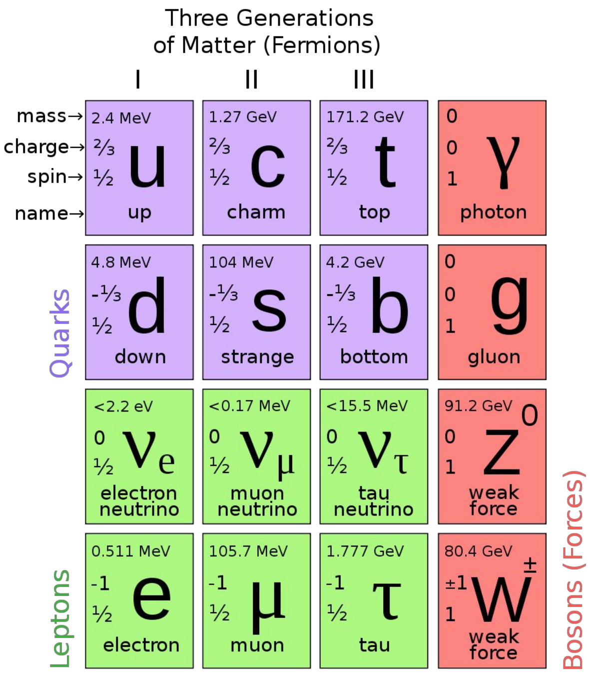
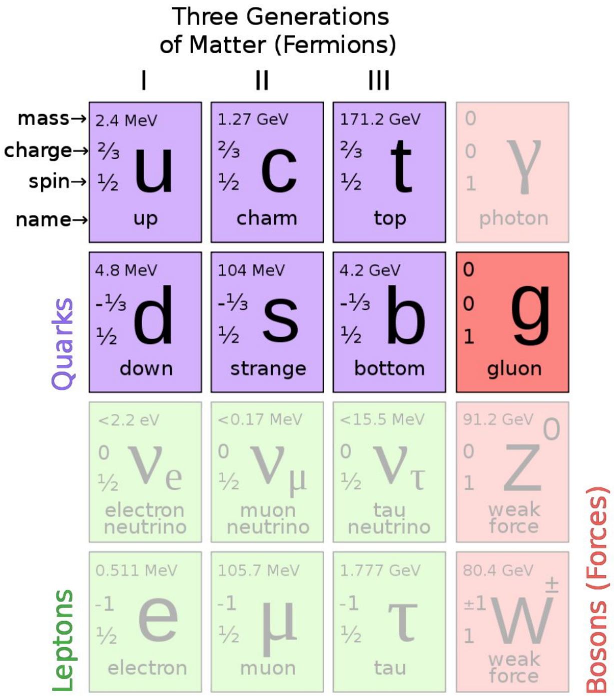
From the "Proof of Concept" to EuroHPC: a user journey across the HPC landscape in Europe

CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS
Dr. Isabel Campos Plasencia

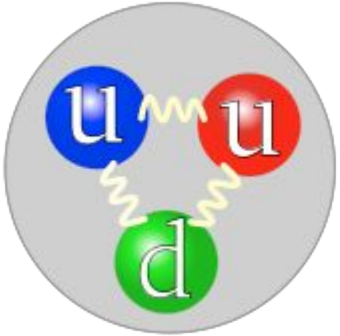
Standard Model

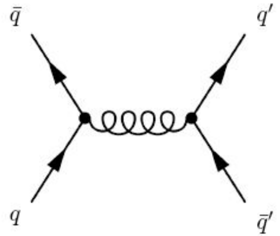


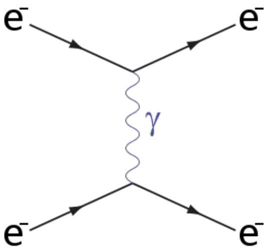
Quantum Chromo Dynamics



QCD is the "regnant" theory to describe "strong interactions"





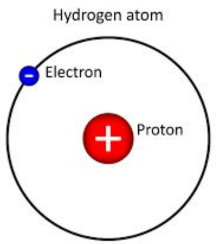


QCD is about gluon exchanges among coloured particles

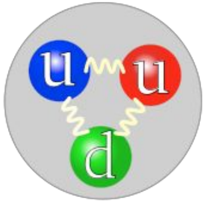
Analogy: QED is about photon exchanges among charged particles

QCD is formulated in terms of **quarks and gluons** → **we believe** those are the basic degrees of freedom ("bricks") that make up hadronic (protons et. al) matter

What do we mean by strong ? comparison with QED



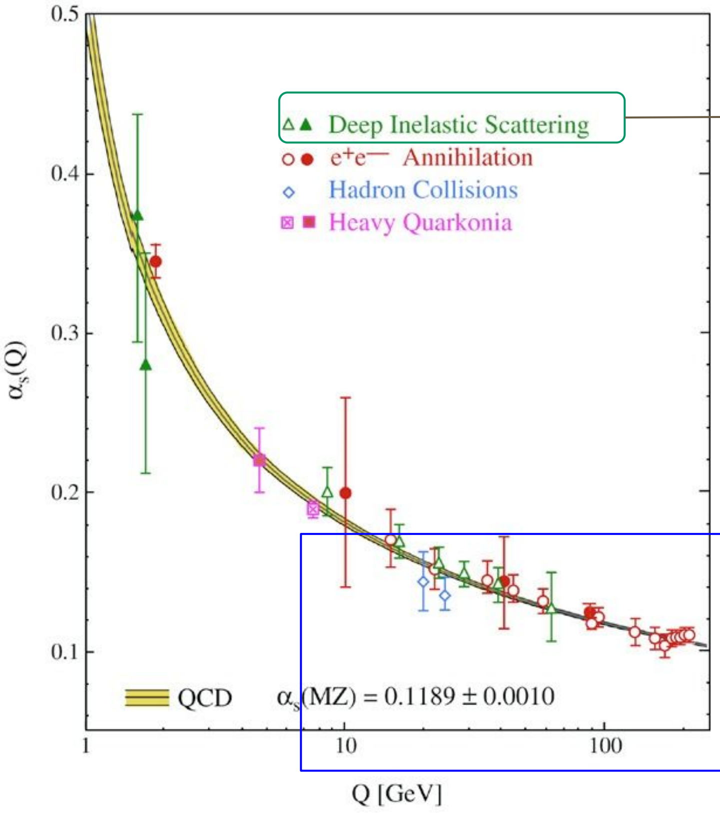
electromagnetism: $$\frac{E_{\rm bind}(H)}{(m_e+m_p)c^2} \simeq 1.4\times 10^{-7}$$

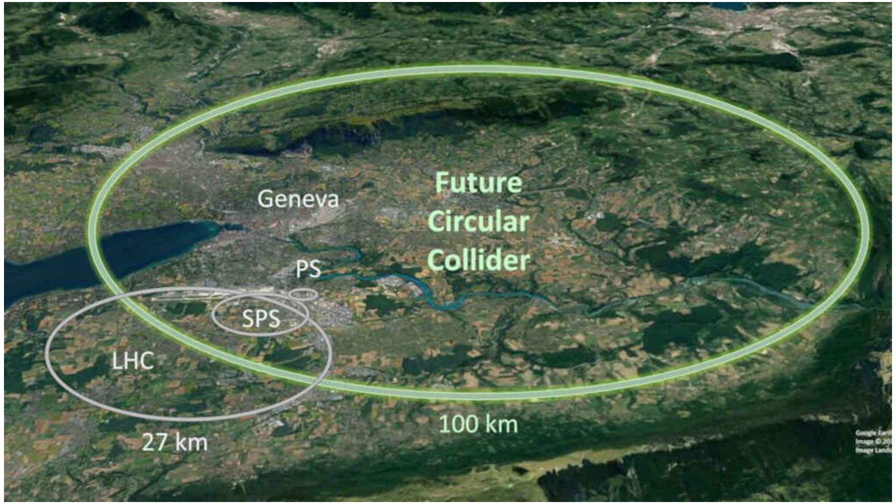


strong interaction: $$\frac{E_{\rm bind}(\text{proton})}{(2m_u+m_d)c^2} \sim 60$$

