Pourquoi le neutron est-il plus lourd que le proton?
Calcul ab initio de la différence de masses neutron-proton

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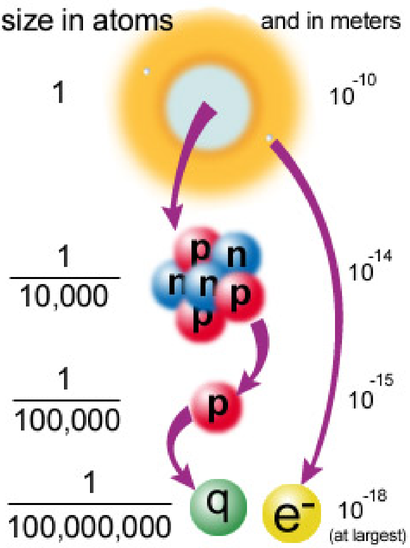
Budapest-Marseille-Wuppertal collaboration (BMWc)

(basé principalement sur Science 347 '15, PRL 111 '13, Science 322 '08)

Ordinary matter and elementary particles



(http://www.particleadventure.org/)

- *p* and *n* are “nucleons”
- Quarks and electrons are elementary particles
- Their interactions are governed by the Standard Model of particle physics
- Include the strong, weak and electromagnetic interactions . . .
- . . . as well as coupling to Higgs field

Importance of nucleon mass difference

Stability of nuclei and matter content of universe depends strongly on $M_n - M_p$ value

Experiment gives (PDG '15)

$$M_n = 939.6\ \mathrm{MeV}, \qquad M_p = 938.3\ \mathrm{MeV}, \qquad m_e = 0.511\ \mathrm{MeV}, \qquad m_{\nu_e} \simeq 0$$
$$\Delta M_N = M_n - M_p = 1.2933322(4)\ \mathrm{MeV} = 0.14\% \times M_N$$

w/ $1\ \mathrm{MeV} \simeq 1.8 \times 10^{-30}\ \mathrm{kg}$ and $M_N = (M_n + M_p)/2$

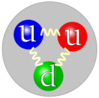
Imagine instead

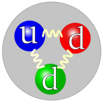
- $\Delta M_N > 0.14\% \times M_N$
  $\Rightarrow$ much more rapid $n \to p + e^- + \bar{\nu}_e$
  $\Rightarrow$ easily get a universe w/out n and heavier elements
- $0.14\% \times M_N > \Delta M_N \gtrsim m_e - m_{\nu_e} \simeq 0.05\% \times M_N$
  $\Rightarrow$ universe would have much less $^1\mathrm{H}$
- $\Delta M_N \lesssim 0.05\% \times M_N$
  $\Rightarrow$ $^1\mathrm{H}$ unstable ($p + e^- \to n + \nu_e$) or even $p \to n + e^+ + \nu_e$
  $\Rightarrow$ very boring universe w/ mostly n and few atoms

$\to$ understand physics behind ΔM_N and similar phenomena in terms of the fundamental theory

Why are n and p so similar?

Quarks bound together into hadrons by strong interaction

proton: 

neutron: 

u and d quarks are quite different

	u	d
m_q [FLAG '13]	$2.16(11)\,\mathrm{MeV}$	$4.68(16)\,\mathrm{MeV}$
$e_q = Q_q e$	$\frac{2}{3}e$	$-\frac{1}{3}e$

However differences are very small compared to strong interaction scale
$\Rightarrow$ theory has an $SU(2)$ isospin symmetry ($u \leftrightarrow d$) broken by small effects

$$3\,\frac{m_d - m_u}{M_N} \sim 1\% \qquad \text{and} \qquad \alpha = e^2/(4\pi) \sim 1\%$$

$\rightarrow$ to first approximation, need only strong interaction, i.e. QCD (quantum chromodynamics) w/ $m_d = m_u$ and w/out QED (quantum electrodynamics)

What is quantum chromodynamics (QCD)?

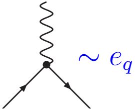
Fundamental theory of the strong force whose d.o.f. are quarks and gluons:

- ordinary matter: (u, d), g
- two more families: (c, s) and (t, b)

Responsible for a wealth of phenomena ever since the early universe: binds quarks into hadrons, binds hadrons into nuclei, governs Big Bang nucleosynthesis, powers stars and nuclear power plants, . . .

