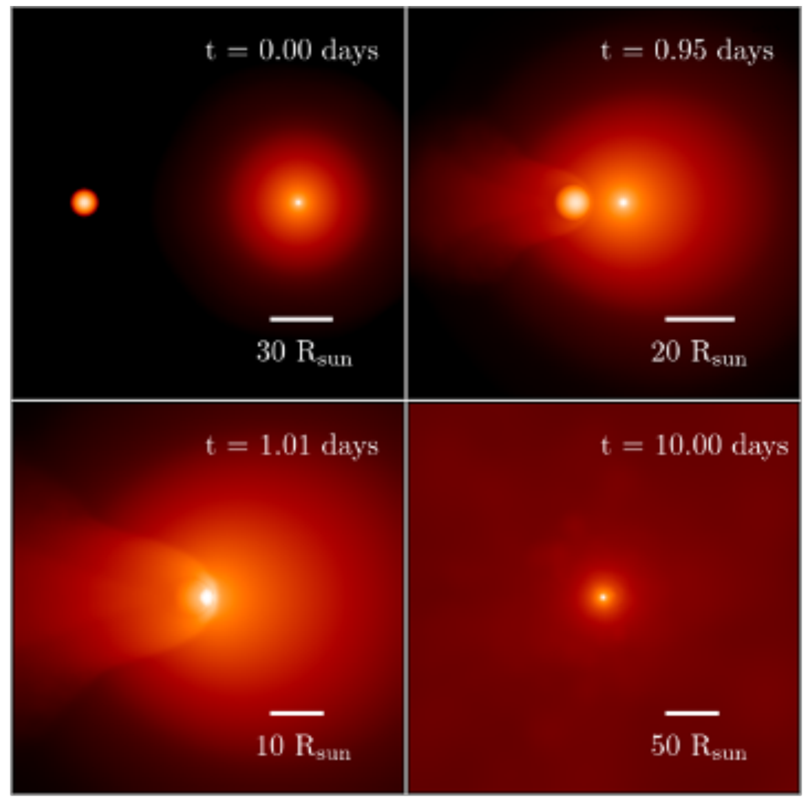
**TEONGRAV**

## 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*)

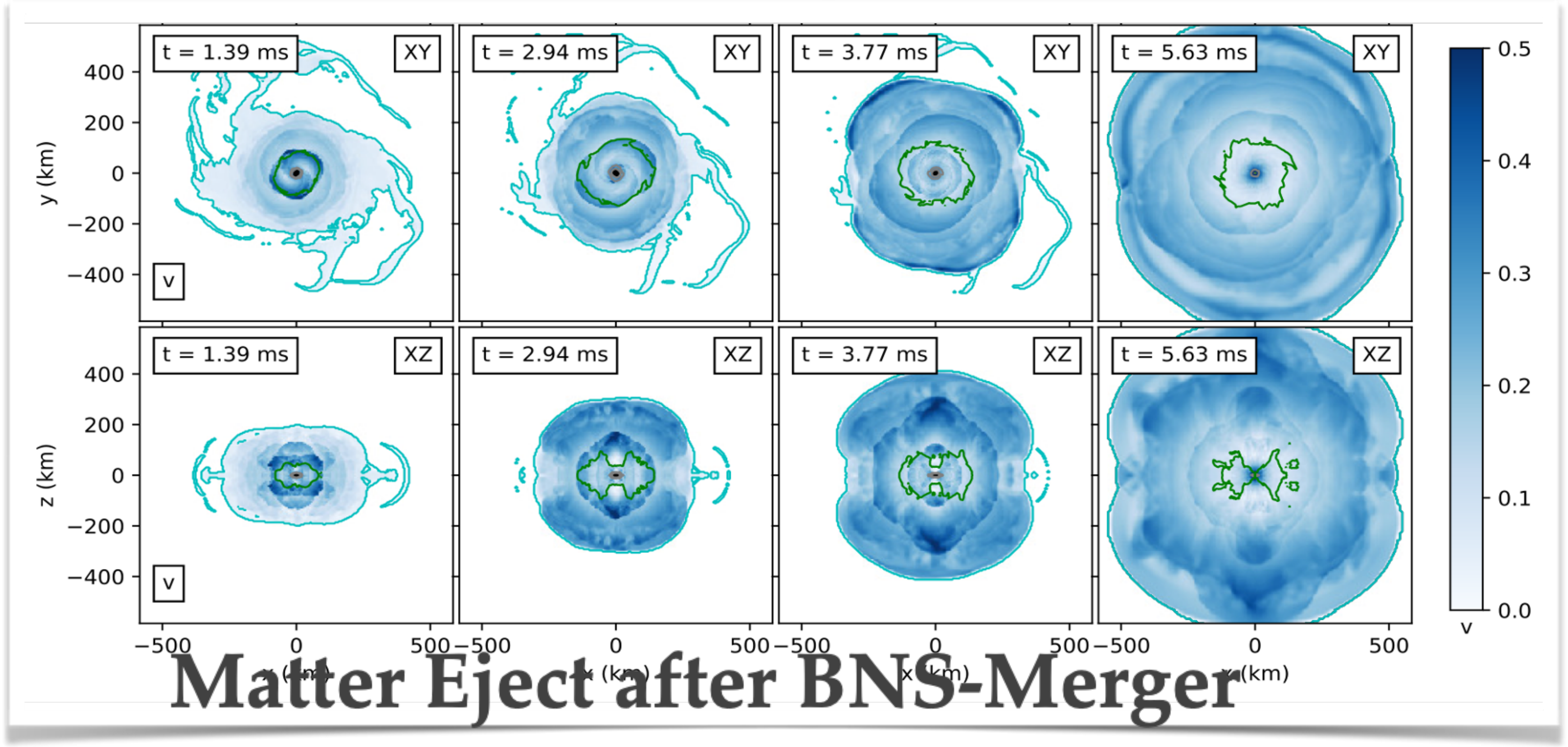
**Hydrodynamics and magnetohydrodynamics simulations using state of the art codes in both the Newtonian and the General Relativistic regime**
(*e.g. Model dynamical evolution and formation of stellar-mass and supermassive black holes via N-body simulations* )



