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

QCD in Extreme Conditions

Use case for the WP1

of the CN-HPC of the PNRR

M I C H E L E P E P E

I N F N Sez. Milano – Bicocca

Context

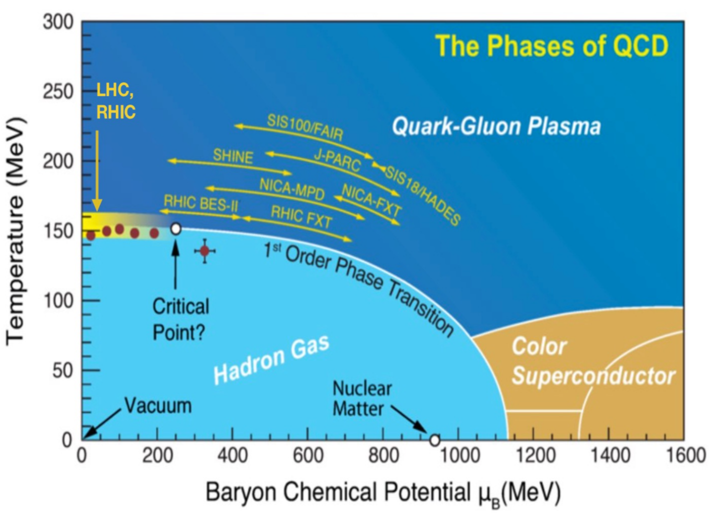
- Forces in Nature: Strong, Weak, Electro-magnetic and Gravitational

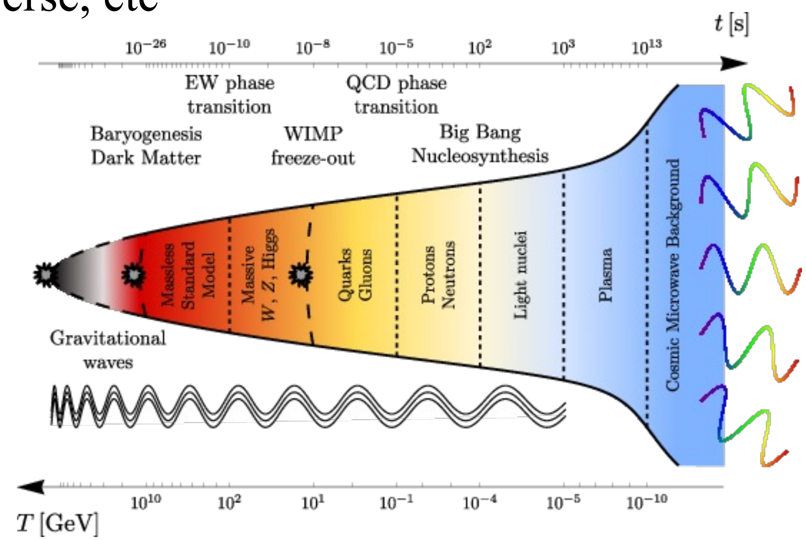
strong but short range:
scale of particle physics

weak but long range:
macroscopic scale

- Strong Interactions: responsible of the formation of protons and neutrons, and of their binding to form atomic nuclei (almost 100% of the mass of our body and of what we see)

- Strong Interactions play a crucial role also in nuclear physics and in astrophysics: Quark-Gluon plasma, neutron stars, early Universe, etc





- Extreme Conditions: high temperature, finite density, background fields, etc

Context

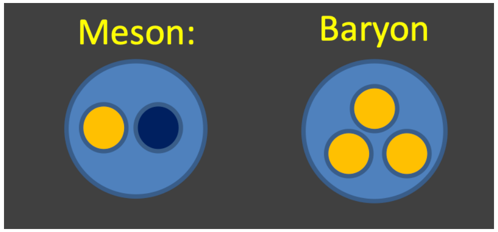
- Thanks to experimental results at particle colliders and to their interpretation and understanding by theorists we have a fundamental quantum theory of Strong Interactions

Quantum ChromoDynamics (QCD)

Matter fields

Quark and AntiQuarks:

Up, Down, Strange, Charm, Bottom, Top



Gauge fields

Gluons:

carrier of the interaction

"glue" that binds quarks

$$\sigma \simeq (\mathbf{0.4Gev})^2 \simeq \mathbf{10^5 N}$$

$$\sigma = \mathbf{M\,g} \qquad \mathbf{M} \sim \mathbf{100}\,\text{people}$$

As strong as a cm-thick steel cable but 13 orders of magnitude thinner

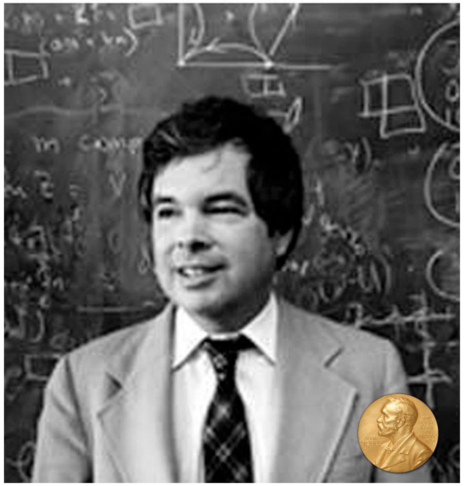
The Yang-Mills cableway

QCD sets the rules but to extract theoretical predictions we need to play all the games

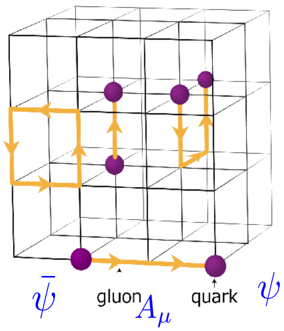
BUT

it is not possible to do it analitically

Lattice Field Theory and HPC

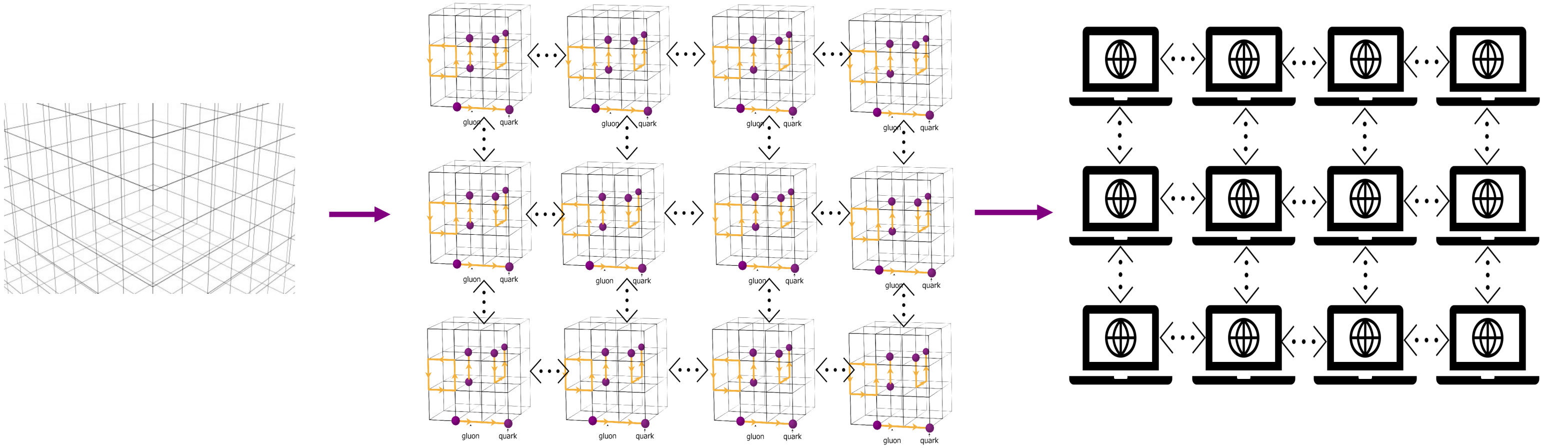


1974: K. Wilson proposes to define QCD on a space-time lattice



! The theory is formulated in terms of a **discrete** number of variables (=complex numbers);

- Lattice QCD is the only currently known formulation allowing to study QCD non-perturbatively from first principles; the theory can be put on a computer and solved numerically;
- A very demanding computational challenge: order 10^{10} variables