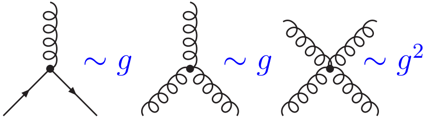
QED

q and γ interact through electric charge:
$e \sim \sqrt{\alpha}$



QCD

q and g interact through color charge: $g \sim \sqrt{\alpha_s}$



Additional g-g interactions in QCD
$\Rightarrow$ QCD binds q and g in a highly non-linear fashion, leading to confinement
$\Rightarrow$ solve theory numerically using lattice QCD

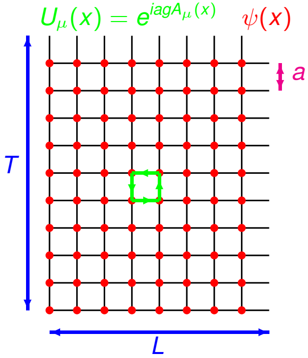
What is lattice QCD (LQCD)?

To describe ordinary matter, QCD requires $\geq$ 104 numbers at every point of spacetime
$\rightarrow \infty$ number of numbers in our continuous spacetime
$\rightarrow$ must temporarily "simplify" the theory to be able to calculate *(regularization)*
$\Rightarrow$ Lattice gauge theory $\longrightarrow$ mathematically sound definition of NP QCD:

- UV (& IR) cutoff $\rightarrow$ well defined path integral in Euclidean spacetime:

$$\langle O \rangle = \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi \, e^{-S_G - \int \bar{\psi} D[M] \psi} \, O[U,\psi,\bar{\psi}]$$
$$= \int \mathcal{D}U \, e^{-S_G} \det(D[M]) \, O[U]_{\mathrm{Wick}}$$

- $\mathcal{D}U e^{-S_G} \det(D[M]) \geq 0$ & finite # of dofs $\rightarrow$ evaluate numerically using stochastic methods



LQCD is QCD when $m_q \rightarrow m_q^{\mathrm{phys}}$, $a \rightarrow 0$ (after renormalization), $L \rightarrow \infty$ (and stats $\rightarrow \infty$)

HUGE conceptual and numerical ($\sim 10^9$ dofs) challenge

Significant recent progress

Thanks to work of physicists from around the world in past years:

- New field theoretical techniques (Wilson flow, twisted boundary conditions, . . .)
- More effective discretizations of QCD
- Better understanding of physics and mathematics of algorithms has allowed many improvements (mass preconditioning, multiple timescale integration, domain decomposition, deflation, all-mode averaging . . .)
- Highly optimized codes
- Arrival of supercomputers capable of Tflop/s and now Pflop/s performance, some of which are derived from computers developed by physicists to solve QCD

(© CNRS/IDRIS)

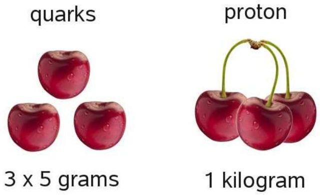
e.g. IBM Blue Gene/Q

- Turing @ IDRIS: 98,304 cores, 1.3 Pflop/s peak, 96 TB of RAM
- JUQUEEN @ FZ Jülich: 458,752 cores, 5.9 Pflop/s peak, 448 TB of RAM

$\longrightarrow$ have tools to perform fully controlled computations in non-perturbative QCD

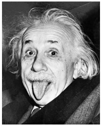
Where does most of p and n mass come from?

- Mass of object is usually the sum of the mass of its constituents
- Not true for light hadrons



- Light hadron masses generated by QCD energy imparted to q and g via:

$$m = E/c^2$$



(Arthur Sasse

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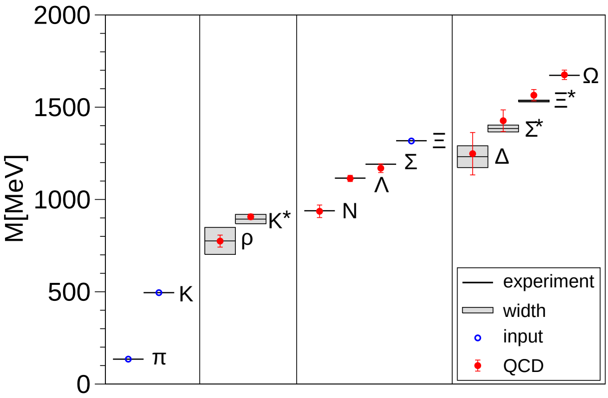
- mechanism at origin of more than 95% of mass of visible universe
- Higgs "only" gives mass to the q in p, whose sum $< 2\%$ of M_p