8 orders of magnitude compared with QED

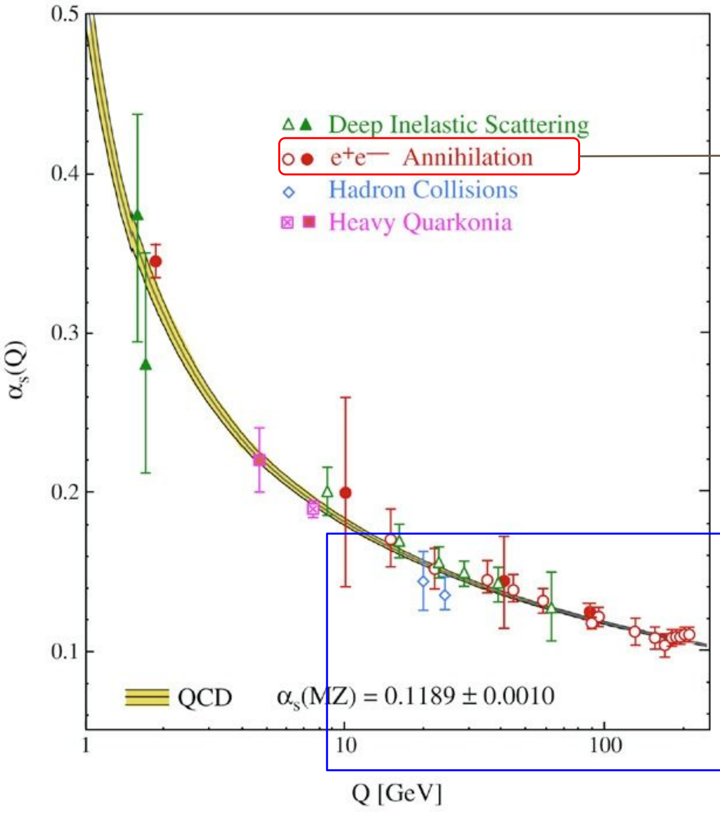
The strength of the coupling between quarks, α, is not constant: it depends on the energy of the quarks

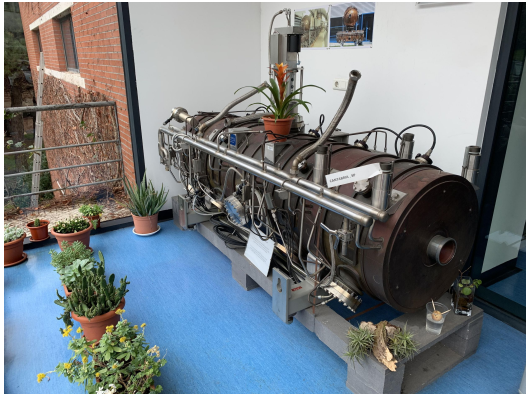


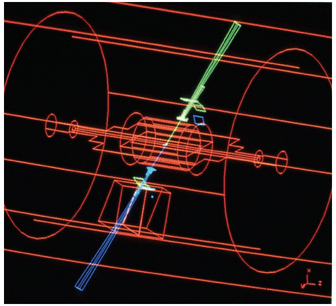


At High energies the quarks are weakly coupled.
Launching sufficiently energetic probes,
they can be “seen” as individual entities

"Asymptotic freedom" at high energies: α is very small







At High energies the quarks are weakly coupled.
By launching sufficiently energetic probes,
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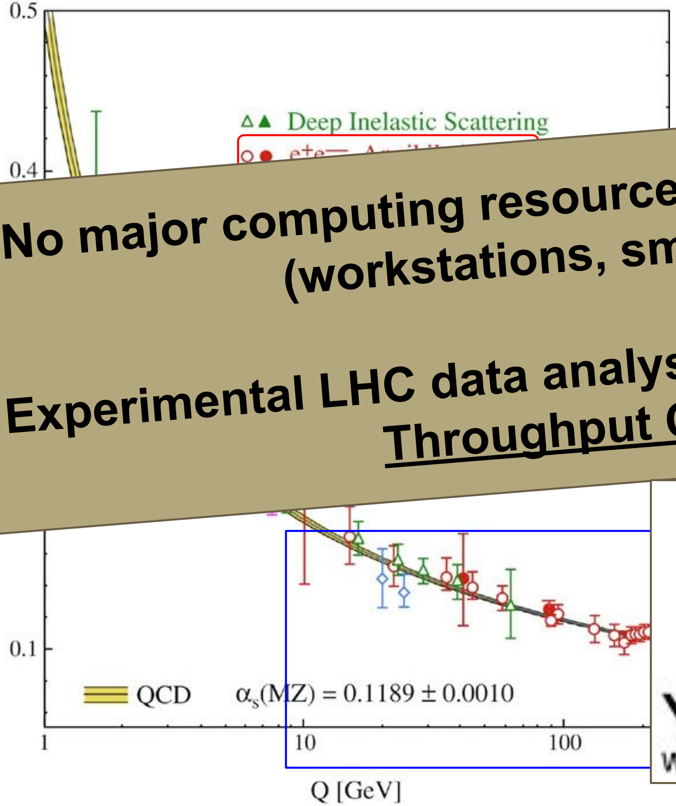
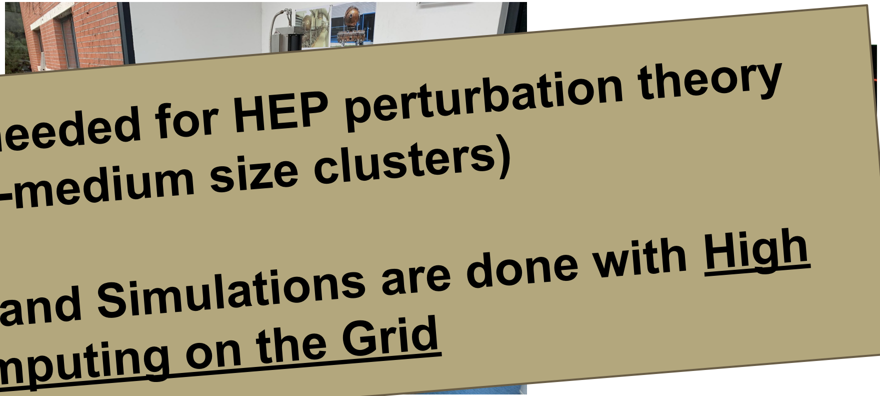
"Asymptotic freedom" at high energies: α is very small





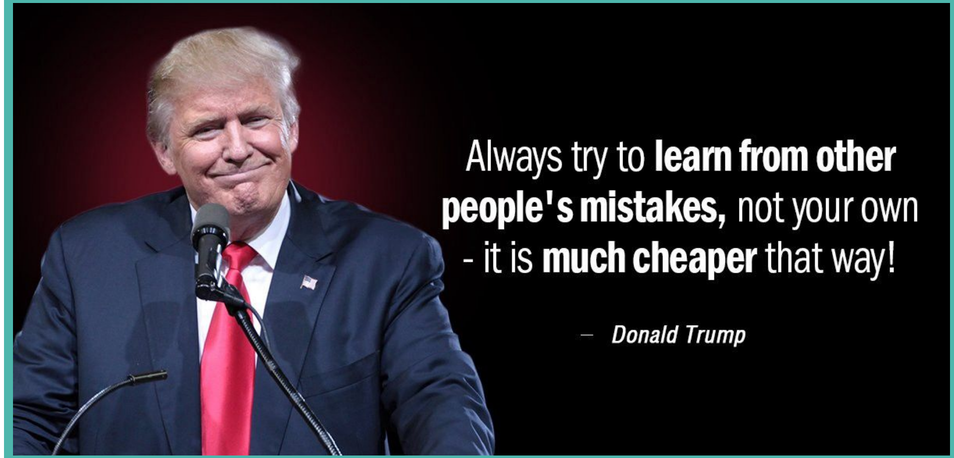
No major computing resources needed for HEP perturbation theory (workstations, small-medium size clusters)

Experimental LHC data analysis and Simulations are done with <u>High Throughput Computing on the Grid</u>

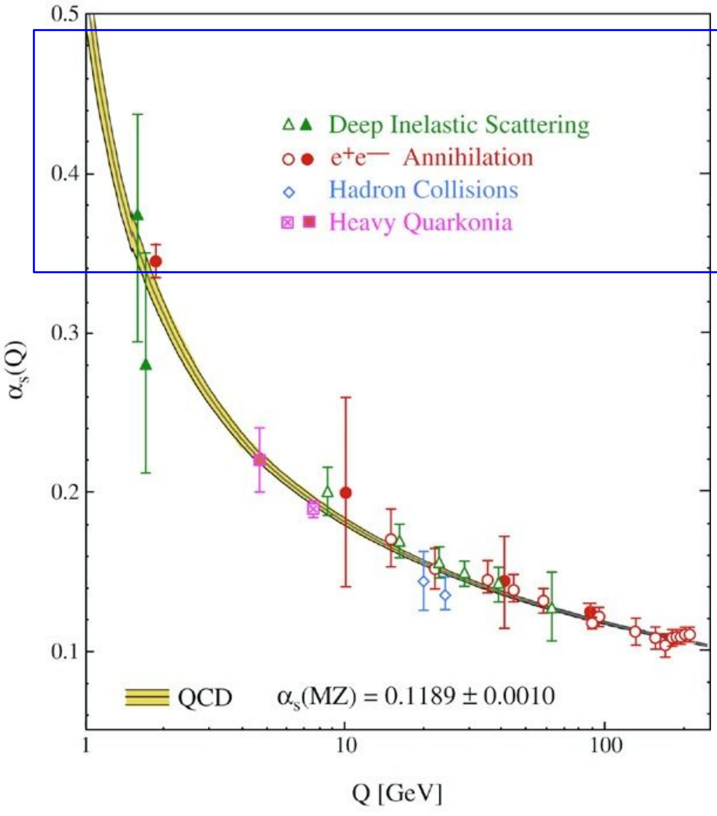
WLCG
Worldwide LHC Computing Grid

…ies the quarks are weakly coupled.
…ching sufficiently energetic probes,
…can be "seen" as individual entities

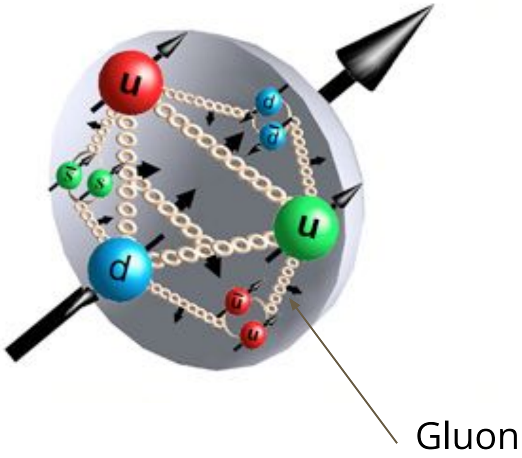
This is the reason why many HEP colleagues go about their careers not caring about Lattice QCD at all...