## 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.



**Matter Eject after BNS-Merger**

## 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

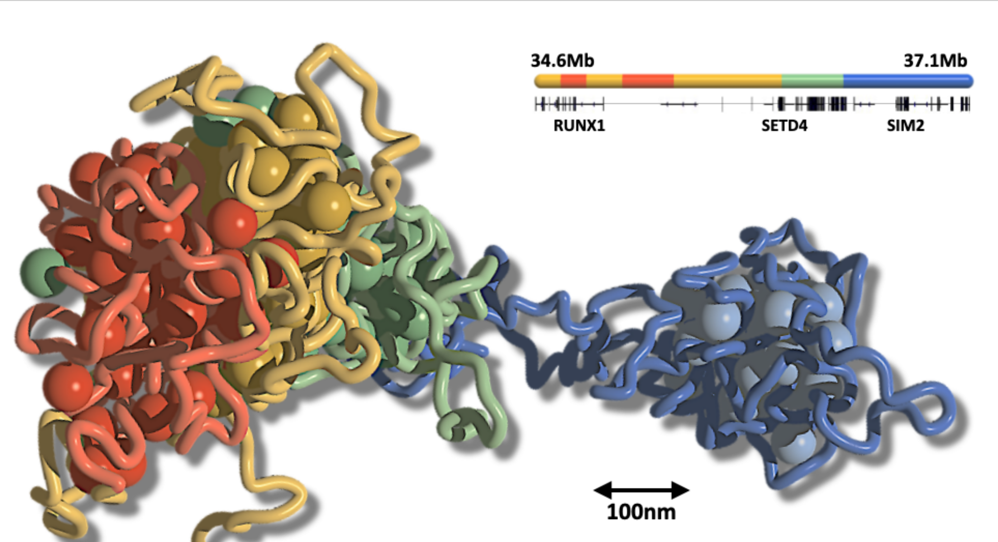
**BIOPHYS** **ENESMA** **FIELDTURB**

## 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.

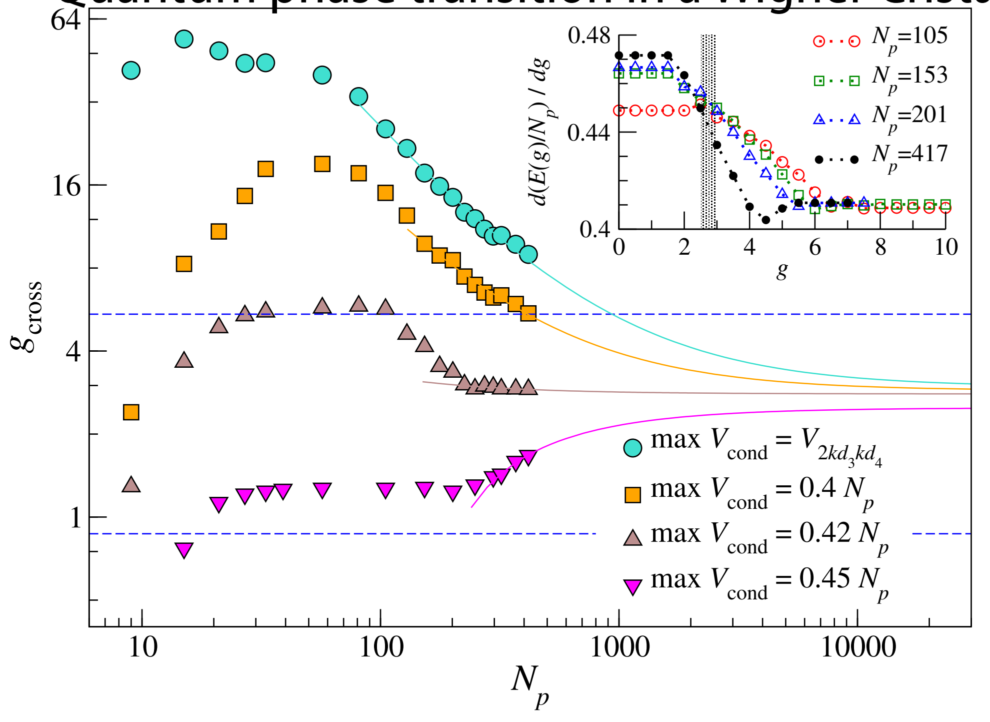


DNA Folding

## 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...).

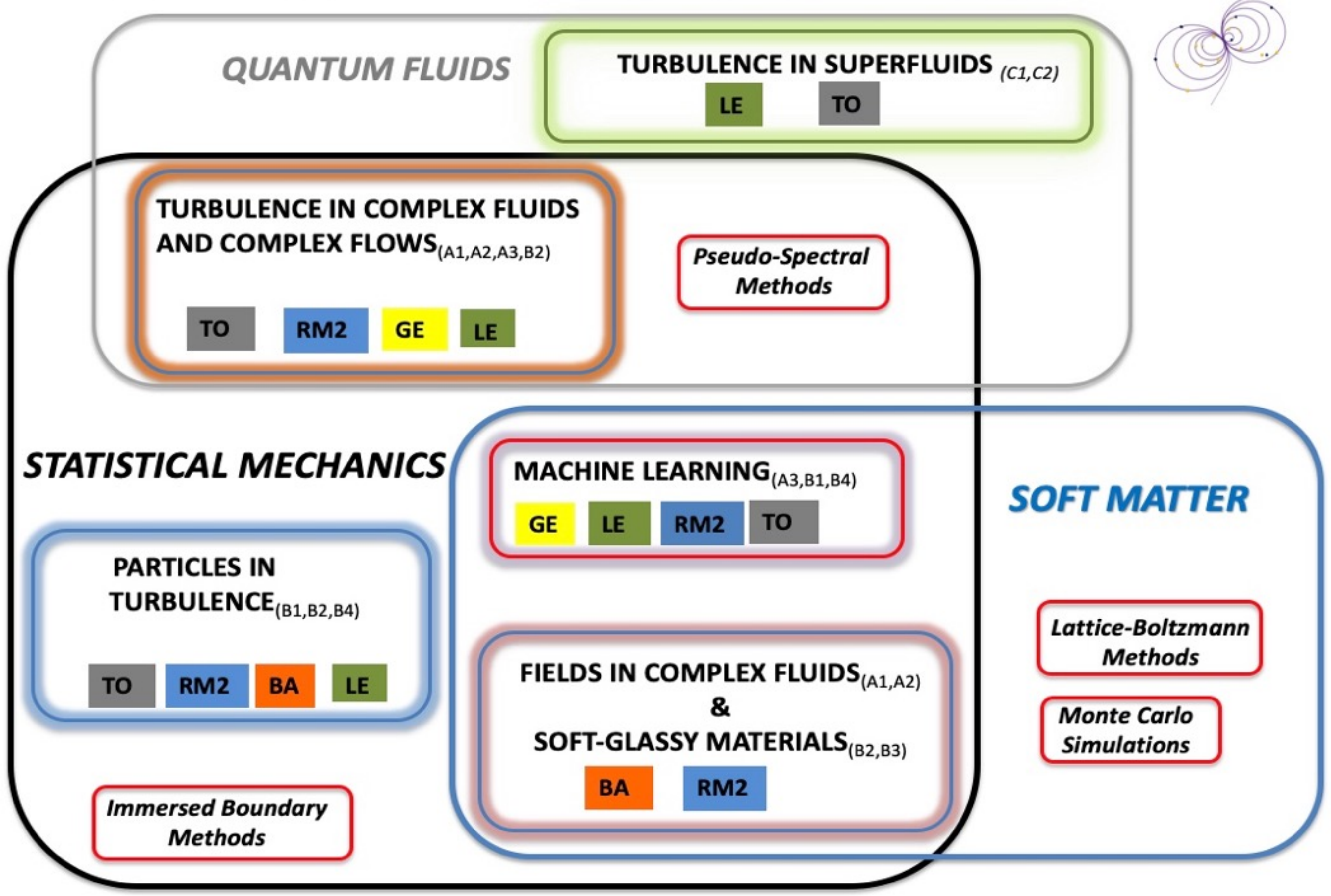
Quantum phase transition in a Wigner Cristal