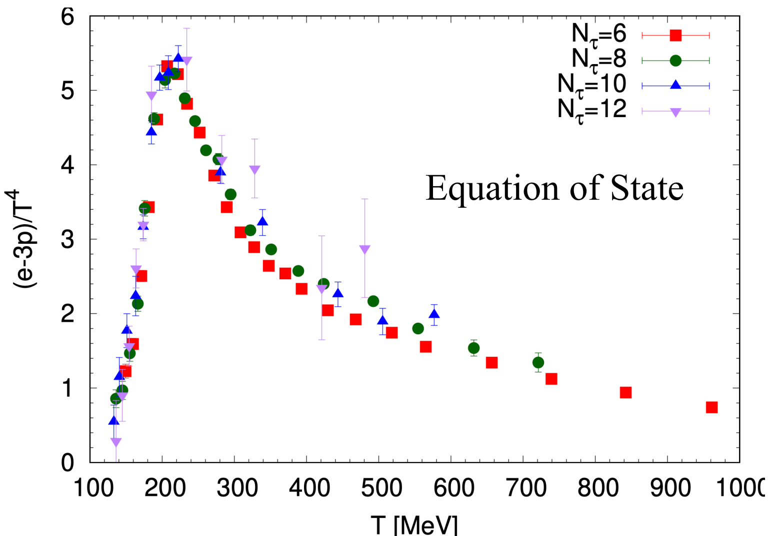


QCD in Extreme Conditions

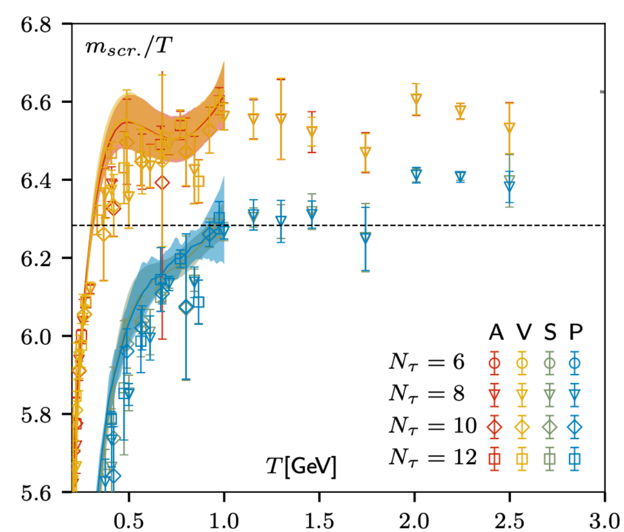
- The steady increase of computing power is essential but in many cases is not enough: it is necessary to develop new algorithms and computational methods

- The study of QCD in Extreme Conditions, namely, high temperature, finite density, with external background fields is numerically demanding

- The study of QCD at finite temperature T is challenging, T_{max}~1 GeV: two very different energy scales (=length scales), T and T=0, have to simulated at the same time (!)



Bazavov et al. (2021)



Mesonic screening masses

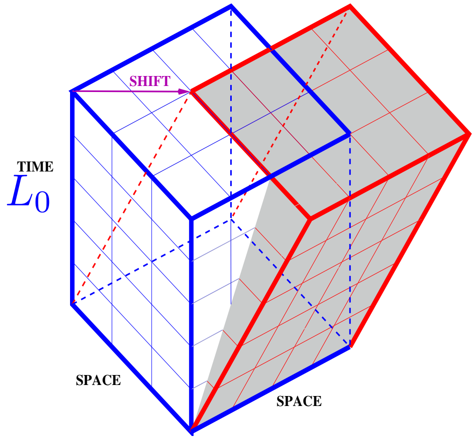
Bazavov et al. (2019)

QCD at high temperature

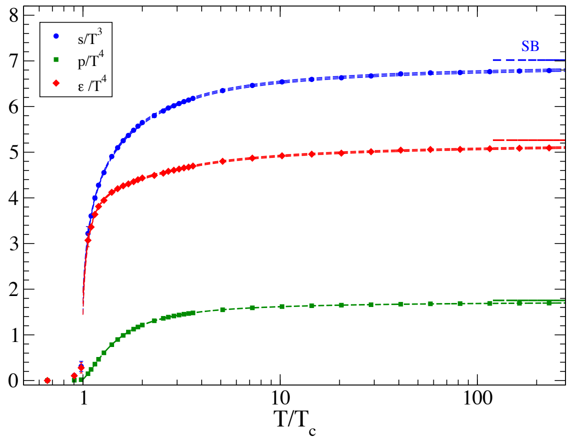
- solution: formulation of QCD in a moving reference frame