However at low energies deep in the hadronic world (~ 1 GeV, ~1 fermi, coupling α_s ~ 1) life is different

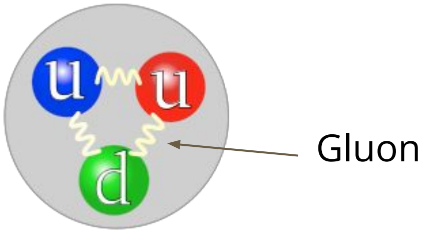


The quarks are strongly coupled, and thus the relevant degrees of freedom are the hadrons themselves



The Hadronic world is responsible for intriguing properties, with deep consequences

- **Confinement:** Quarks and gluons are confined into colourless bound states that we call hadrons.
- QCD has as free parameters:
  - **Quarks masses**: u,d,s,c,b,t
  - **Strong coupling constant**: α_s



The **conceptual beauty** resides in the fact that **all the physical observables can be calculated from those 7 free parameters**: hadron masses, branching ratios,decay constants, etc...

QCD is “believed” to be the right theory → but it remains to proven : this is the task of lattice QCD practicioners

At the scale of the Proton, 1 GeV, α_s ~ 1 we are in **the realm of Lattice QCD**

Which Physical Observables are in the “Lattice QCD side of life” ?

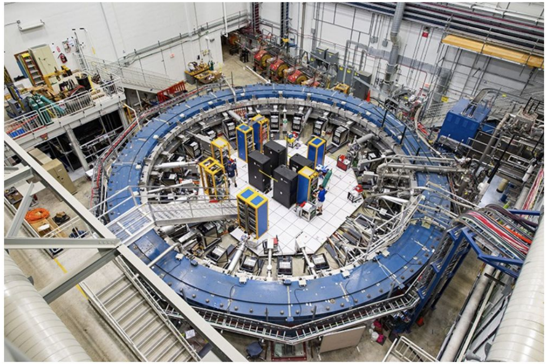
- Properties of **mesons and hadrons** in general;
- Fundamental parameters of the QCD:
  - Is **confinement** a property of QCD ?
    - So far, we have only the experimental observation of quark confinement.
  - Strong coupling **alpha constant, and quark masses determination**
- Possibilities to **probe** the Physic beyond the **Standard Model**:
  - Hadronic contributions to the anomalous magnetic moment of the muon (**g-2**)

NEWS | 07 April 2021

Is the standard model broken? Physicists cheer major muon result

The muon’s magnetic moment is larger than expected — a hint that new elementary particles are waiting to be discovered.

Davide Castelvecchi



The storage-ring magnet used for the *g* – 2 experiment at Fermilab. Credit: Reidar Hahn/Fermilab

QCD is “believed” to be the right theory, but it remains to proven : this is the task of Lattice QCD practitioners

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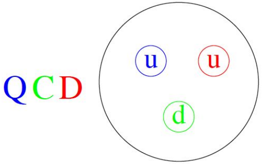
If we suppose that we know all the physical laws perfectly, of course we don't have to pay any attention to computers.

Quote from the Lectures on:
“Simulating Physics with Computers”,
by Richard Feynman, (1981) Caltech

Why is the Proton mass so intriguing ?



Proton

- $m_u = 2.3^{+0.7}_{-0.5}$ MeV/c^2
- $m_d = 4.8^{+0.7}_{-0.3}$ MeV/c^2
- $M_P = 938.3$ MeV/c^2

(Strong force)

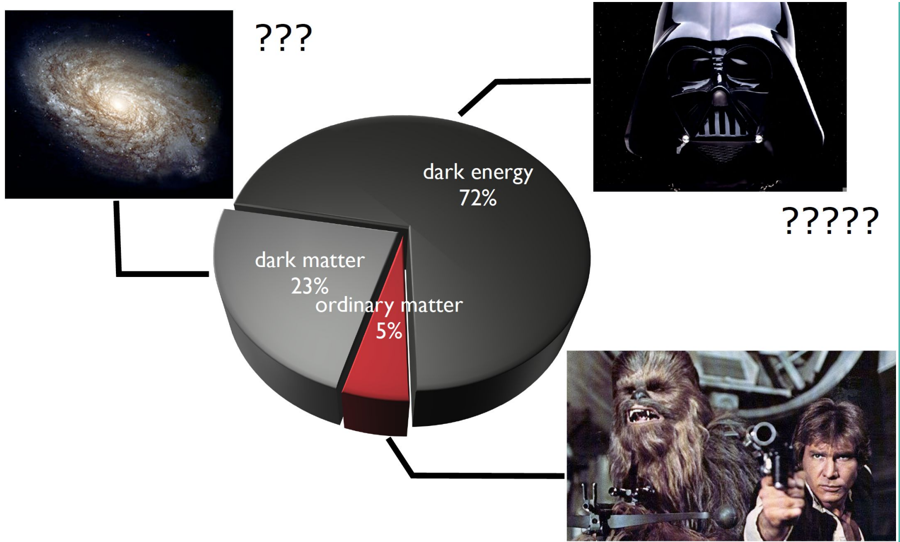
- Almost all the mass of the proton is attributed to **strong non-linear interactions** of the gluons
- Massless gluons and almost massless quarks interact - generating most of the mass.
  - **Only** 1% of the proton's mass comes from the constituent quarks' intrinsic masses.

- **Even switching-off the mass of the quarks, the proton would still have a mass**

The Proton is an emergent (long-range) phenomena resulting from the collective behaviour of quarks and gluons - QCD!

"A ´paradox´ is only a conflict between reality and your feeling of what reality is ´ought´ to be"

Such strong Force is a source of highly non-linear effects: Could the source of new physics be found there?



Lattice QCD as the non-perturbative approach

- **Lattice QCD is not a model, is QCD itself**
- The only mathematically well-defined implementation of QCD at Low energies
    - Incidentally also well-defined at High energies
    - Should we have an infinite Computer, we could QCD exactly ;)

Current reach of Lattice QCD simulations

- The current reach of the simulations is in the range **2 - 4 GeV**
    - *up*, *down*, *strange* and *charm* quarks can be directly simulated
- For the *bottom* quark no direct simulations are possible
    - the results you may see quoted use effective theories to include the *b* quark (HQET)

Lattice QCD as the non-perturbative approach

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Curre

JUST WAITING FOR MORE COMPUTER POWER <u>IS AN INTELLECTUAL DEFEAT</u> (and would not be enough anyway)

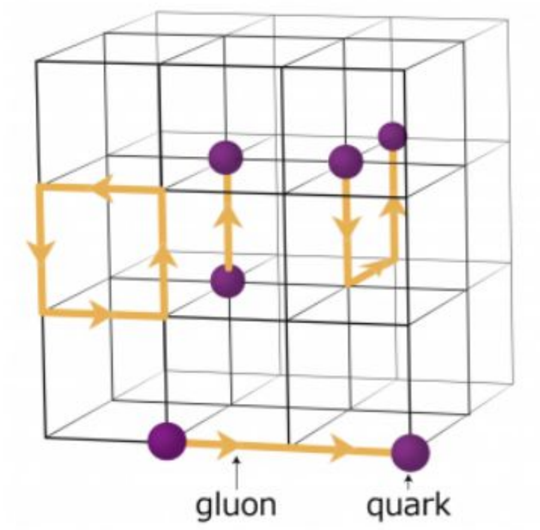
Smarter algorithms and new ideas need to be developed in the upcoming years

be directly simulated

direct simulations are possible

- the results you may see quoted use effective theories to include the *b* quark (HQET)

Background on Lattice QCD



- Gluon fields are place on the links of a four dimensional lattice (hypercube);
- Quark fields are placed on sites.
- We substitute Derivatives → by finite differences (we are discrete people)

$$\langle O \rangle = \mathcal{Z}^{-1} \int [DU] e^{-S[U]} O(U) \approx \frac{1}{N} \sum_{i=1}^{N} O[U_i]$$

Very high dimensional integral → Monte-Carlo methods

Lattice simulations are based on **Markov chains** and the concept of **importance sampling.**

How does it work (in a nutshell):

Lattice simulations are based on **Markov chains** and the concept of **importance sampling.**

Mike Creutz

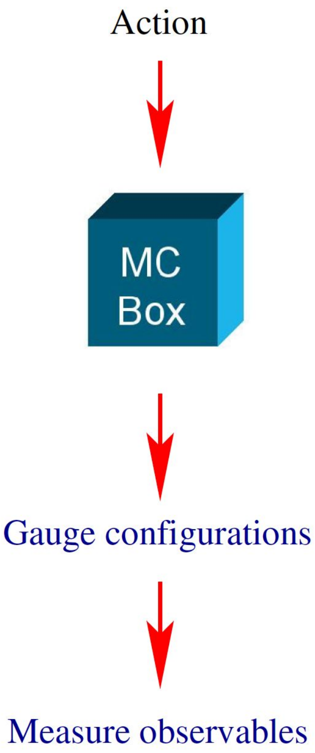
www.latticeguy.net

First Lattice QCD simulation ever:

Monte Carlo study of Quantized SU(2) Theory
Phys.Rev. D21 (1980)
(**over 1000 citations**)

Let’s compute:

- Start with some (e.g. hot or cold) configuration.
- Update each link of the configuration = one sweep.
- Run for many equilibrating sweeps.
- Continue sweeping and measure observables every k sweeps (k depends on the autocorrelation time).