## FIELDTURB

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

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



*QUANTUM FLUIDS*

**TURBULENCE IN SUPERFLUIDS** $_{(C1,C2)}$
LE TO

**TURBULENCE IN COMPLEX FLUIDS AND COMPLEX FLOWS** $_{(A1,A2,A3,B2)}$
TO RM2 GE LE

*Pseudo-Spectral Methods*

*STATISTICAL MECHANICS*

**MACHINE LEARNING** $_{(A3,B1,B4)}$
GE LE RM2 TO

*SOFT MATTER*

**PARTICLES IN TURBULENCE** $_{(B1,B2,B4)}$
TO RM2 BA LE

**FIELDS IN COMPLEX FLUIDS** $_{(A1,A2)}$
&
**SOFT-GLASSY MATERIALS** $_{(B2,B3)}$
BA RM2

*Lattice-Boltzmann Methods*

*Monte Carlo Simulations*

*Immersed Boundary Methods*

# 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.

# Nuclear Physics

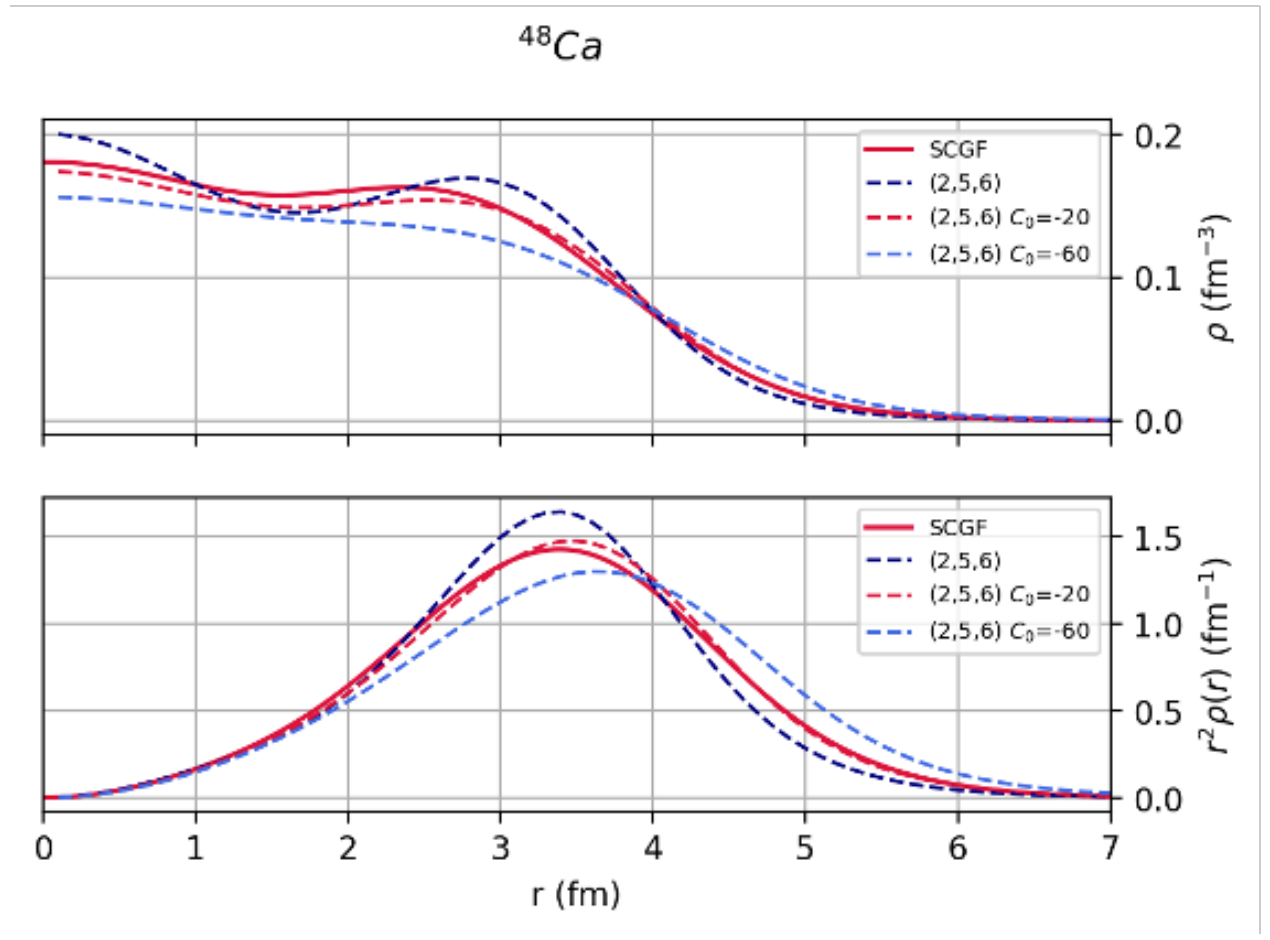
***MONSTRE***
***NUCSYS***

## *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

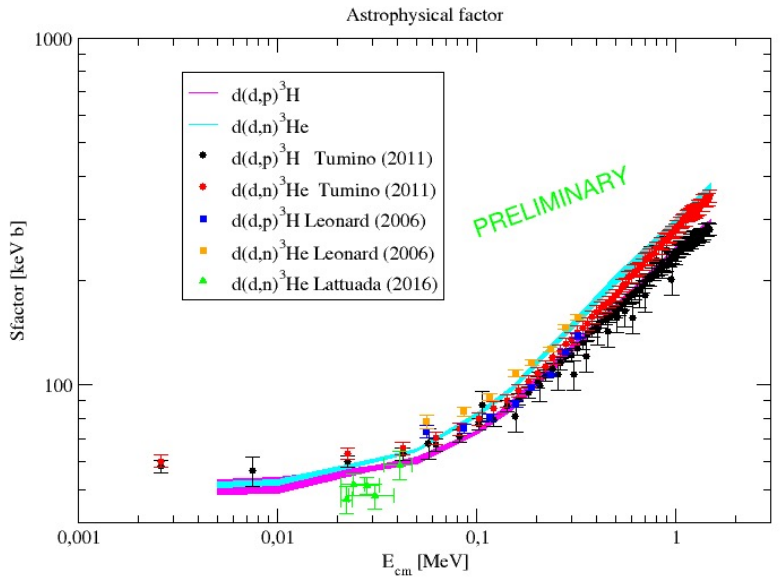
**Calcoli *ab initio***

- 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)

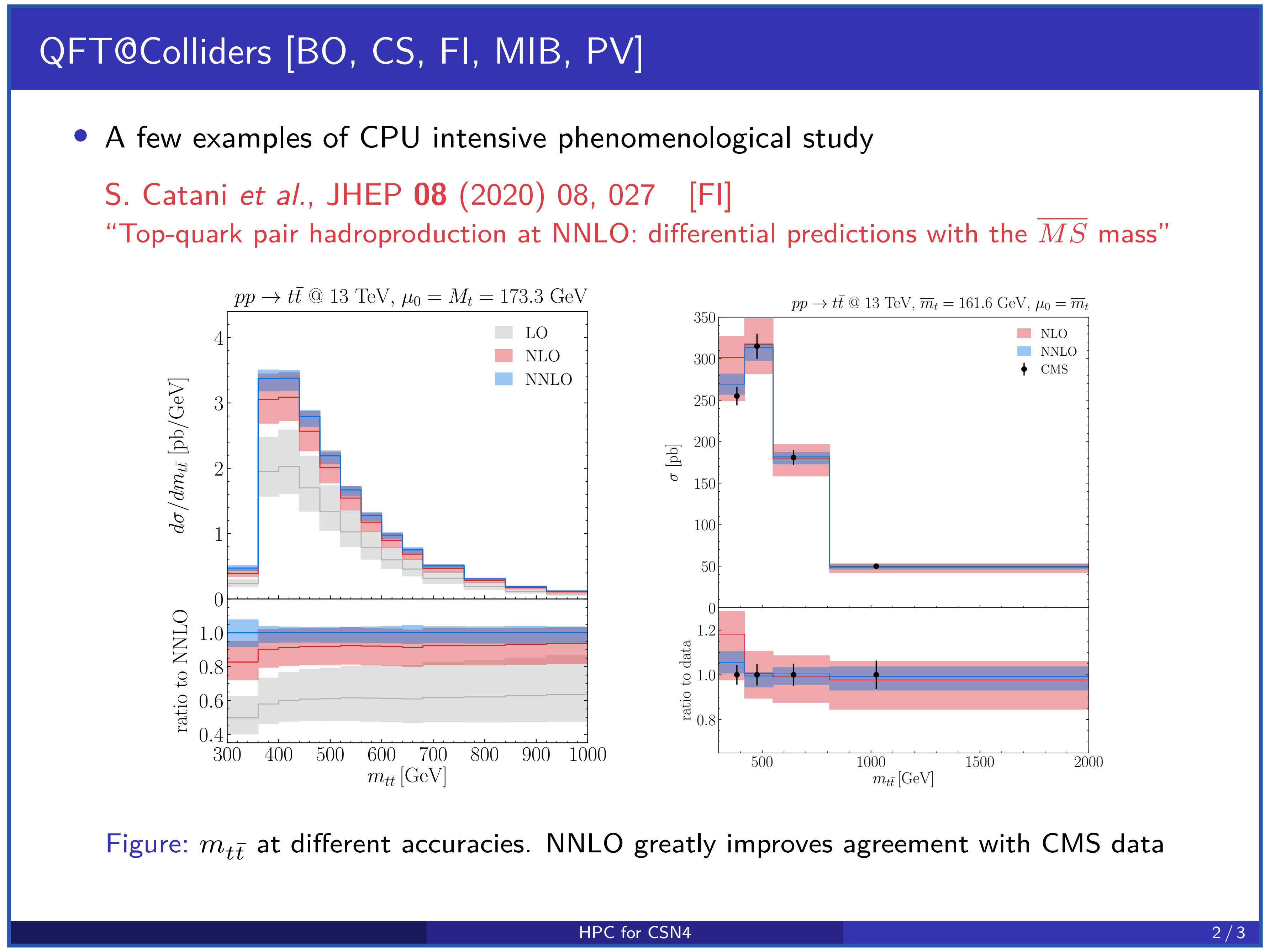
**NEXT: implementation using GPUs, extension up to A=6**