Shifted boundary conditions

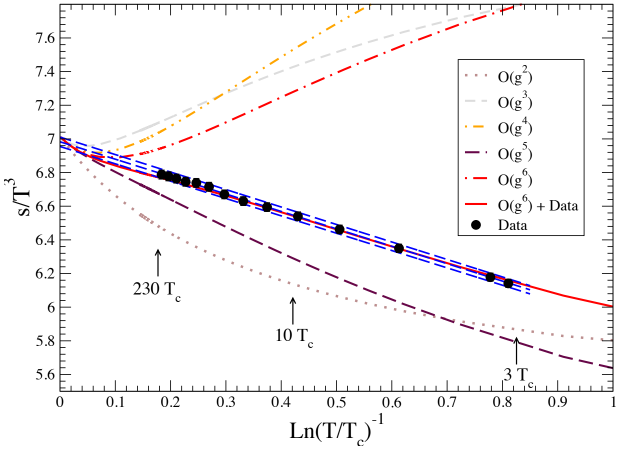
$$\phi(\vec{x}, L_0) = \phi(\vec{x} + \vec{\xi}, 0)$$



One measures the thermodynamics quantities **only at the temperature T of interest**



Yang-Mills SU(3)
(pure gauge sector of QCD)



- Both the theoretical formulation and its computational implementation turn out to be very effective and efficient

- We would like to apply the same technique to QCD

QCD in Extreme Conditions: Use case

- The main target of this use case is to deploy a parallel code to perform efficient Monte Carlo simulations of QCD in the completely unexplored regime of the very high temperatures

- Definition of the theoretical and algorithmic strategies to compute the entropy density (primary observable) in a moving reference frame

- Development of an efficient **parallel MPI Monte Carlo code** to study **lattice QCD at finite temperature** with shifted boundary conditions with the aim of reaching T∼100 GeV.

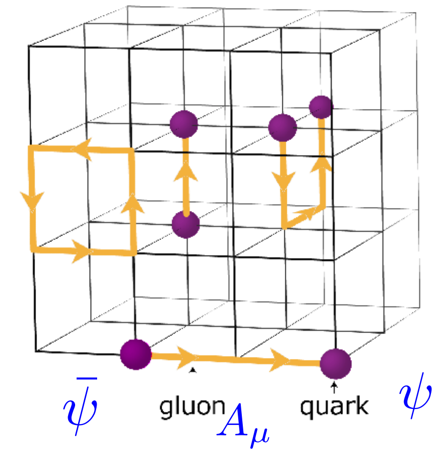
- The parallel code has to have a good strong scaling in order to run efficiently jobs requiring up to about **5000 -10000 cores**.

- The code will simulate quarks using the O(a)-improved Wilson formulation; it will be a development of the open source OpenQCD code.

- The use case has also two additional activities:

1) preparation of parallel codes to investigate QCD at finite density and in external background fields with Monte Carlo simulations on the lattice.
2) development of a code to study the spin polarization in the QCD plasma

An example of target simulation



- Monte Carlo simulation of Lattice QCD: generation of many gauge field configurations; numerically it corresponds to solving many times the Dirac equation

$$\eta = D\chi$$ D: large and sparse (5×10^9 by 5×10^9)

- Global system size: $288^3\times16 = 3.8\times10^8$ sites

- MPI grid: $18\times18\times18$ cores = 5832 cores. Local lattice $V=16^4 = 6.5\times10^4$ sites

- For each site D requires to compute several matrix-vector multiplication U*v

U is 3×3 and v 3×1; we need 8 U and 36 v giving (8×18+36×6)×8=2880 bytes.

Load 2880 bytes and store 4×6×8= 192 bytes, i.e. memory transfer **B=3072 bytes per site** (improved with smart coding)

- The computation consists in multiply&add operations amounting to **F=1400 Flop per site**

- For **I=B/F=2.2 bytes/Flop**

Memory bandwidth limited

- For a Skylake node we have **I= 256 Gb/s/ 3.2 TFlop/s =0.08 bytes/Flop**

- Each core has to pass data continuously to n.n. cores: this is an addition bottleneck w.r.t. the purely computational effort and requires a fast (100-200 GB/s) **infiniband network**

Computational resources required

- Need to access a small-medium cluster for code development (start&stop) with an infiniband network: CNAF. 3 Mch

- Need to access a larger HPC system for advanced tests and for benchmarking on system of realistic size: Cineca. 20 Mch

Exchanges with WP5 activity

- Creation of a repository of gauge configurations once the production phase will be entered

People involved

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