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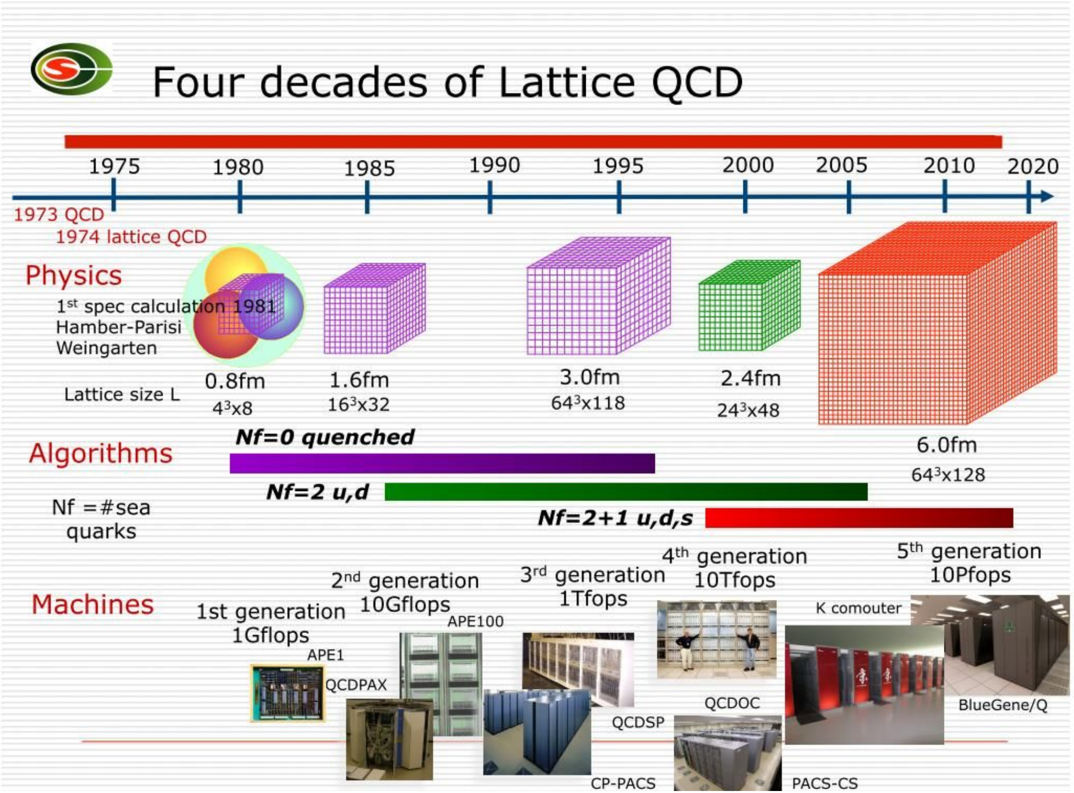


A **pioneering community**: instrumental **driving force** in processors & computing architecture developments:

- APENext machines
- QCDOC → Blue Gene

- **Lattice QCD is one of the largest consumers of HPC** resources in the world (longstanding **PRACE challenge**).

- Very **sophisticated software suites** targeting different architectures, but also MonteCarlo integrators and solvers.

Very interesting, but....
what has Lattice QCD ever done for us ?

Top-level technical contributions of wide applicability

or how inverting the Dirac operator with fermion fields on the Lattice generated true innovation even without being a "Sustainable Development OECD Objective"

RANLUX: used eg. in GEANT4 (*very popular package)
by Martin Lüscher: http://luscher.web.cern.ch/luscher/ranlux

→ ranlux is part of the **C++ standard library**
→ Included in the GNU Scientific Library

Computer Physics Communications
Volume 79, Issue 1, February 1994, Pages 100-110

A portable high-quality random number generator for lattice field theory simulations

Martin Lüscher

Show more

https://doi.org/10.1016/0010-4655(94)90232-1

Abstract

The theory underlying a proposed random number generator for numerical simulations in elementary particle physics and statistical mechanics is discussed. The generator is based on an algorithm introduced by Marsaglia and Zaman, with an important added feature leading to demonstrably good statistical properties. It can be implemented exactly on any computer complying with the IEEE-754 standard for single-precision floating-point arithmetic.

Physics Letters B
Volume 195, Issue 2, 3 September 1987, Pages 216-222

Hybrid Monte Carlo

Simon Duane [1], A.D. Kennedy, Brian J. Pendleton, Duncan Roweth

Show more

https://doi.org/10.1016/0370-2693(87)91197-X

Abstract

We present a new method for the numerical simulation of lattice field theory. A hybrid (molecular dynamics/Langevin) algorithm is used to guide a Monte Carlo simulation. There are no discretization errors even for large step sizes. The method is especially efficient for systems such as quantum chromodynamics which contain fermionic degrees of freedom. Detailed results are presented for four-dimensional compact quantum electrodynamics including the dynamical effects of electrons.

The **Hybrid Monte Carlo algorithm**: widely used in scientific simulations by many research areas. Invented **by the Lattice group of the University of Edinburgh (Tony Kennedy et al.)**

What does this entail from the Computational resources point of view ?

Example: Calculating light quark (u,d,s) masses https://arxiv.org/abs/1911.08025

Simulate the hadronic world with the best possible accuracy to compute **α** and **quark masses,...**

Low Energy (L = 1 fm)

~ 200 Mi CPU hours

SuperMUC - LRZ (Munich)
JUWELS - Jülich HPC,...

LQCD step-scaling
("Finite Size Scaling")

~ 10 Mi. CPU hours

Resources at the RES level:
Marenostrum,
Finisterrae-CESGA
Altamira - IFCA,...

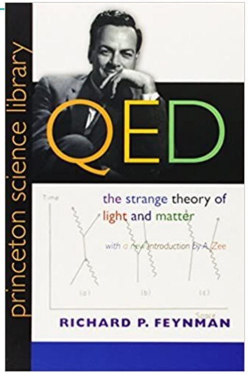
Matching with Perturbation Theory/ High Energy regime to **compare with experiment**

High Energy (L = 0.003 fm)

~ 1 Mi. CPU hours

Workstations, small clusters,...

The Nobel Prize in Physics 1965 was awarded jointly to Sin-Itiro Tomonaga, Julian Schwinger and Richard P. Feynman "for their fundamental work in quantum electrodynamics, with deep-ploughing consequences for the physics of elementary particles"



QCD+QED

Understanding the Stability of the Universe from First Principles

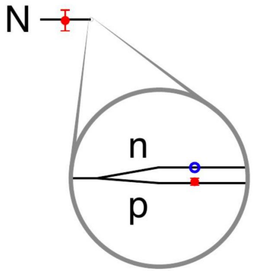
What exactly are we up to ? investigate the Physical consequences of Isospin Symmetry Breaking

- **Isospin is an approximate symmetry of QCD**

  Under an isospin transformation, the up and down quarks are rotated one into another.

- **Isospin-breaking effects** on hadronic observables **are of order of 1%** but very important

SU(2) isospin symmetry: u↔d



SU(2) is violated by
- quark mass difference
- electric charge difference

On the per mil level $\Delta M_N/M_N = 0.14\%$ arising from a competition of the two.

It is because of isospin breaking that we are here today !

The value of ΔM_N is **neccesary for the observed Universe:**
- $\delta M_N < 0.05\% \to$ inverse β-decay leaves only neutrons
- $\delta M_N > 0.14\% \to$ much faster β-decay, no heavy elements

https://workshops.ift.uam-csic.es/files/172/kalman_szabo_xmas14.pdf

Since isospin-breaking effects are generally small, **traditionally lattice QCD simulations are performed in the isospin-symmetric limit**.

This approximation is **no longer justified when observables need to be calculated with a > 1%** precision to match precision of current experiments.

Including QED effects in QCD simulations: small effect in size, but key to probe the Standard Model

At the current levels of experimental precision, the up and down quark mass difference and the coupling to QED cannot be neglected.