# 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

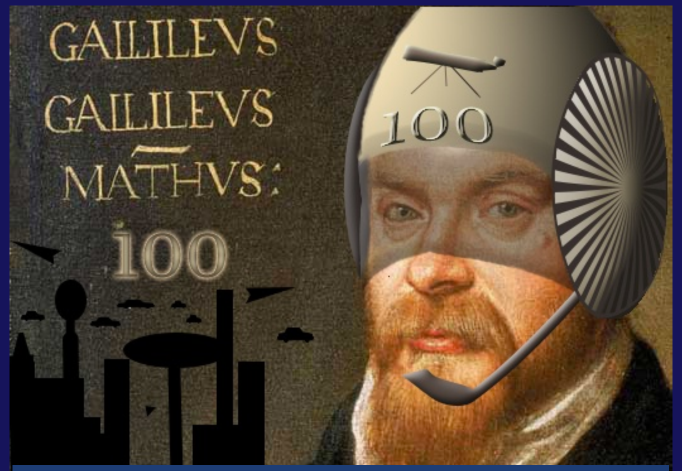
HPC for CSN4 2 / 3

# Computing Resources (*)

## Cineca-INFN agreement

### Cineca-INFN

MARCONI-A3
60 Mcorehours



GALILEO 100
6 Mcorehours

LEONARDO
Booster: 3 Mnodehours

LEONARDO
General purpose

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

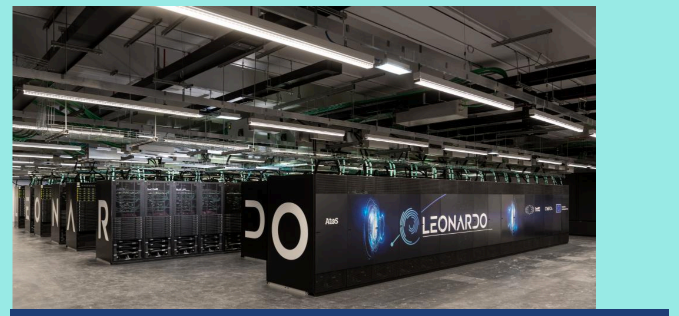
ISCRA
CINECA

## Euro-HPC

### EuroHPC

EuroHPC
Joint Undertaking

LUMI supercomputer
375 PFlop/s -



LEONARDO
supercomputer

MARENOSTRUM 5
205 PFlop/s - SPAIN

HPC Vega IZUM
6.92 PFlop/s -

MELUXINA supercomputer
12.81 PFlop/s -

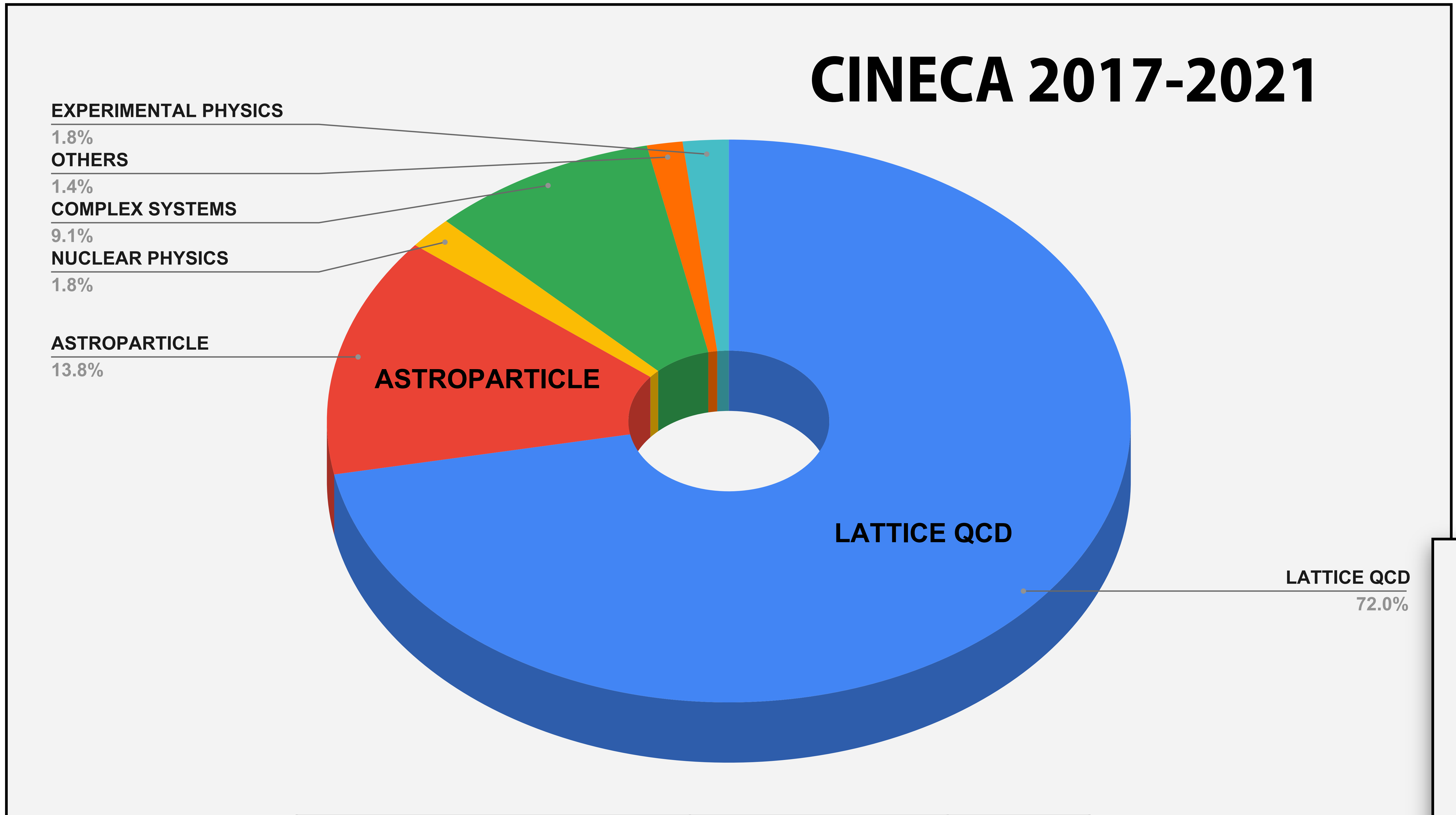
DEUCALION
supercomputer

DISCOVERER
supercomputer

KAROLINA supercomputer
9.59 PFlop/s - CZECH

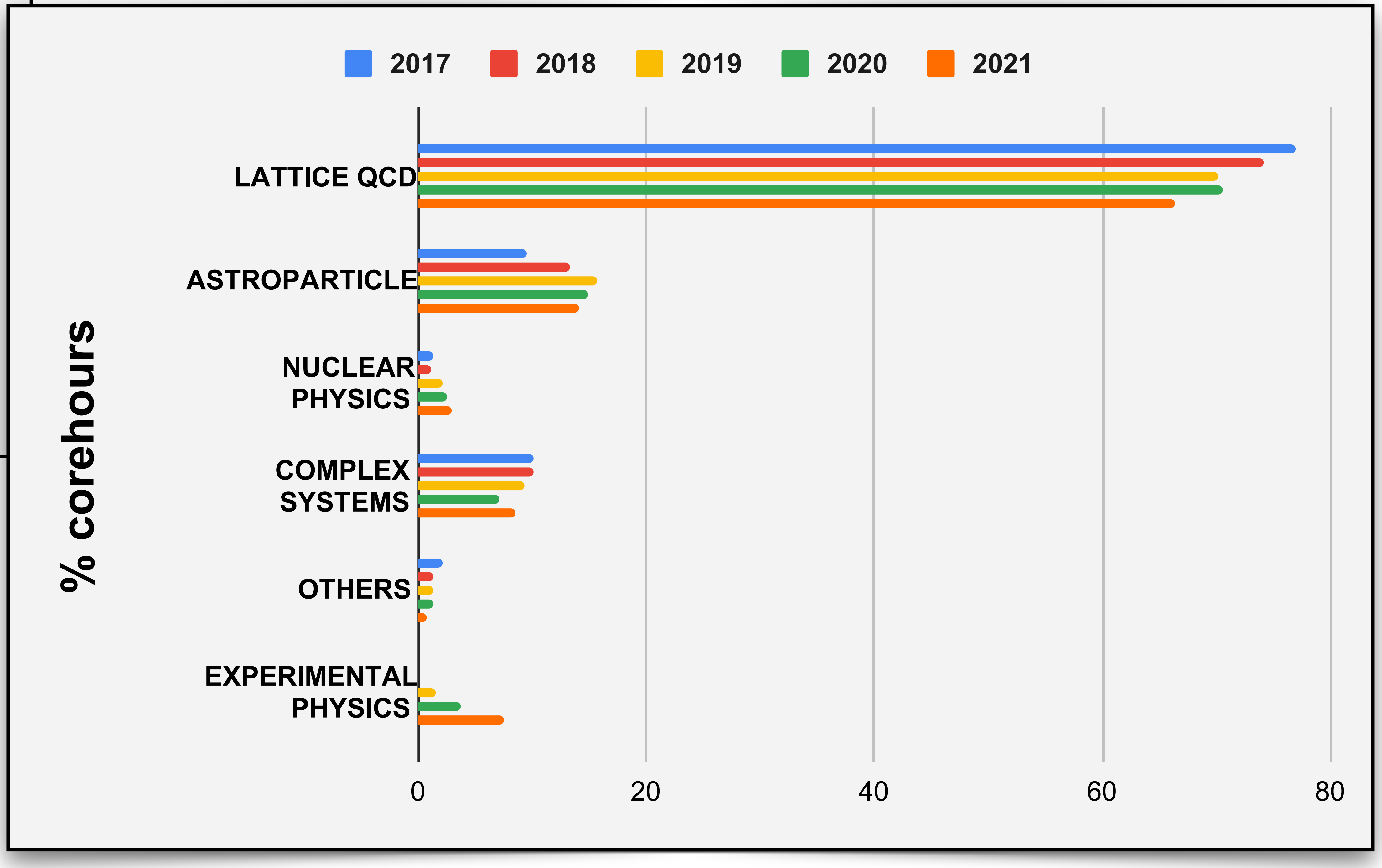
(*) other resources from Tier1/Tier2 (e.g. ReCaS)