Ab initio calculation of light hadron masses

Dürr et al [BMWc], Science 322 (2008) 1224



Performed 20 large-scale simulations in lattice QCD, w/out electromagnetic effects and w/ $m_u = m_d$ (i.e. isospin limit)

All required limits taken in fully controlled way

(Also calculations by ETM '09, MILC '04-'10, RBC-UKQCD '07, Del Debbio et al '07, JLQCD '07, QCDSF '11, Walker-Loud et al '08, PACS-CS '09, Gattringer et al '09, . . .)

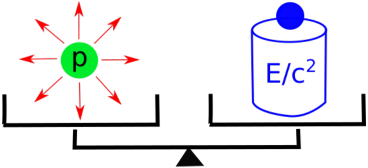
→ QCD mass generation mechanism checked at few % level

→ validation of nonperturbative QCD

Going beyond the isospin limit

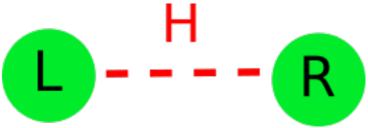
Must add effects associated with the 2 other ways in which the standard model generates mass

ELECTROMAGNETIC



- Charged particles are surrounded by an electromagnetic field which carries energy
- This energy contributes to the mass of these particles via $m = E/c^2$
- Tends to make p more massive than n

HIGGS



- d couples more strongly to the Higgs than u
- So $m_d > m_u$
- Tends to make n more massive than p

We added both these effects to our lattice QCD calculations in a complete way

QCD+QED challenges

Borsayni et al [BMWc], Science 347 (2015) 1452

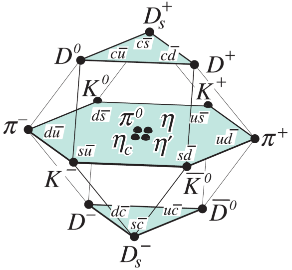
Main challenges addressed in addition to those of a full QCD calculation:

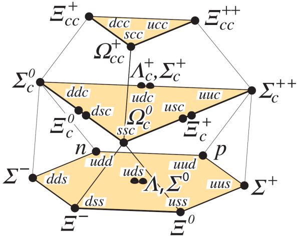
- formulate QED in a finite box (long-range interactions)
- control large finite-volume effects due to long-range interactions
- fight large autocorrelations of QED field
- consistently renormalize QCD+QED theory at hadronic scale
- fight large noise/signal ratio
- unprecedented precision required ($\times$1000 more statistics for ΔM_N than for M_N)
- ...

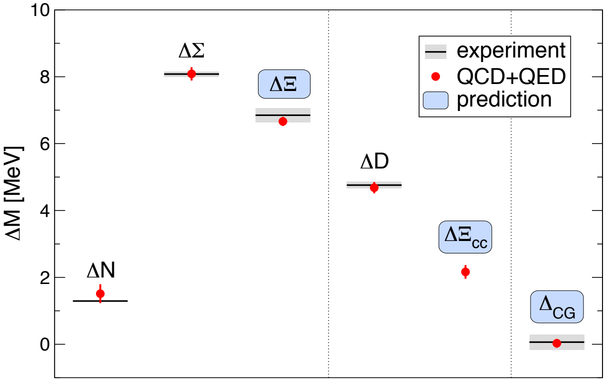
Performed 41 large scale simulations in lattice QCD, including some with QED and $m_d > m_u$

