Colourful calculations – Physics World December 2006

The formidable computational power of lattice QCD is finally allowing researchers to make solid predictions about the force that binds quarks inside protons and neutrons, describes Christine Davies

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Understanding how the universe works at the most fundamental scale is often likened to peeling away the layers of an onion. The outermost layer of the onion represents atoms, and we have known about these for a century or so. The next layer of structure, which was unearthed by Rutherford in 1911, is the atomic nucleus -- a much smaller object which contains almost all of the atomic mass. Some 20 years after that, physicists realized that the nucleus is composed of more fundamental objects called protons and neutrons. However, peeling back the next layer of the onion has turned out to be much more of a challenge.

It is now universally accepted that protons and neutrons are made up of fractionally charged particles called quarks: two "up" quarks and a "down" quark in a proton, and two downs and an up in a neutron. There are six types of quarks in total, but the problem is that none of them has ever been observed as a free particle (see Box 1). Smashing protons together at enormous energies in particle accelerators, for instance, reveals not single quarks but yet more particles made of quarks. Such particles are called hadrons, and there are hundreds of them: some are "baryons", which contain three quarks and include protons and neutrons, while the rest are "mesons" made up of quark--antiquark pairs. It might therefore seem, as indeed it did to particle physicists in the 1960s, that the core of the onion is forever hidden.

The only way we can understand the properties of quarks is to compare experimental measurements of hadrons with calculations based on the theory of the "strong force" which binds quarks together: quantum chromodynamics or QCD. Despite being around for over 30 years, however, the equations of QCD have proved eye-wateringly difficult to solve. Indeed, to the immense frustration of particle physicists, it has been impossible to calculate properties of hadrons with an accuracy of better than 10%.

In recent years, this situation has changed remarkably thanks to the huge progress that has been made in a field of computational physics known as lattice QCD. We can now solve the equations of QCD numerically with an accuracy of a few percent, allowing us to make testable predictions about the properties of hadrons. Such a prediction involving the mass of the "charmed B meson" was dramatically confirmed last year at the Tevatron collider in the US. Now, we are in the exciting position of being able to determine the properties of quarks themselves and to reveal what the final layer of the onion might look like.

A discrete theory

Lattice QCD started life in a paper written by the future Nobel laureate Ken Wilson of Cornell University in the US in 1974, shortly after QCD itself became established. A key ingredient of the Standard Model of particle physics, QCD is a quantum field theory which describes the interaction between quarks as being due to the exchange of massless particles called gluons. These interactions are quite different to the classical interactions between billiard balls for example, which can be calculated with absolute certainty. Rather, QCD describes the interactions between quarks and gluons in terms of an integral over quantum fields that represent those particles at different points in space—time. The integrand is weighted by the probability that such a field configuration will appear in the vacuum.

Although impossible to solve analytically, Wilson realized that the integral could be tackled numerically by representing space--time as a 4D lattice and expressing the equations of QCD in terms of the quantum fields at the individual lattice sites (since by definition there is nothing in between). The first stage in actually evaluating the integral is to generate "snapshots" of the QCD vacuum which contain the gluon fields that have the highest probability to appear. We calculate the quantities of interest on each gluon field configuration and then, finally, average over many hundreds of these “snapshots”. A typical lattice QCD calculation has a "box size" of 2.5::fm (1::fm::=::10^{--15}::m), which is somewhat larger than a hadron in order to avoid "squeezing" it unnaturally, and a lattice spacing of about 0.1::fm. This means that about 400::000 lattice points are involved in calculating the properties of a hadron (see Box 2).

Early lattice QCD calculations, beginning with those of Mike Creutz at Brookhaven National Laboratory in 1979, concentrated on a stripped-down version of QCD which included only gluons. This provided a self-consistent theory that proved the effectiveness of the lattice approximation to QCD. But since we know from experiments that hadrons do contain quarks -- indeed for most hadrons it is obvious what type of quarks they contain from the way they decay to other hadrons -- this basic version of QCD could never allow us to predict the properties of a real quark--gluon system such as a hadron.