# HPC COMPUTING RESOURCES 2017-2021

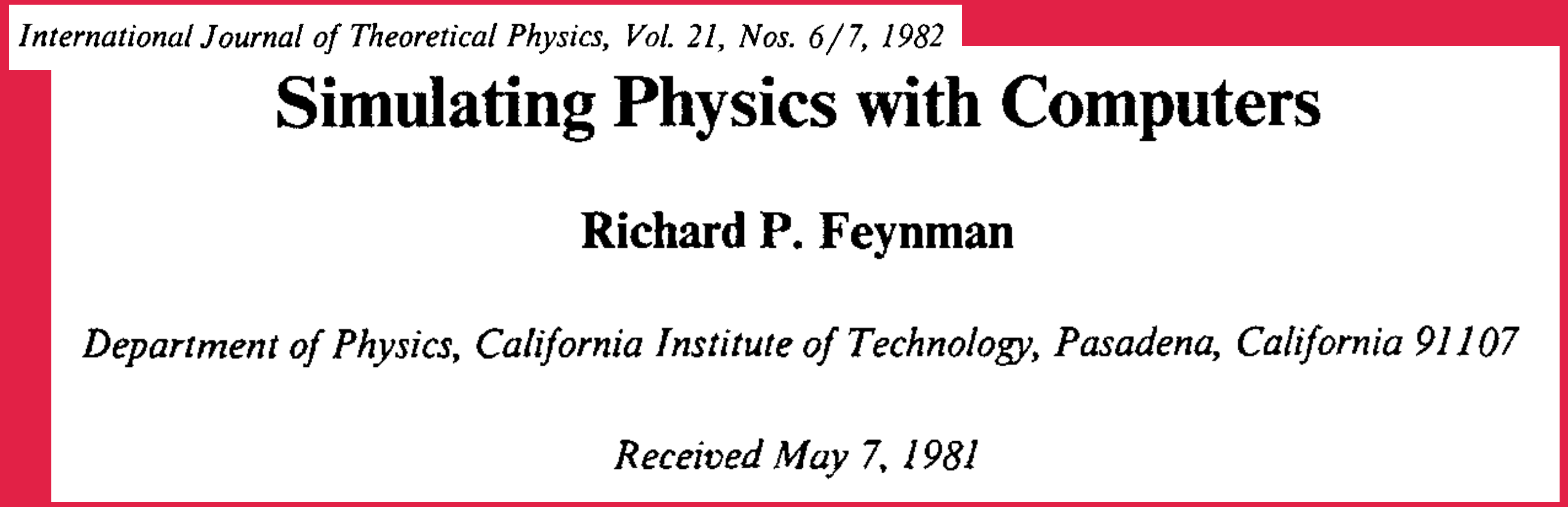


| AREA | corehours | % |
|---|---:|---:|
| LATTICE QCD | 687,787,117 | 72.0 |
| ASTROPARTICLE | 131,826,951 | 13.8 |
| NUCLEAR PHYSICS | 17,546,676 | 1.8 |
| COMPLEX SYSTEMS | 87,396,389 | 9.1 |
| OTHERS | 13,724,017 | 1.4 |
| EXPERIMENTAL PHYSICS | 17,596,432 | 1.8 |
| *TOTAL* | *955,877,582* | *100*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

| %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 |



# HPC + Quantum Computing ?



*International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982*

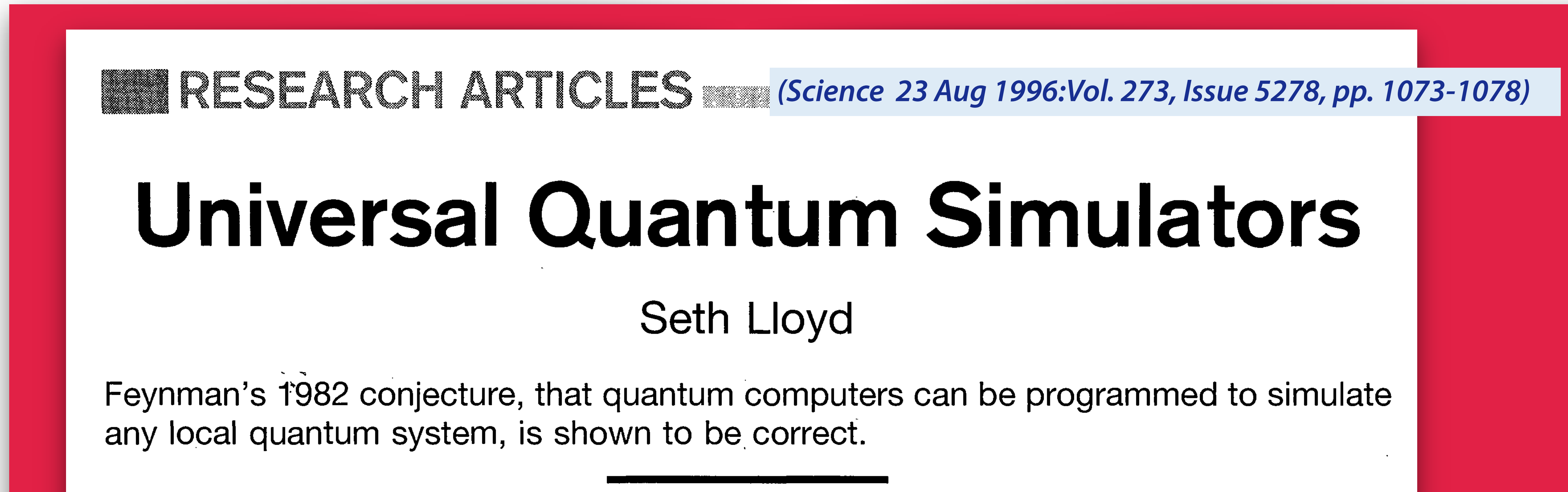
**Simulating Physics with Computers**

**Richard P. Feynman**

*Department of Physics, California Institute of Technology, Pasadena, California 91107*

*Received May 7, 1981*

"Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws."