All required limits taken in fully controlled way

Results for isospin mass splittings



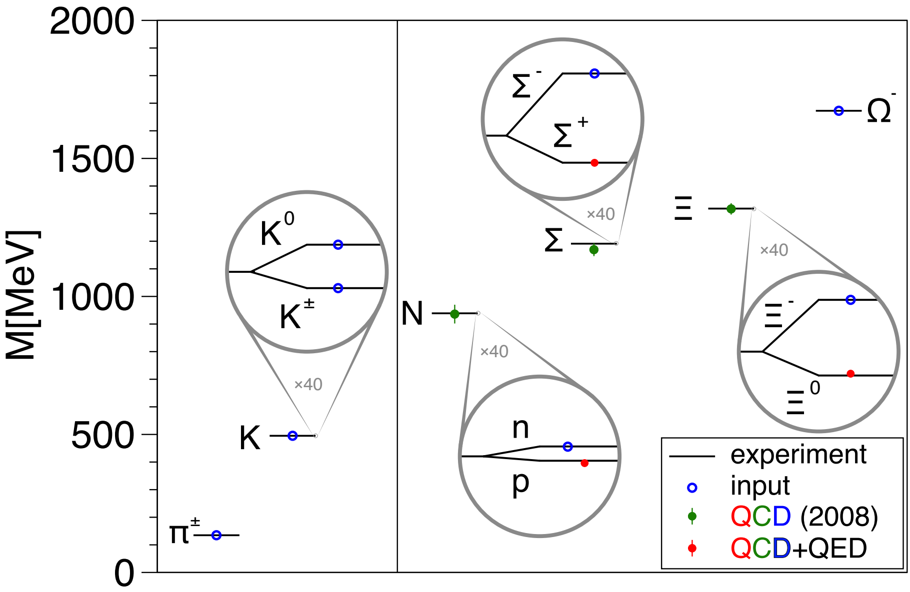




- 5σ signal for $M_n - M_p$
- 3 predictions
- $\Delta_{CG} = \Delta N - \Delta\Sigma + \Delta\Xi = O(\alpha(m_s - m_{ud}), \delta m(m_s - m_{ud})^2)$ (Coleman-Glashow relation)
- Full calculation: all systematics are estimated

Strong + Higgs + Electromagnetism = Experiment

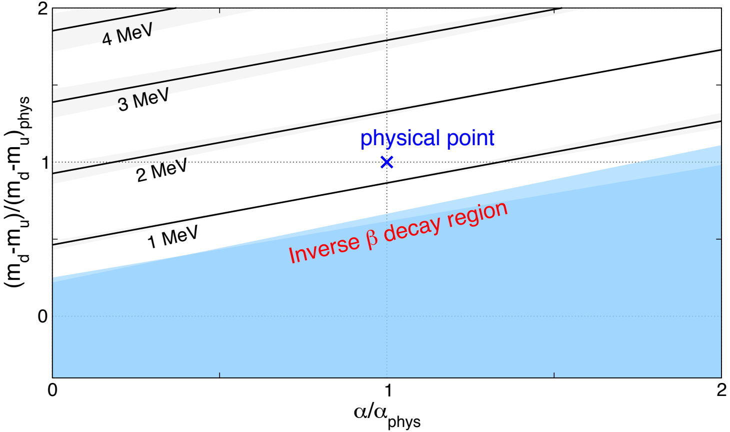
Progess since 2008



Quantitative anthropics

Also have dependence of ΔM_N on α and $(m_d - m_u)$

- $\Rightarrow$ can separate QED and $(m_u - m_d)$ contributions
- $\Rightarrow$ can be used first principle answer to: what would the universe be made of if these fundamental constants were different?



Conclusions

- The n-p mass difference is tiny but hugely important
- It is due to a competition between two small effects: electromagnetism and u-d quark mass difference
- We now have the theoretical, algorithmic and computational tools to fully include these effects in lattice QCD calculations of important hadronic properties
  $\Rightarrow$ determined $M_n - M_p$ and other mass splittings with w/ full control over uncertainties
- Confirm: Strong $+$ Higgs $+$ Electromagnetism $\rightarrow$ experimental hadron masses
- Also have dependence of ΔM_N on α and $(m_d - m_u)$ $\Rightarrow$ first principle anthropics
- Approach provides description low-energy Standard Model w/ intrinsic accuracy increased by $\sim \times 10$ compared to standard state-of-the-art simulations
- Added precision required to continue testing Standard Model and searching for new fundamental physics in increasingly precise experiments

NEWS & VIEWS

doi:10.1038/nature14381

PARTICLE PHYSICS

A weighty mass difference

The neutron–proton mass difference, one of the most consequential parameters of physics, has now been calculated from fundamental theories. This landmark calculation portends revolutionary progress in nuclear physics.

FRANK WILCZEK

Nuclear physics, and many major aspects of the physical world as we know it, hinges on the 0.14% difference in mass between neutrons and protons.