<u>**Including in the simulations of Lattice QCD the fact that quarks have an electric charge**</u>

→ Besides the **Theoretical complexity** (solved only very recently), the **cost of the simulation** increases considerably (order of magnitude)

What can we measure ?

- To <u>explain the mass splitting</u> between Proton and Neutrons
  - Protons and Neutrons have a tiny mass difference (0.14%)
  - How does it arise? Electromagnetic effects: the charge of the constituent quarks is different: up (+⅔) ; down (-⅓)
- Improve the <u>determination of observables that have reached the 1% precision</u> and are relevant for the LHC decay rates of light mesons
- Electromagnetic corrections to key observables involved in <u>testing the existence of New Physics</u>: Anomalous magnetic moments (eg. **g-2**)

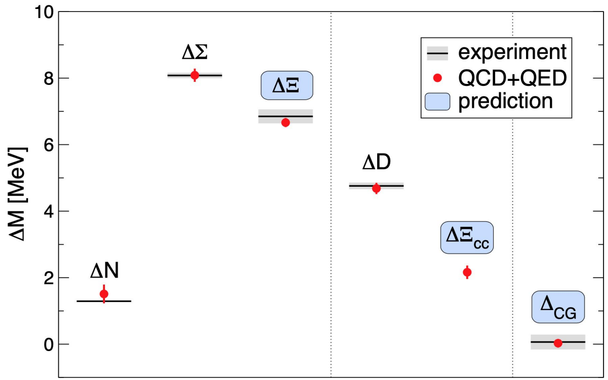
Science News *from research organizations*

Theory of the strong interaction verified: Supercomputer calculates mass difference between neutron and proton

Date: March 26, 2015

Source: Forschungszentrum Juelich

https://doi.org/10.1126/science.1257050



Investigating the effect of Quantum ElectroDynamics in QCD

→ **We included QED effects on the QCD code in a theoretically sound way:** imposing C* boundary conditions to avoid that Gauss law destroyed the theory on the lattice **(RC* collaboration)**

- Starting from the most advanced open source Lattice QCD code

  OpenQCD: http://luscher.web.cern.ch/luscher/openQCD

- **Adhering to Open Source principles (GPLv2 license)**
- **We added QED**, and called it **OpenQ*D**:
- The code is used to generate gauge configurations and measure physical observables.

https://gitlab.com/rcstar/openQxD

Requirements in terms of HPC resources:

★ **Exploratory studies** require about 512 - 1024 cores (months)...
★ **Production** runs require a minimum of 8000 cores/year (several years)

Collaboration:

- Humboldt University (Berlin), **Agostino Patella**
- Tor Vergata U. & INFN (Rome), **Nazario Tantalo**
- Trinity College (Dublin): **Patrick Fritzsch**
- ETH (Zurich): **Marina Krstic Marinkovic**
- IFCA - CSIC (Santander): **Isabel Campos**

\+ **.... 12 students, postdocs...**

https://pages.cms.hu-berlin.de/lattice-field-theory/lft-website/research/qcd+qed/

April 7th 2021: news

NEWS | 07 April 2021

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The muon's magnetic moment is larger than expected — a hint that new elementary particles are waiting to be discovered.

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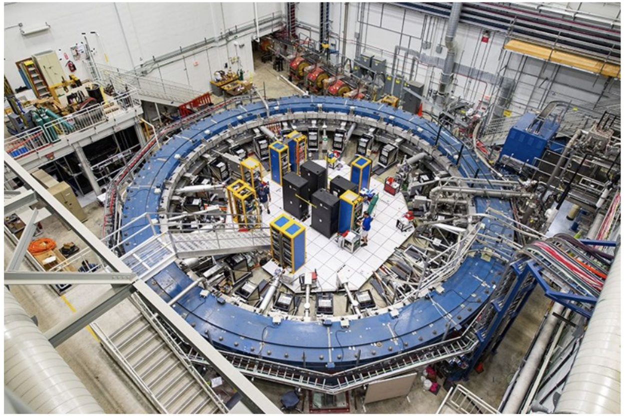


The storage-ring magnet used for the *g* – 2 experiment at Fermilab. Credit: Reidar Hahn/Fermilab

News

First results from Fermilab's Muon g-2 experiment strengthen evidence of new physics

April 7, 2021

Share Tweet Email

Media contact

- Tracy Marc, Fermilab, media@fnal.gov, 224-290-7803

The long-awaited first results from the Muon g-2 experiment at the U.S. Department of Energy's Fermi National Accelerator Laboratory show fundamental particles called muons behaving in a way that is not predicted by scientists' best theory, the Standard Model of particle physics. This landmark result, made with unprecedented precision, confirms a discrepancy that has been gnawing at researchers for decades.

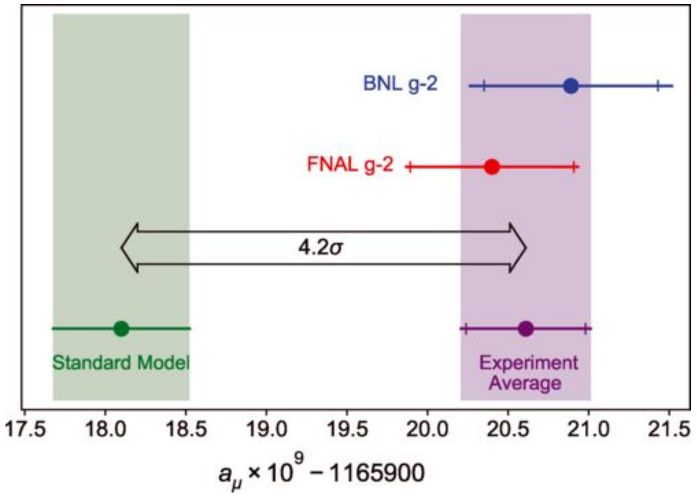
The strong evidence that muons deviate from the Standard Model calculation might hint at exciting new physics. Muons act as a window into the subatomic world and could be interacting with yet undiscovered particles or forces.

"Today is an extraordinary day, long awaited not only by us but by the whole international physics community," said Graziano Venanzoni, co-spokesperson of the Muon g-2 experiment and physicist at the Italian National Institute for Nuclear Physics. "A large amount of credit goes to our young researchers who, with their talent, ideas and enthusiasm, have allowed us to achieve this incredible result."

Experimental versus Theoretical prediction of (g-2): is the Standard Model broken?

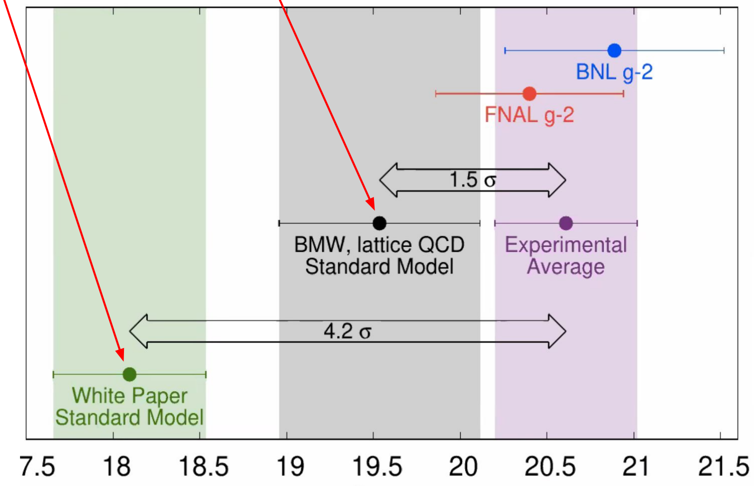
Computing the prediction of the Standard Model using **perturbation theory**

Computing the prediction of the Standard Model using **Lattice QCD**, and comprare with the experimental prediction



Ops!

Maybe not!



Standard Model (g-2) value from: https://muon-gm2-theory.illinois.edu/white-paper

A last minute update

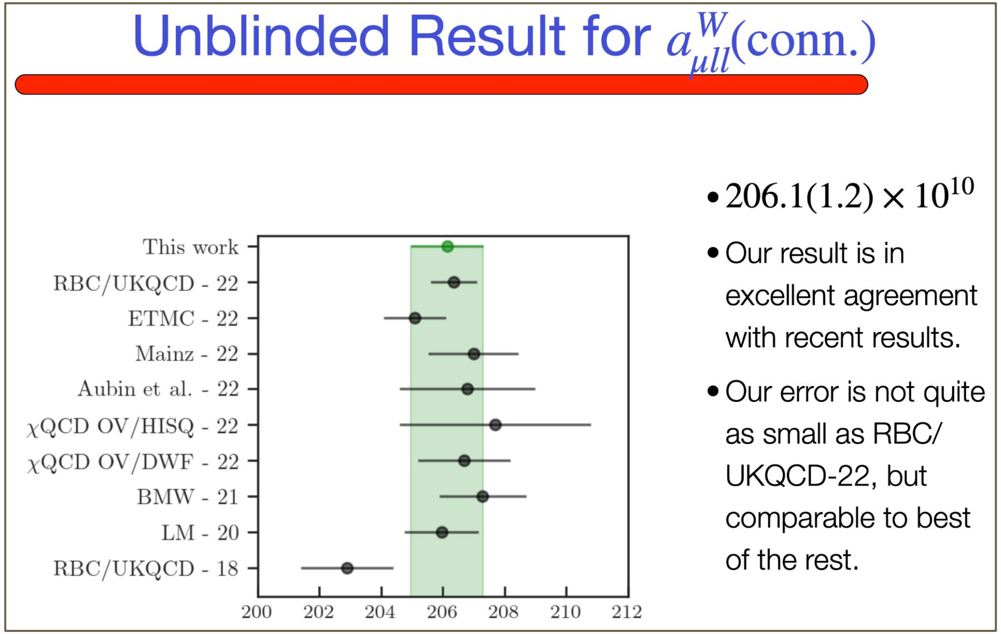
The Standard Model is tough!