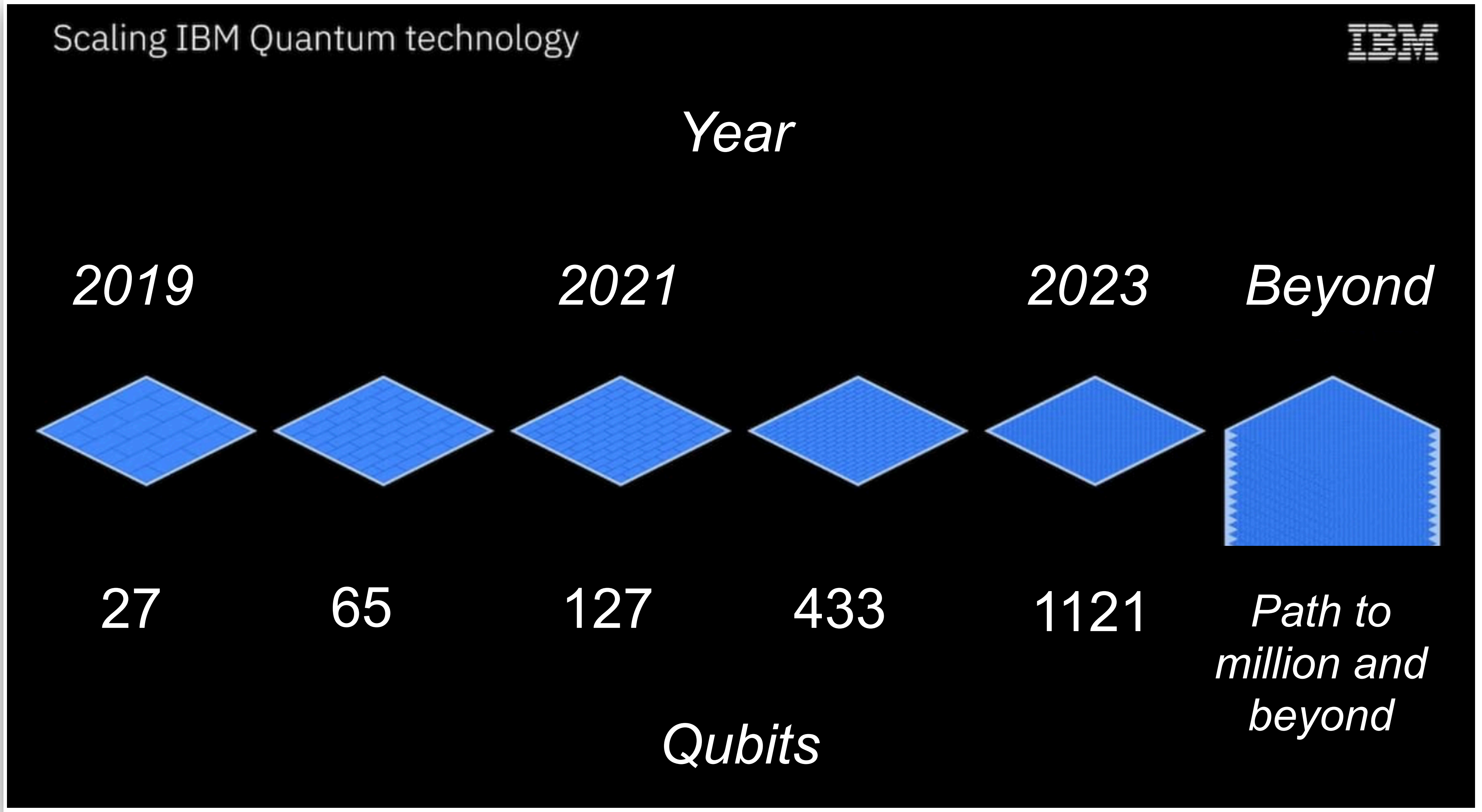
RESEARCH ARTICLES *(Science 23 Aug 1996:Vol. 273, Issue 5278, pp. 1073-1078)*

**Universal Quantum Simulators**

Seth Lloyd

Feynman's 1982 conjecture, that quantum computers can be programmed to simulate any local quantum system, is shown to be correct.

Universal simulator: by appropriately changing the sequence of quantum operations (the code), it can simulate problems that are very different from each other.



**Quantum computing will play a huge role in the future of HPC**

**Develop a hybrid programming platform that combines quantum simulations with classical high-performance computing to accelerate the computing speed of classical supercomputers.**

ICSC

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

# Supercomputing shaping the future

# Lo scopo e gli obiettivi di ICSC

Creare un'infrastruttura digitale nazionale per ricerca e innovazione, partendo dalle attuali infrastrutture in HPC, HTC e Big Data…

… evolvere verso un modello di **cloud datalake**, accessibile dalle comunità scientifiche e industriali attraverso interfacce web cloud flessibili e uniformi, affidandosi a un team di supporto di alto livello …

… costituire un **ecosistema attrattivo a livello globale basato su partenariati strategici pubblico-privato** per sfruttare appieno l'infrastruttura digitale di alto livello per il calcolo scientifico e tecnico e per promuovere lo sviluppo di nuove tecnologie informatiche

# 5 pilastri del programma d'azione

- Costruire **un'infrastruttura cloud di supercalcolo** di livello mondiale per archiviare, gestire ed elaborare tutti i dati prodotti
- Istituire **centri di eccellenza** con team di esperti di alto livello per sviluppare applicazioni del settore
- Creare forti legami tra il **mondo accademico**, l'**industria** e la **pubblica amministrazione**

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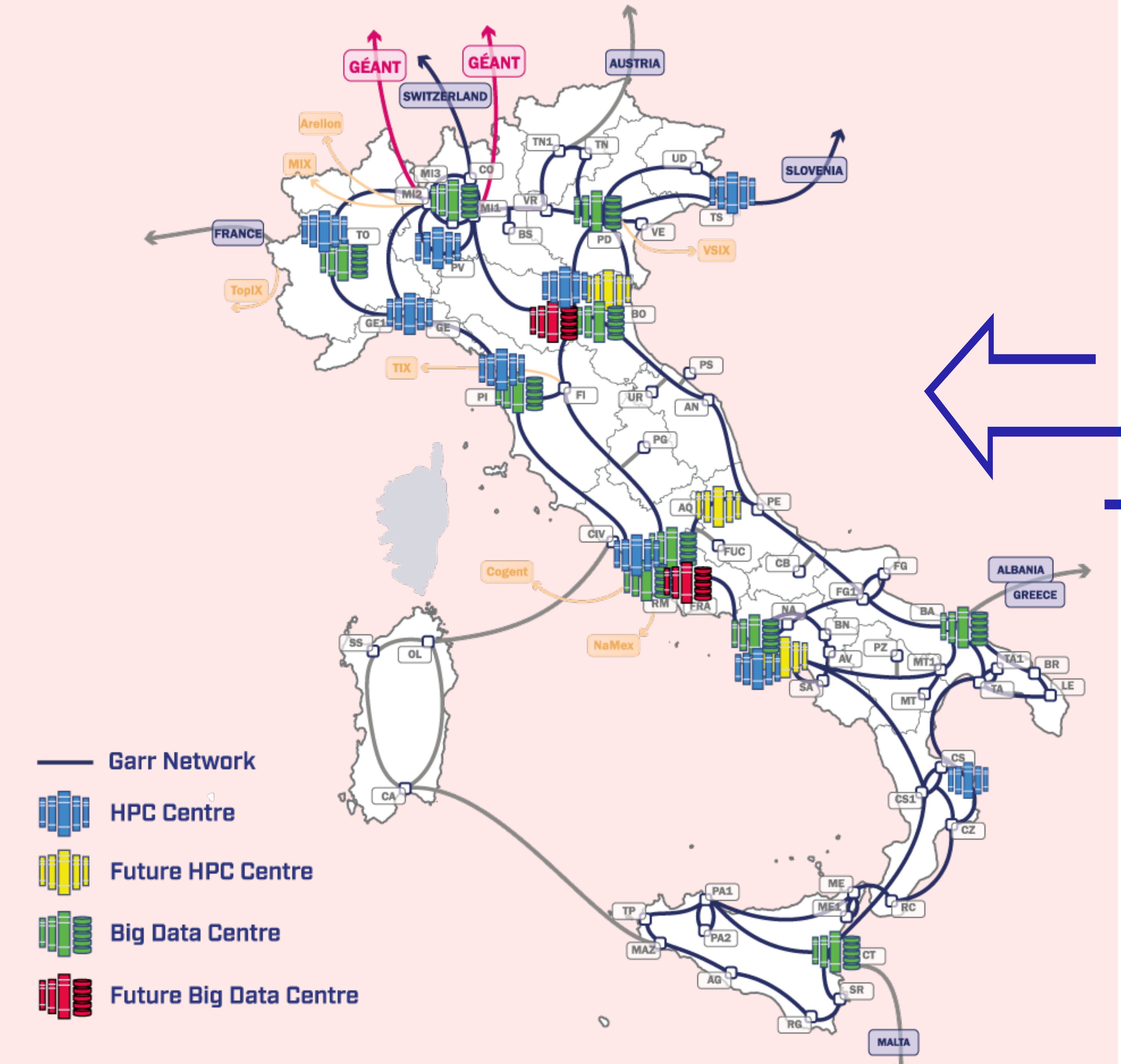
1010100100001
1010100100101

- **Formare** la prossima generazione di data scientist e manager affinché diventino **esperti** nella transizione digitale
- Attuare **misure strutturali per l'innovazione** e la **divulgazione**

# L'ICSC include
# **10 Spoke tematici**
# e
# **1 Spoke infrastruttura**

## 0 SUPERCOMPUTING CLOUD INFRASTRUCTURE



dotato di un team di esperti di alto livello che integrano i gruppi di lavoro degli Spoke (gruppi misti trasversali)