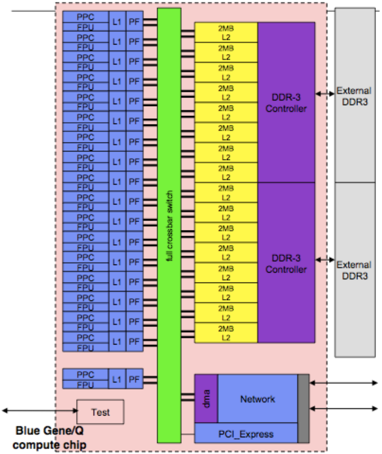
applications[3,4]. We can thus identify, with confidence and precision, the fundamental contributions to the neutron–proton mass difference. There are two: electromagnetic interactions and differences in the masses of quarks (the particles that make up hadrons, such as neu-

and different electric charges, but identical strong interactions. Thus, the two sources of neutron–proton mass difference that figured in our heuristic discussion also underpin the rigorous theory.

If the only place where the mass difference between the *u* and *d* quarks occurred were in the proton–neutron mass difference, we would simply be trading one number for another. But the *u* and *d* (and strange) quarks occur inside dozens of different quark-containing subatomic particles, all of whose masses must be obtained using the same quark-mass values in the QCD and QED equations. Therefore, the quark masses have been determined in a vast number of cases, and the theory is stringent. Borsanyi and colleagues actually calculated the masses of a large number of particles (among them the neutron and proton) and obtain a consistent fit to the observed values.

- **Selected writings about this work (English and French)**
  - A weighty mass difference (Frank Wilczek, Nature 520 (2015) 303)
  - Proton et neutron: une différence de masse enfin expliquée par le calcul (Sean Bailly, Pour la Science, n^{o} 241, mai 2015)
  - Ajustement fin (La Recherche, n°499, mai 2015)
  - Le neutron est plus lourd que le proton, et l'on sait pourquoi (Mathilde Fontez, Science & Vie, n^{o} 241, p. 219, juin 2015)
  - Masse du neutron: la fin du mystère (Azar Khalatbari, Sciences et Avenir, n^{o} 819, p. 15, mai 2015)
  - Clé de la cosmologie, la masse du neutron a été calculée (Laurent Sacco, Futura-Sciences, 29 mars 2015)
  - Pourquoi le neutron est-il plus lourd que le proton ? (Alerte presse du CNRS, Français)
  - Why is the neutron heavier than the proton? (CNRS press alert, English)
  - A trip to the heart of matter with Turing (GENCI News, 3 April 2015)
  - Plongée au coeur de la matière avec Turing (Actualités GENCI, 3 avril 2015)

BG/Q Implementation



Features:

- 16+1 SMP cores @ 1.6 GHz w/ 16 GB RAM
- 4 threads/core
  $\rightarrow$ overlap load/store and FP ops
- 4-way mult.-add SIMD FPU
  $\rightarrow$ vectorize code w/ XL C intrinsics
- Programmable MU w/ DMA
  $\rightarrow$ overlap FP ops with communication
  $\Rightarrow$ persistent communication instead of MPI

5D toroidal network

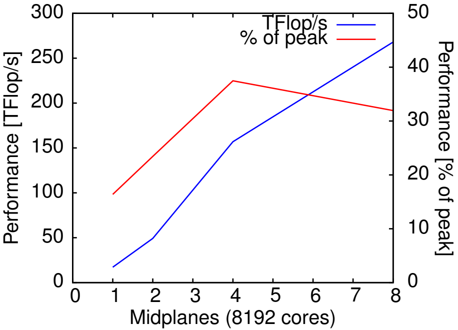
- node: $1 \times 1 \times 1 \times 1 \times 1(\times 16)$
- midplane: $4 \times 4 \times 4 \times 4 \times 2(\times 16)$

Fold 2×2 dimensions pairwise, e.g. midplane $\rightarrow 4 \times 8 \times 16(\times 16)$, and embed 4D spacetime lattice into this configuration

BG/Q Implementation (cont'd)

- Excellent performance
- Strong scaling less linear than on BG/P
- Sweet spot on 2 racks for $64^3 \times 128$ lattice
- Up to 37.5% of peak

(Right: strong scaling analysis on a $64^3 \times 128$ lattice)



Performed 41 large-scale simulations with $a \searrow 0.064\,\mathrm{fm}$, $L \nearrow 8.\,\mathrm{fm}$, $e = 0 \nearrow 3e^{\mathrm{phys}}$, $M_\pi \searrow 200\,\mathrm{MeV}$ and $(m_d - m_u)$, m_s & m_c scattered around their physical values