The main quarks inside a hadron, which are responsible for its charge, **spin** and other properties, are known as valence quarks. However, real life -- at least that which is described by quantum field theories such as QCD -- is not quite so simple.
For a proton, for example, 99% of its mass comes from the “binding energy” that results from the valence quarks living in a complicated "soup" of gluons and quark--antiquark pairs, known as “sea quarks”. These fluctuate in and out of existence by borrowing energy from the vacuum for a short period in accordance with the uncertainty principle.

Quarks are the biggest headache for lattice QCD. In the first calculations to include them, the valence quarks were simply dropped into Creutz's gluons-only theory and allowed to propagate and interact with the gluons. This so-called "quenched approximation" led to equations that were just about solvable on the computers of the early 1980s, and launched an entire industry of lattice QCD calculations based around expanding supercomputer facilities. As the calculations got more precise, however, dissatisfaction with the results grew because the size of systematic errors from the quenched approximation became clearer.

During the 1990s theorists therefore realized that they needed full QCD calculations which also included the sea quarks. Because the sea quarks are the result of gluons inside hadrons momentarily "splitting" into quark--antiquark pairs, which themselves can radiate more gluons that split into further quark- or gluon-pairs, they are numerically much more expensive to include in the calculations than valence quarks.

By the early 2000s, however, computing power had increased sufficiently to enable 26 lattice QCD theorists from four collaborations -- FNAL, based at Fermilab; HPQCD, which stands for High Precision QCD; MILC, comprising US researchers; and the UK-based UKQCD -- to perform realistic calculations for the first time. These calculations, which are based on a very efficient way of including sea quarks, have heralded the era of precision lattice-QCD.

Mass predictions

The best theories in physics have as broad as possible predictive power based on a small number of input parameters. QCD is no exception. The only parameters it requires are a mass for each quark and a value for the "colour charge", *g*, more usually expressed as the strong coupling constant: α_s::=::$g^2/4\pi$. These parameters have to be fixed by comparing a theoretical result from QCD with the corresponding experimental value obtained by studying hadrons. After that, however, the theory is completely determined and can make general predictions.

For simplicity, the latest lattice QCD calculations contained the masses **of** just four quarks, by taking the masses of the lightest up and down quarks to be the same and ignoring the very heavy "top" quark. These parameters were fixed from the measured masses of four hadrons -- the π (which contains up and down quarks), K (up/down and strange quarks), D_s (charm and strange quarks) and Y (bottom quarks) -- by adjusting the value of each quark mass until the calculated mass of its associated hadron best matched its measured value. To fix the strong coupling constant, which turns out to be equivalent to determining the value of the lattice spacing, we used the difference in mass between the Y and its excited state, the Y'.

After this we were able to calculate the masses of nine other hadrons as well as a well-measured decay rate of the π and K mesons. Performing the calculations was a massive team effort between physicists at Cornell and Ohio State Universities in the US and Glasgow University in the UK (as part of the HPQCD and UKQCD collaborations), who dealt with hadrons that contain bottom quarks; Fermilab physicists in the FNAL team, who concentrated on charm quarks; and physicists across the US in the MILC collaboration, who worked on hadrons that contained the lightest up, down and strange quarks.

The calculations took about two years to perform, including the time taken to generate the gluon configurations (which is the most time-consuming part). The results started to come together towards the end of 2002, and to our delight early the following year the results matched experiment across the board

QCD scores direct hit

The new results using full lattice QCD are not just down to brute processing power. They have been made possible by many years of research and development to improve the way QCD is discretized onto the lattice. This led researchers at Cornell University, Arizona University and the Argonne national laboratory in 1998/99 to a relatively fast method for handling the light up, down and strange quarks called the "improved staggered formulation". Using this, and a lot of help from a supercomputer, it was possible to generate sample gluon field configurations that included the effect of the up, down and strange sea quarks.

One unwanted side-effect of the staggered formulation is that it contains four copies of every quark, which means that the calculations have to "divide by four" at appropriate points. This has caused some controversy in the lattice-QCD community because practically it means taking the fourth root of the determinant of a large matrix – a process which only becomes strictly correct if the lattice spacing approaches zero. However, the fact that the method was able to correctly predict the properties of so many hadrons means that, while it may be ugly, it appears to work well at the values of the lattice spacing that we are using.