**ISTRUZIONE E FORMAZIONE, IMPRENDITORIALITÀ, TRASFERIMENTO DI CONOSCENZE, POLICY, OUTREACH**

**1** FUTURE HPC & BIG DATA

**2** FUNDAMENTAL RESEARCH & SPACE ECONOMY

**3** ASTROPHYSICS & COSMOS OBSERVATIONS

**4** EARTH & CLIMATE

**5** ENVIRONMENT & NATURAL DISASTERS

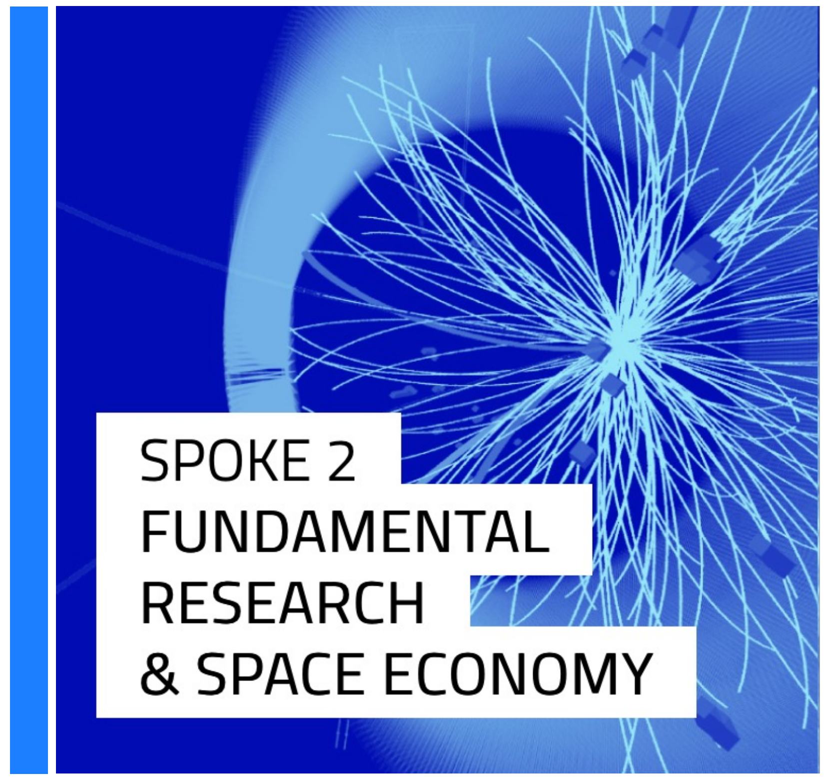
**6** MULTISCALE MODELING & ENGINEERING APPLICATIONS

**7** MATERIALS & MOLECULAR SCIENCES

**8** IN-SILICO MEDICINE & OMICS DATA

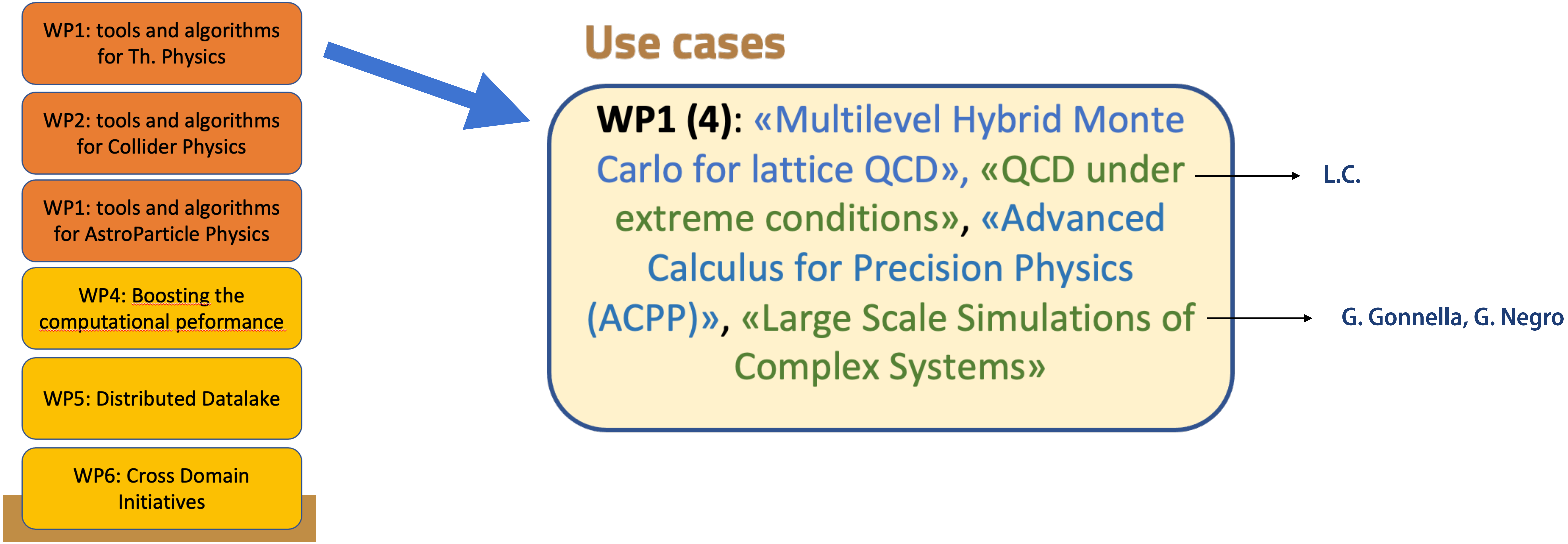
**9** DIGITAL SOCIETY & SMART CITIES

**10** QUANTUM COMPUTING



## 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.



- 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

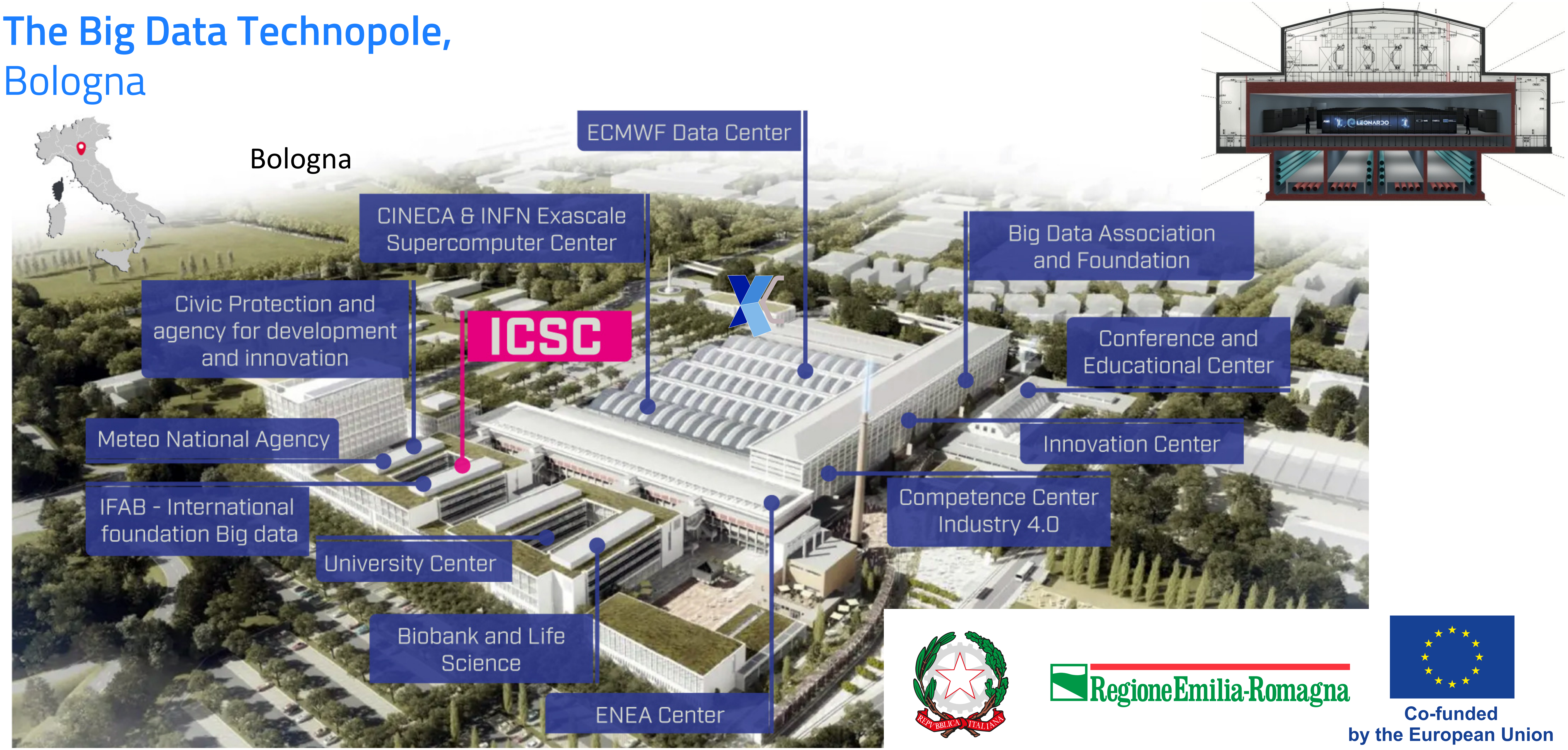
### Use cases

**WP1 (4)**: «Multilevel Hybrid Monte Carlo for lattice QCD», «QCD under extreme conditions», «Advanced Calculus for Precision Physics (ACPP)», «Large Scale Simulations of Complex Systems»

→ L.C.