https://www.benasque.org/2022lattice_workshop/talks_contr/158_Gottlieb_gm2_LatticeNET.pdf

Update in September 2022 (Benasque workshop)

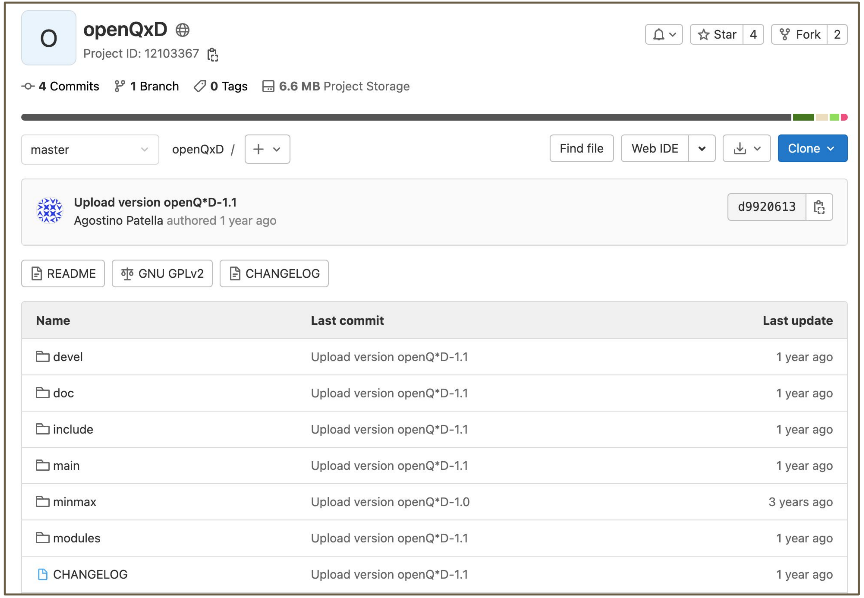
Steve Gottlieb updating the LQCD simulations results related to g-2

Updated results from major LQCD collaborations tend to agree with the BMW estimation



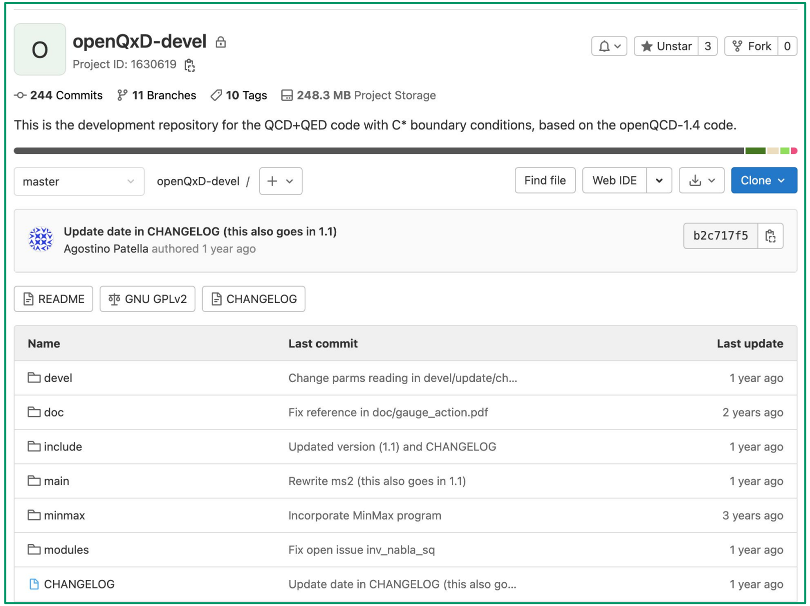
Our code: openQxD

https://gitlab.com/rcstar/openQxD



Devel branch:

https://gitlab.com/rcstar/openQxD-devel



Software Quality approach

A set of Common Software Quality Assurance Baseline Criteria for Research Projects

A DOI-citable version of this manuscript is available at http://hdl.handle.net/10261/160086.

https://indigo-dc.github.io/sqa-baseline

A taste our own medicine

→ **Code Accessibility and Licensing: open source under GPLv2 license**

- **[QC.Acc01]** Following the open-source model, the source code being produced **MUST** be open and publicly available to promote the adoption and augment the visibility of the software developments.
- **[QC.Acc02]** Source code **MUST** use a Version Control System (VCS)
- **[QC.Lic01]** As open-source software, source code **MUST** adhere to an open-source license **[QC.Lic02]** License **MUST** be compliant with the Open Source Definition [3].
- **[QC.Lic03]** Licenses **MUST** be physically present (e.g. as a LICENSE file) in the root of all the source code repositories related to the software component.

→ **Code Style: Written in Standard ANSI C**

→ **Code Metadata: No**

Software Quality approach

Unit and Functional testing

For the purpose of testing and code development, the programs can also be run on a desktop or laptop computer. All what is needed for this is a compliant C compiler and a local MPI installation such as Open MPI.

- The code has a **./devel/** directory where the codes for testing are located
- Testing involves
  - **Consistency tests**: very stringent as it implies fulfilling basic properties of the theory under transformation of the variables: (gauge invariance, fields normalized to "1" etc...)
  - **Algorithmic tests**: convergence and performance of certain operations such as inversions of operators with a given precision
  - **Linear Algebra tests:** making sure that basic algebra operations do what they should do:
    - Specially in the parts of the code programmed in assembly language
  - **I/O test** : making sure the code reads and writes properly
    - Read and write configurations

```
INDEX   1.68 KiB

MD force programs

check1       Gauge and translation invariance of the SU(3) gauge action

check2       SU(3)  gauge action of constant Abelian fields

check3       Check of force0() and action0()

check4       Check of sw_su3frc(), hop_su3frc(), sw_u1frc() and hop_u1frc()

check5       Check and performance of the CG solver

check6       Check of force1() and action1()

check7       Check of force2() and action2()

check8       Check and performance of the multi-shift CG solver
```

```
#if (defined AVX)
#include "avx.h"

#if (defined FMA3)

complex spinor_prod(int vol,int icom,spinor *s,spinor *r)
{
   complex z;
   complex_dble v,w;
   spinor *sm;

   __asm__ __volatile__ ("vxorpd %%ymm12, %%ymm12, %%ymm12 \n\t"
                         "vxorpd %%ymm13, %%ymm13, %%ymm13 \n\t"
                         "vxorpd %%ymm14, %%ymm14, %%ymm14"
                         :
                         :
                         :
                         "xmm12", "xmm13", "xmm14");

   sm=s+vol;
```

Software Quality approach

Unit and Functional testing

QC.Unit01: Yes

We do test the possible flows in the code by adjusting the input parameters to different situations (boundary conditions, number of quarks, number of interacting gauge fields).

- Coverage is close to 90% in general and close to 100% for physically relevant cases.
  - Example 1: our code reproduces QCD results when we switch off QED fields (photon)
  - Example 2: the code reproduces compact QED when we switch off in the input QCD fields (gluon)

QC.Uni02 Yes

QC.Uni03 Yes

QC.Uni04 Nope (could be done yes, but things pile up)

https://indigo-dc.github.io/sqa-baseline

4.5. Unit Testing [QC.Uni]

Unit testing evaluates all the possible flows in the internal design of the code, so that its behavior becomes apparent. It is a key type of testing for early detection of failures in the development cycle.

- **[QC.Uni01]** Minimum acceptable code coverage threshold **SHOULD** be 70%.
  - **[QC.Uni01.1]** Unit testing coverage **SHOULD** be higher for those sections of the code identified as critical by the developers, such as units part of a security module.
  - **[QC.Uni01.2]** Unit testing coverage **MAY** be lower for external libraries or pieces of code not maintained within the product's code base.
- **[QC.Uni02]** Units **SHOULD** reside in the repository code but separated from the main code.
- **[QC.Uni03]** Unit testing coverage **MUST** be checked on change basis.
- **[QC.Uni04]** Unit testing coverage **MUST** be automated.
  - **[QC.Uni04.1]** When working on automated testing, the use of testing doubles is **RECOMMENDED** to mimic a simplistic behavior of objects and procedures (c.f. section 4.6.).