The new sets of gluon field configurations, which were made available by the MILC collaboration, also allowed us tackle those hadrons that contain the heavier charm and bottom quarks in realistic QCD. Such particles are currently the focus of several particle-physics experiments worldwide because they provide a good way to look for inconsistencies in the Standard Model. Charm and bottom quarks are too heavy to be produced by the quantum fluctuations inside hadrons, and so do not contribute to the sea quarks. But that does not mean the calculations were easy. In fact, even when treated as valence quarks the large masses of these quarks complicate lattice QCD calculations of bottom- and charmed-hadrons considerably. This is because the wavelength associated with such a large-mass particle is short enough to be readily distorted by the discretization of space—time on a lattice.

Fortunately, although the quark masses are large their binding energies inside hadrons are not -- and it is these energies that have to be handed accurately. Thanks to a lot of work carried out in the 1990s, researchers realized how to do this. In fact, mesons made of bottom quarks and antiquarks are now one of the best studied sets of hadrons in lattice QCD, and the agreement between the predicted and measured masses of bottom-hadrons tells us that we are handling bottom quarks correctly.

Lattice QCD has had similar successes for hadrons that contain charm quarks, which are known as Ψ or "charmonium" states. This gave theorists the confidence to predict the mass of a hadron containing a bottom and a charm quark ahead of experiment for the first time. Indeed, in 2004, precisely such an opportunity arose when members of the HPQCD collaboration from Glasgow and Fermilab heard that researchers working on the CDF experiment at the Tevatron were close to discovering the "B_c meson", which has as its valence quarks a bottom and a charm quark or antiquark. Since the mass of this particle had never been measured before, this was our chance to put three decades of lattice QCD research on the line.

To calculate the mass of the B_c meson we simply had to allow charm and bottom quarks to move through the sample gluon field configurations generated by the MILC collaboration. We were then able to "reconstruct" the mass of the B_c by calculating how much it differed from the average mass of the lightest Y and Ψ mesons. In fact, the present author and the Glasgow lattice QCD team had performed this calculation five years earlier in the quenched approximation, but we had been dismayed by the large systematic error that we had to include in order to allow for the absence of sea quarks. Thanks to the improved staggered formulation, which allowed the lightest sea-quarks to be included, we were finally able to dispense with that error.

At a conference in June 2004, my graduate student Ian Allison presented our measurement of the B_c mass: 6.304::±::0.020 GeV/c^2 (for comparison, the mass of the proton is 0.938::GeV/c^2). The result took about six months to achieve, but that was only because much of the work in generating the gluon configurations and calculating the Ψ and Y masses had already been done. The rest of the summer was spent checking and polishing the result for publication -- an activity which became increasingly frantic as rumours began to circulate that the experimentalists had found the first signs of the B_c using a very thorough "blind" analysis.

Stress levels mounted as we posted our result on the arXiv preprint server and waited for their experimentalists to announce their result, and we all considered how much easier it would be to sleep at night if we were string theorists! Then, at a seminar at Fermilab in December 2004, Saverio D'Auria of Glasgow University announced that the CDF collaboration had measured the B_c mass to be 6.287::±::0.005::GeV/c^2. The agreement was close enough for us to feel huge relief, but work continues both theoretically and experimentally to tighten up these numbers.

Getting to the core of QCD

Lattice QCD has finally allowed theorists to calculate the inner workings of hadrons which the strong force has kept hidden. But this is not the end of the story. The calculations also provide a direct way of accessing the core parameters of QCD: the individual quark masses and the strong coupling constant. Indeed, without lattice QCD it is hard to even define the mass of a particle that you cannot directly weigh. Although we may never actually observe individual quarks, knowing how heavy they are is important because their masses appear as parameters in many other calculations. In particular, some theories which attempt to unify the basic forces of nature predict how the quark masses are related to the masses of "leptons" such as electrons and neutrinos.