→ G. Gonnella, G. Negro

# The Big Data Technopole, Bologna



Bologna

ECMWF Data Center

CINECA & INFN Exascale Supercomputer Center

Big Data Association and Foundation

Civic Protection and agency for development and innovation

ICSC

Conference and Educational Center

Meteo National Agency

Innovation Center

IFAB - International foundation Big data

Competence Center Industry 4.0

University Center

Biobank and Life Science

ENEA Center

RegioneEmilia-Romagna

Co-funded by the European Union

- 5092 computing nodes subdivided in:

**Booster module (GPUs)**

- **Model:** BullSequana X2135 "Da Vinci" single node GPU Blade
  **Nodes**: 3456 booster nodes
  **Processors**: Intel Xeon 8358 32 cores, 2.6 GHz
  **Cores:** 110592 (32 cores/node)
  **Accelerators:** 4XNvidia custom Ampere GPU 64GB HBM2

**General Purpose module (CPUs)**

- **Model:** BullSequana X2140 three-node CPU Blade
  **Nodes**: 1536 data-centric nodes
  **Processors**: Intel Saphire Rapids 2x56 cores, 4.8 GHz
  **Cores:** 172032 (112 cores/node)
  **RAM:** (48x32) GB DDR5 4800 MHz
  **Network:** 3xNvidia HDR cards 1x100Gb/s

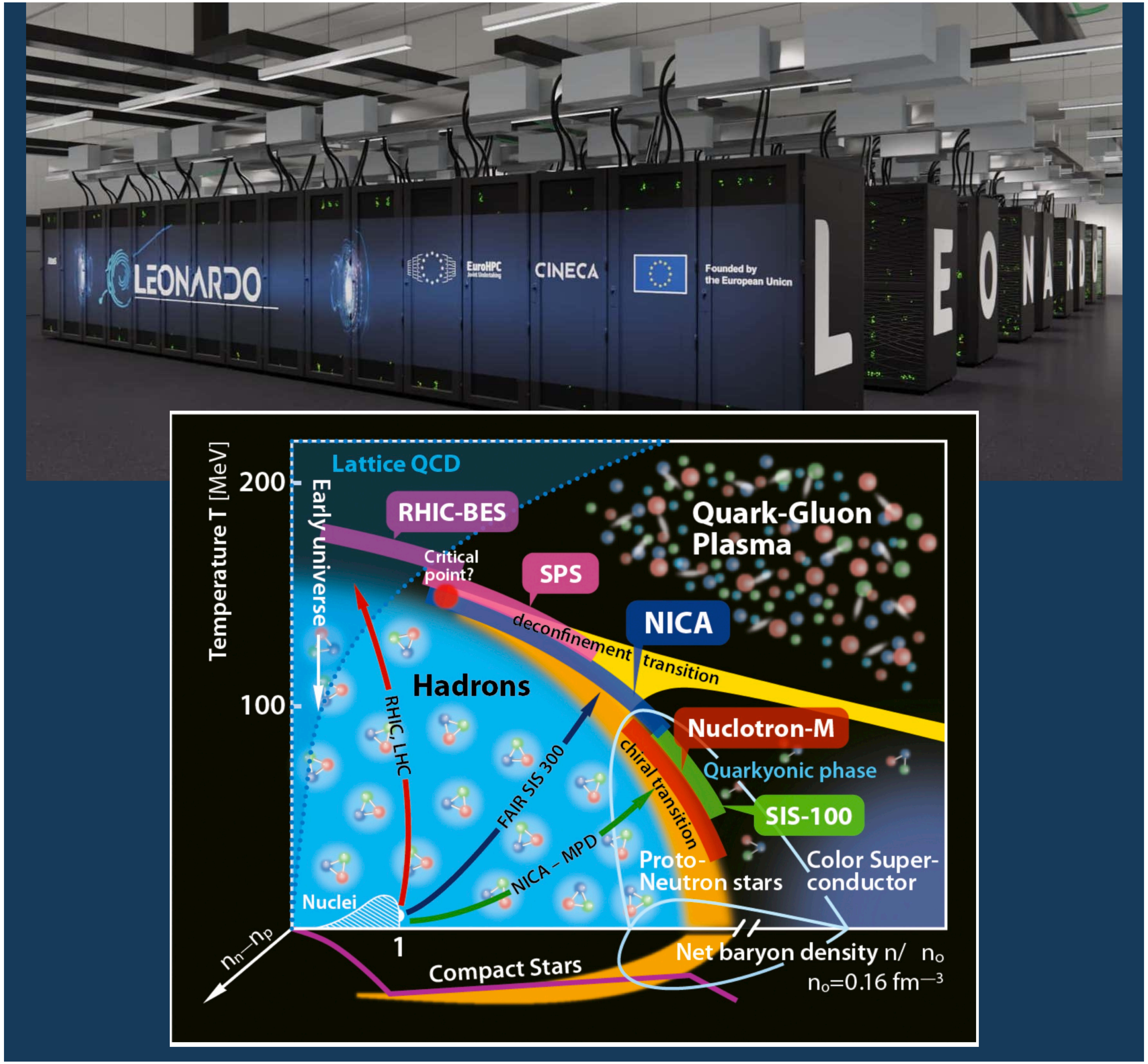
# TOP500.org (as of June 2023)

| Rank (previous) | Rmax<br>Rpeak<br>(PetaFLOPS) | Name | Model | CPU cores | Accelerator (e.g. GPU) cores | Interconnect | Manufacturer | Site country | Year |
|---|---|---|---|---|---|---|---|---|---|
| 1 — | 1,194.00<br>1,679.82 | Frontier | HPE Cray EX235a | 561,664 (8,776 × 64-core Optimized 3rd Generation EPYC 64C @2.0 GHz) | 36,992 × 220 AMD Instinct MI250X | Slingshot-11 | HPE | Oak Ridge National Laboratory 🇺🇸 United States | 2023 |
| 2 — | 442.010<br>537.212 | Fugaku | Supercomputer Fugaku | 7,630,848 (158,976 × 48-core Fujitsu A64FX @2.2 GHz) | 158,976 x<br>Fujitsu A64FX | Tofu interconnect D | Fujitsu | RIKEN Center for Computational Science 🇯🇵 Japan | 2020 |
| 3 — | 309.10<br>428.70 | LUMI | HPE Cray EX235a | 150,528 (2,352 × 64-core Optimized 3rd Generation EPYC 64C @2.0 GHz) | 9,408 × 220 AMD Instinct MI250X | Slingshot-11 | HPE | EuroHPC JU 🇪🇺 European Union, Kajaani, 🇫🇮 Finland | 2022 |
| 4 — | 238.70<br>304.47 | Leonardo | BullSequana XH2000 | 110,592 (3,456 × 32-core Xeon Platinum 8358 @2.6 GHz) | 15,872 × 108 Nvidia Ampere A100 | Nvidia HDR100 Infiniband | Atos | EuroHPC JU 🇪🇺 European Union, Bologna, 🇮🇹 Italy | 2023 |
| 5 — | 148.600<br>200.795 | Summit | IBM Power System AC922 | 202,752 (9,216 × 22-core IBM POWER9 @3.07 GHz) | 27,648 × 80 Nvidia Tesla V100 | InfiniBand EDR | IBM | Oak Ridge National Laboratory 🇺🇸 United States | 2018 |


ICSC

# Conclusions

- **Scientific computing has become one of the fundamental pillars of science, combining theory and experiment.**
- **Computational theoretical physics @INFN: a rich and enduring tradition that has made fundamental contributions to the advancement of high-performance computing (HPC) endeavors.  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, which necessitates a considerable amount of human resources —> ICSC.**
- **The availability of cutting-edge computing resources is vital for maintaining competitiveness on an international scale —> ICSC.**



# Thank you for your attention!