Software Quality approach

Documentation

QC.Doc01: Yes

QC.Doc02: We wrote in Latex. Should be translatable:

pandoc -s example4.tex -o example5.md

QC.Doc03: Yes

QC.Doc04: Yes

QC.Doc05: Yes

QC.Doc06: We only have one target audience: our peers

https://indigo-dc.github.io/sqa-baseline

4.8. Documentation [QC.Doc]

- **[QC.Doc01]** Documentation **MUST** be treated as code.
    - **[QC.Doc01.1]** Version controlled, it **MAY** reside in the same repository where the source code lies.
- **[QC.Doc02]** Documentation **MUST** use plain text format using a markup language, such as Markdown or reStructuredText.
    - **[QC.Doc02.1]** It is **RECOMMENDED** that all software components delivered by the same project agree on a common markup language.
- **[QC.Doc03]** Documentation **MUST** be online and available in a documentation repository.
    - **[QC.Doc03.1]** Documentation **SHOULD** be rendered automatically.
- **[QC.Doc04]** Documentation **MUST** be updated on new software versions involving any substantial or minimal change in the behavior of the application.
- **[QC.Doc05]** Documentation **MUST** be updated whenever reported as inaccurate or unclear.
- **[QC.Doc06]** Documentation **MUST** be produced according to the target audience, varying according to the software component specification. The identified types of documentation and their RECOMMENDED content are:

Lattice QCD+QED computing project workflow

In a Lattice QCD project there are typically 3 phases regarding computing requirements

- **Development** (code development, including code testing)
- **Production runs at small scale**
    - Small lattices sizes, or parameter space areas where a maximum of 256 - 512 cores were needed
    - Used for complex consistency tests: eg. we checked at CESGA that the limiting cases of QCD and QED are correctly reproduced using 512 cores
- **Production runs at large scale**
    - What "large scale" means, and if it is needed obviously depends on the problem
    - Current LQCD challenges require several projects of ~50 Million CPU hours in large HPC systems, possibly in several iterations.
    - Very complex cases such as (g-2) we go to several 100s of millions
        - Only collaborations with very good access to HPC resources can afford working on those problems.

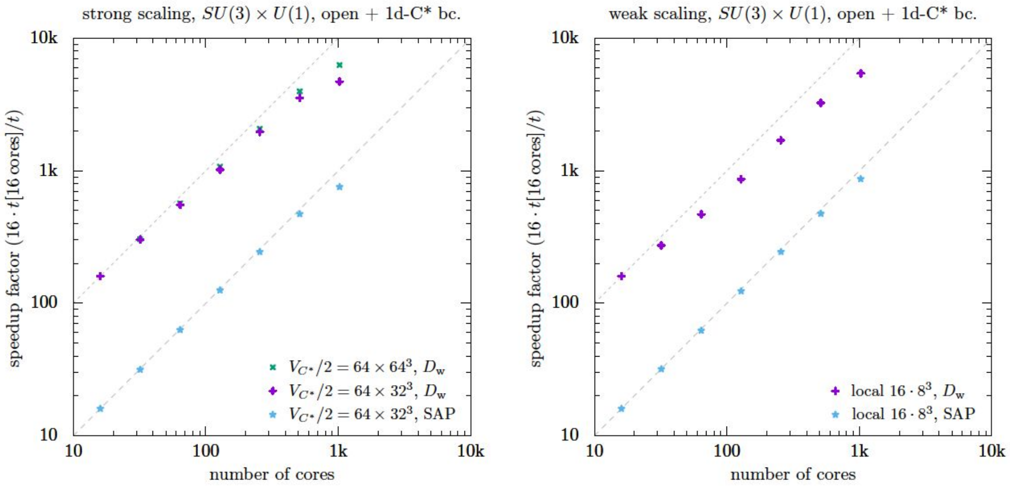
Workstation, Laptop

Local Linux farm

National / International usually peer reviewed applications

Scaling tests: where can we run?

We need to do <u>"scaling tests"</u> to prove that the code scales properly in order to apply to large production runs in peer reviewed applications



Thanks to CESGA we could do the scaling tests in FT-2

"OpenQ*D code: a versatile tool for QCD+QED simulations"

Eur. Phys. J. C (2020) 80:195 (https://arxiv.org/abs/1908.11673)

I. Campos, P. Fritzsch, M. Hansen, M. Marinkovic, A. Patella, A. Ramos and N. Tantalo

Things are slowly changing...

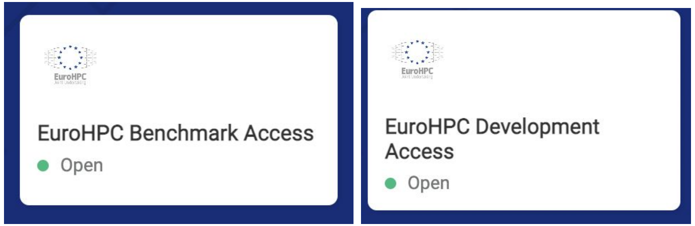
EuroHPC Joint Undertaking

It is now possible to apply for <u>Benchmark time</u> in EuroHPC

- Call designed exclusively to support code scalability tests,
- The outcome is can be used to be included in the future application to EuroHPC regular Access call or other HPC facilities
- Users receive a limited number of node hours; the maximum allocation period is three (3) months.
- At the moment **1 M CPU hours** (they go by quickly)

It is <u>also possible</u> to apply for <u>Development time</u> in EuroHPC

- Allocates maximum **2M CPU hours/year**
- Dedicated exclusively to **code and algorithm development** and optimisation.
- **Renewable up to 2x** (in total a maximum of 3 years)



→ Applications are sent directly to the HPC center where you request the resources, and evaluated there.

→ Easy application (short web form 1-2 pages)

→ Immediate answer from the HPC center (evaluated 1st day of the next month)

https://pracecalls.eu

Applying for large scale production

There is a clear need for simplification

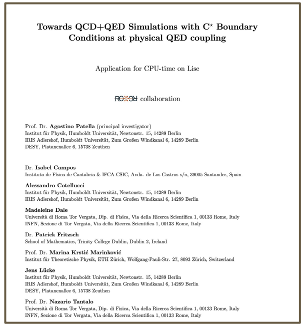
- **Simplification in the access to small scale resources**
  - Less than 10M hours / year is small scale.
  - Should be possible for researchers to apply to this level with minimum overhead (should exclude having to write a 10 pages of proposal)
- Large scale production (PRACE, EuroHPC)
  - In PRACE it amounts almost to write a research paper (deprecated model….)
  - The **process has been simplified in EuroHPC** (max. 10 pages, to the point, etc…)

→Complex application processes have been for us a blocking factor in the progress of the research progra

→ A typical discussion we have in RC* is: "*who has time to write the CPU application this time?*"
Once per year someone has the time

→ Usually deadlines are missed because researchers are too busy on other duties (teaching, project running, etc…)

https://pages.cms.hu-berlin.de/lattice-field-theory/lft-website/research/qcd+qed/bep00102.pdf


Towards QCD+QED Simulations with $C^\star$ Boundary Conditions at physical QED coupling

Application for CPU-time on Lise

RC* collaboration

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Applying for large scale production

What means large scale production for our project ?

- Starting with times above 10M CPU hours/year are considered medium-large scale

We obtained CPU competitively (peer review) in:

- Jan. 2020 **HLRN** → 14 Million hours
- Mar. 2020 **PNSC** → 10 Million hours
- Jun. 2021 **HLRN** → 35 Million hours
- Sep. 2022 **HLRN** → **47M hours current grant starting**
- Sep. 2022 **CSCS** → **11M x2 years current grant starting**

Benchmark time in EuroHPC

- So far we have been able to run the code up to 4096 cores
- Progress in generating configurations is not so fast
- We recently obtained **Benchmark CPU in LUMI** to analyze the scalability up to 16,000 cores
- If using 2x the number of cores progress will be of course faster

The estimation is that we will need **order ~100 Million hours more to be able to set the physical scale** of our simulation (eg. by computing the mass of the Omega meson)

Time scale

“Lab Reports” (Lattice 2021, Lattice 2022)

High Energy Physics – Lattice

[Submitted on 26 Aug 2021]

An update on QCD+QED simulations with C* boun

Lucius Bushnaq, Isabel Campos, Marco Catillo, Alessandro Cotellucci, Madelei

We present two novelties in our analysis of fully dynamical QCD+QED ensembles with C* that provides a significant speedup compared to traditional methods. The second one is QCD+QED ensembles with pions at $m_{\pi^\pm} \approx 400$ MeV, a lattice spacing of $a \approx 0.05$ fm, a

Comments: RC* Collaboration, Lattice 2021
Subjects: High Energy Physics – Lattice (hep-lat)
Report number: HU-EP-21/26-RTG
Cite as: arXiv:2108.11989 [hep-lat]
(or arXiv:2108.11989v1 [hep-lat] for this version)
https://doi.org/10.48550/arXiv.2108.11989

High Energy Physics – Lattice

[Submitted on 23 Dec 2021]

Baryon masses from full QCD+QED$_C$ s

Lucius Bushnaq, Isabel Campos, Marco Catillo, Alessandro

In these proceedings we present preliminary results for the masse boundary conditions. These results are part of the ongoing effort electromagnetic coupling is $\alpha_{em} \sim 0.04$, the physical volume is L unphysical ensemble that baryon masses can be calculated with sa effectiveness of the strategy presented here also in the case of sin