To estimate the quark masses using lattice QCD we simply adjust the input quark masses used in our calculation (or interpolate between or extrapolate values that we have used) until the mass of a hadron sensitive to that quark mass matches its measured value. The hadrons used for each quark mass were given earlier and are chosen so that this can be done accurately. The only difficulty is finding a way to convert these quark masses to the values appropriate to real-world QCD in continuous space--time.

To do this we have to perform a "matching calculation" whereby we work out the effect of short-wavelength gluons that are emitted and absorbed by quarks and other gluons inside the hadron. In particular we need to consider wavelengths that are shorter than the lattice spacing, since these are forbidden on the lattice but present in continuous space--time. Because the strong force is relatively weak at such short distances, the matching calculations can be performed analytically as a power series expansion in terms of the strong coupling constant, α_s. Early last year, members of the HPQCD collaboration from Cambridge, Cornell and Simon-Fraser Universities used such an expansion (which included terms up to α_s^2) to calculate the real-world masses of the lightest quarks, giving smaller errors than previous non-lattice methods. A similar approach allows us to determine the strong coupling constant itself. Instead of directly using the parameter from our lattice QCD calculations, it turns out to be more accurate to "measure" α_s on the sample gluon field configurations. We do this by calculating the value of small "loops" of gluon fields which, although they have no directly observable characteristics, can be compared with very precise power-series expansions in α_s . Such calculations performed by the HPQCD team in 2004/5, which included terms up to α_s^3, enabled α_s to be determined with better accuracy than had been achieved by any other method before.

Pinning down the properties of quarks and the strength of the strong interaction also impacts the sector of the Standard Model that is not governed by QCD. In particular, the way quarks feel the *weak* nuclear force is important for understanding the mechanism by which nature distinguishes between matter and antimatter -- which is one of the biggest challenges in particle physics. The weak force was first seen in nuclear beta decay, whereby a down quark inside a nucleus transforms into an up quark by radiating a W boson which instantaneously decays into an electron and an antineutrino. All six quarks can change "flavour" in this way, and the probability of this occurring is described by a 3::×::3 array of numbers called the Cabibbo Kobayashi Maskawa (CKM) matrix.

Hundreds of particle physicists around the world are trying to measure the elements of this matrix as precisely as possibly so that they can check whether or not the Standard Model picture of quark-mixing is correct or whether inconsistencies will appear. But although the numbers themselves relate to individual quark decays, determining them -- as always -- comes from studying hadrons, mainly B mesons containing bottom quarks. In order to work out how the confinement of quarks inside hadrons affects the quark decay rate, we need lattice QCD calculations that are accurate to a few percent. There was no hope of performing such a precise calculation using the old quenched approximation, but the latest lattice QCD results are cause for great optimism.

As part of this process, it is important to keep testing lattice QCD against experiment to check that the calculations really are as accurate as we think they are. To this end, particle physicists in the CLEO collaboration working on an electron--positron collider at Cornell University have recently set theorists a challenge by undertaking to measure various decay parameters of D mesons, which contain charm quarks. Because the CKM numbers relevant to these decays are known, they can be used as tests of lattice QCD predictions and thus of the confidence that we can place in our results for B mesons.

In 2003, lattice QCD theorists in the FNAL and MILC collaborations took up the gauntlet, and in June last year they announced results for the "annihilation rate" of the D meson via a W boson into an electron and antineutrino. This rate is described in the form of the decay constant, f_D, which is the same quantity as the one calculated for the decay of pi and K mesons shown in figure 2. The lattice QCD value came out at 201::±::17::MeV, while CLEO announced a value of 223::±::17 shortly afterwards. Neither result is yet accurate enough to count as a few-percent determination, but the CLEO researchers hope that they will reach 4% as their experiment continues. The lattice QCD calculation, meanwhile, is limited by the accuracy of the discretization of QCD for charm quarks, and work is underway to improve this.

Getting real

Lattice QCD calculations are starting to pay back the effort of over 30 years of development, and to take their place among the precision tools that particle physicists can use to peel back further layers of the proverbial onion and understand nature's fundamental particles and interactions. A significant number of tests against experiments have now been carried out and predictions made for subsequent confirmation. And theorists are beginning to test other ways of including sea quarks that are becoming possible as computer power continues to grow.

Over the next few years the calculations for the weak decay-rates of B and D mesons will be honed down to an accuracy of a few percent to help experimentalists pin down the elements of the CKM matrix. This may lead to more sleepless nights as we grapple with new lattice QCD results, but it is a small price to pay for the chance to confront experiment at last with real lattice QCD.

More about: lattice QCD

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At a glance: lattice QCD

- The sub-atomic world of quarks and gluons is elegantly described by a powerful theory called quantum chromodynamics (QCD)
- Since quarks and gluons are "confined" inside hadrons such as protons, however, the real-world equations of QCD are almost impossible to solve for hadron properties
- Lattice QCD allows researchers to solve the QCD equations at certain points in a 4D lattice which represents discretized space--time

- Handling quarks in lattice QCD is extremely difficult and costly in terms of computer resources, forcing theorists to use the "quenched approximation" for most of the last 30 years
- The last five years have heralded the era of precision lattice QCD, whereby it has become possible to predict the properties of hadrons based on full lattice-QCD

Forever confined [Box 1]

The strong force differs fundamentally from nature's other three basic forces because it does not die away at long distances. A useful analogy is the outdoor game "swing-ball" whereby players hit a tennis ball, which is tethered to a pole by a piece of elastic, in opposite directions.

When struck, the ball behaves as if it is free, but in fact it cannot escape. Similarly, when quarks interact with each other at very short distances (less than about 10^{--16}::m), the strong force behaves in a similar way to electromagnetism with a strength that is proportional to g^2/r^2, where g is the magnitude of the colour charge on a quark and r is the distance. As r is reduced, however, the effective value of g becomes smaller so that the strong force becomes weaker and weaker.

This is because the gluons exchanged between quarks to mediate the strong force can create both quark--antiquark pairs, which "screen" the colour charge just as electric charge is screened inside a dielectric, and gluon pairs which "anti-screen" the charge.

It turns out that anti-screening wins over the screening, a result for which three QCD theorists were awarded the 2004 Nobel Prize for Physics. The flip-side of this short-distance simplicity, however, is that the strong force is very strong at large distances and does not allow particles with colour-charge to escape from each other. The only option is for them to be forever confined in "colourless" combinations of quarks, antiquarks and gluons called hadrons.

Solving the mother of all matrices [Box 2]

Lattice QCD allows theorists to solve the otherwise intractable equations of QCD by approximating space--time as a four-dimensional lattice. The equations of QCD are transcribed onto the lattice according to standard numerical procedures, such as representing derivatives by finite differences, and this discretization process incurs well-known systematic errors. These can be reduced by making the lattice spacing shorter or by using a higher-order differencing scheme, but not without penalty. Halving the lattice spacing increases the number of calculations required by a factor of 2^6. Higher-order differencing schemes are complicated by the short-wavelength gluon emission mismatch between QCD on the lattice and in continuous space-time. Luckily, the strong force becomes weaker at short distances, so we can account for this analytically and implement these schemes. They reduce discretization errors to a few percent at a lattice spacing that existing computers can handle. An example is the improved staggered formulation that has enabled sea quarks to be included in the calculations.

Because they have half-integer spin and therefore obey the exclusion principle, the quantum fields of quarks must be represented by "anticommuting" numbers that computers cannot handle. To get round this we perform the integral over quark quantum fields analytically (which is easy) and then write the result in terms of complicated functions of the gluon fields. The effect of valence quarks then appears as the inverse of the huge quark matrix, M, which has a number of rows and columns several times the number of lattice points and its elements are functions of the gluon fields.

Calculating the inverse of this matrix is equivalent to allowing valence quarks to "move through" the gluon field and interact with it as required by QCD. Including only valence quarks is called the quenched approximation. Including the effect of sea quarks -- which allows gluons to make quark--antiquark pairs -- is thousands of times more costly because it requires the determinant of M to be included in the probability with which the sample gluon field configurations are generated. The final blow for lattice QCD theorists is that the most important sea quarks -- the lightest "up" and "down" quarks -- are also the most numerically expensive.