Comments: 8 pages, 5 figures; for the 38th International Symposium on Lattice
Subjects: High Energy Physics – Lattice (hep-lat)
Cite as: arXiv:2112.12767 [hep-lat]
(or arXiv:2112.12767v1 [hep-lat] for this version)
https://doi.org/10.48550/arXiv.2112.12767

High Energy Physics – Lattice

[Submitted on 24 Jan 2022]

Implementing noise reduction t

Lucius Bushnaq, Isabel Campos, Marco Catillo, Al

We present the results of testing a new technique for s action, with periodic boundary conditions and pion ma traditional methods, owning to the failure of its underl

Comments: The 38th International Symposium on Lattice Field Th
Subjects: High Energy Physics – Lattice (hep-lat)
Cite as: arXiv:2201.09729 [hep-lat]
(or arXiv:2201.09729v1 [hep-lat] for this version)
https://doi.org/10.48550/arXiv.2201.09729

Several PhD. thesis
PostDoctoral career development
Not so many publications (but good ones)

Development, testing, first complete release (Apr. 2019) → Code in production at large scale

2016 2017 2018 2019 2020 2021 2022

“Lab Report” (Lattice 2017)

Open Access

Issue	EPJ Web Conf. Volume 175, 2018 35th International Symposium on Lattice Field Theory (Lattice 2017)
Article Number	09005
Number of page(s)	16
Section	9 Software Development
DOI	https://doi.org/10.1051/epjconf/201817509005
Published online	26 March 2018

EPJ Web of Conferences **175**, 09005 (2018)
https://doi.org/10.1051/epjconf/201817509005

openQ*D simulation code for QCD+QED

https://doi.org/10.1051/epjconf/201817509005

Published in EPJC

Special Article - Tools for Experiment and Theory | Open Access | Published: 03 Mar

openQ*D code: a versatile tool for QCD+QED simulations

RC*☆ collaboration

Isabel Campos, Patrick Fritzsch, Martin Hansen, Marina Krstic Marinkovic, Agostin Ramos & Nazario Tantalo

The European Physical Journal C **80**, Article number: 195 (2020) | Cite this article

1033 Accesses | **2** Altmetric | Metrics

https://link.springer.com/article/10.1140/epjc/s10052-020-7617-3

just Submitted to JHEP

High Energy Physics – Lattice

[Submitted on 27 Sep 2022]

First results on QCD+QED with C* boundary

Lucius Bushnaq, Isabel Campos, Marco Catillo, Alessandro Cotellucci

Accounting for isospin-breaking corrections is critical for achieving subperce lattice QCD calculations is to impose C* boundary conditions in space. Here, in this setup, which preserves locality, gauge and translational invariance all t renormalized fine-structure constant at the U-symmetric point, correspondin tuning strategy and, to the extent possible, a cost analysis of the simulations

Comments: 38 pages, 8 figures
Subjects: High Energy Physics – Lattice (hep-lat)
Report number: HU-EP-22/29-RTG
Cite as: arXiv:2209.13183 [hep-lat]
(or arXiv:2209.13183v1 [hep-lat] for this version)
https://doi.org/10.48550/arXiv.2209.13183

https://arxiv.org/abs/2209.13183

What have we achieved so far in our research program? after ~80 Million CPU hours (which is not that much)

Our approach works : by no means obvious as it is completely new theoretical approach to implement QCD+QED on the Lattice

- The signal could have been killed by statistical noise (even if the theoretical implementation is correct)
- Algorithms could have been unstable or not converge at all (eg. the new field (photon) could have induced instabilities).

The generated configurations will be used to explore a variety of physics observables.

- Primarily **meson** and **baryon correlators** and **masses**, **leptonic decay rates**
- In a more distant future **semileptonic decay rates** of mesons, the hadronic contributions to the **anomalous magnetic moment of the muon (g-2)**

https://arxiv.org/abs/2209.13183

First results on QCD+QED with C⋆ boundary conditions

RC⋆ collaboration

Lucius Bushnaq[a], Isabel Campos[b], Marco Catillo[c], Alessandro Cotellucci[d], Madeleine Dale[e,f], Patrick Fritzsch[a], Jens Lücke[d,g], Marina Krstić Marinković[c], Agostino Patella[d,g], Nazario Tantalo[e,f]

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arXiv:2209.13183v1 [hep-lat] 27 Sep 2022

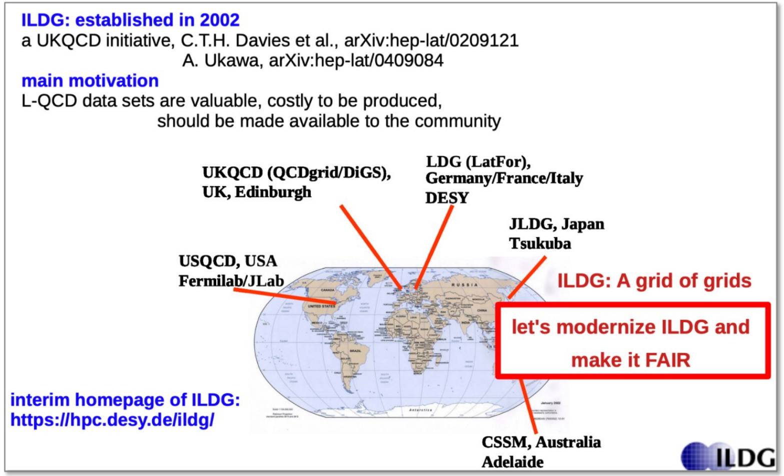
Abstract

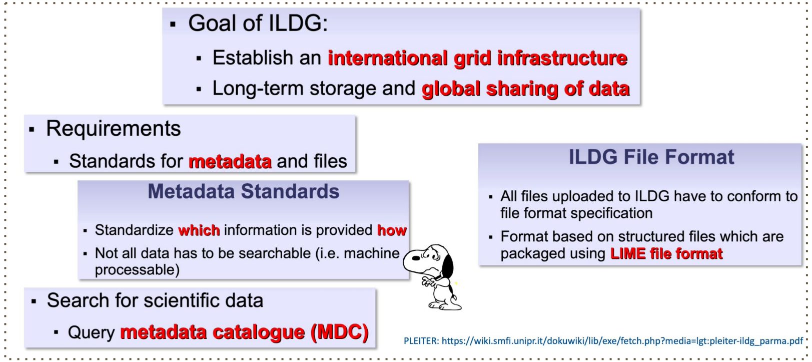
Accounting for isospin-breaking corrections is critical for achieving subpercent precision in lattice computations of hadronic observables. A way to include QED and strong-isospin-breaking corrections in lattice QCD calculations is to impose C⋆ boundary conditions in space. Here, we demonstrate the computation of a selection of meson and baryon masses on two QCD and five QCD+QED gauge ensembles in this setup, which preserves locality, gauge and translational invariance all through the calculation. The generation of the gauge ensembles is performed for two volumes, and three different values of the renormalized fine-structure constant at the U-symmetric point, corresponding to the SU(3)-symmetric QCD in the two ensembles where the electromagnetic coupling is turned off. We also present our tuning strategy and, to the extent possible, a cost analysis of the simulations with C⋆ boundary conditions.

Keywords: Lattice QCD and QED, High Performance Computing
PACS: 11.15.-q, 11.15.Ha, 12.20.-m, 12.38.Gc, 12.38.-t, 02.70.-c, 02.70.Uu

Data preservation ?

- **Global consensus about the necessity** to keep configurations available and shareable within the community (very expensive to simulate)
  - In an organized way: i.e. searchable, with metadata, etc...
  - Not just dumped in a storage area
- If people gets into that **"huge burden"** it has to be worth it
  - Keep the configurations for ~10 years (i.e. not only until Xmas)
  - Requires also funding: storage is not for free
- LQCD was the first community to come up with a standard for metadata (**2002**): **ILDG**
  - To tag Lattice QCD configurations





See the nice compilation of Patrick Fuhrmann for Lattice QCD students in our school in Benasque:
https://indico.ifca.es/event/2452/contributions/12495/attachments/1456/2090/2022-09-19-LaticeNET-SummerSchool-Lecture.pdf

Final take outs

"There was a Princess Somebody of Denmark sitting at a table with a number of people around her, and I saw an empty chair at their table and sat down.
She turned to me and said, "Oh! You're one of the Nobel-Prize-winners. In what field did you do your work?"
"In physics," I said.
"Oh. Well, nobody knows anything about that, so I guess we can't talk about it."
"On the contrary," I answered. "It's because somebody knows something about it that we can't talk about physics. It's the things that nobody knows anything about that we can discuss. We can talk about the weather; we can talk about social problems; we can talk about psychology; we can talk about international finance--gold transfers we can't talk about, because those are understood--so it's the subject that nobody knows anything about that we can all talk about!"
I don't know how they do it. There's a way of forming ice on the surface of the face, and she did it!"

― Richard P. Feynman, Surely You're Joking, Mr. Feynman!: Adventures of a Curious Character

https://sistemas.fciencias.unam.mx/~compcuantica/RICHARD%20P.%20FEYNMAN-SURELY%20YOU'RE%20JOKING%20MR.%20FEYNMAN.PDF