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First High-Precision Calculations of Hadron Properties (2004)

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For almost 30 years, precise numerical studies of nonperturbative QCD, formulated on a space-time lattice, had been stymied by the inability to include the effects of realistic quark vacuum polarization. A milestone was reached in 2004 when improved algorithms and faster computers allowed unquenched lattice-QCD simulations with much smaller (and more realistic) quark masses than previously possible. Researchers compared experimental results with a variety of nonperturbative calculations in QCD drawn from a restricted set of well-established quantities. They found agreement to within statistical and systematic errors of 3% or less.

Physicists who work in the field of lattice quantum chromodynamics — lattice QCD for short — are nothing if not patient. For 30 years they have been trying to use the basic QCD equations to calculate the properties of hadrons — particles (including protons and neutrons) composed of quarks, antiquarks, and gluons. Limited by the speed of available computers, they have had to simplify their simulations in order to get results in a reasonable amount of time, and those results typically had an error rate of around 15% when compared with experimental data.

But in 2004, with faster computers, improved algorithms that employ fewer simplifications of physical processes, and better-performing codes, four QCD collaborations involving 26 researchers reported calculations of nine different hadron masses, covering the entire range of the hadron spectrum, with an error rate of 3% or less. This marks the first time that lattice QCD calculations have achieved such precise results for such diverse physical quantities using the same QCD parameters.

QCD is the theory of the "strong force," by which gluons bind quarks together to form hadrons. QCD theorists use computer simulations to determine the most probable arrangements of gluons and quarks inside a particle and then use these configurations to determine the particle's properties. Calculating all the possible positions of quarks and gluons would be impossible, so theorists simplify the problem by imagining space and time not as a continuum, but as a lattice — a four-dimensional grid of discrete points at which quarks and gluons can reside. This approach, called lattice QCD, transforms an impossible problem into one that is extremely difficult but, in principle, solvable.

"Lattice QCD simulations are needed to obtain a quantitative understanding of the physical phenomena controlled by the strong interactions, to determine a number of the basic parameters of the Standard Model, and to make precise tests of the Standard Model's range of validity," explains Doug Toussaint, Professor of Physics at the University of Arizona and a member of the MILC Collaboration, one of the four teams that co-authored the "QCD confronts experiment" paper.

"Despite the many successes of the Standard Model," Toussaint says, "high energy physicists believe that to understand physics at the shortest distances a more general theory will be required, which unifies all four of the fundamental forces of nature" — the strong force; the weak force, electromagnetism, and gravity.

One way of determining the validity of the Standard Model is to tabulate the rates at which heavy quarks decay into lighter ones. Unfortunately, it is impossible to directly measure the decay of an individual heavy quark into a lighter one, because every quark is bound by a swarm of gluons to other quarks or to an antiquark. Experimenters have to measure the decays of composite particles, such as B mesons, and then try to calculate the CKM numbers by subtracting the effects of the extra quarks and

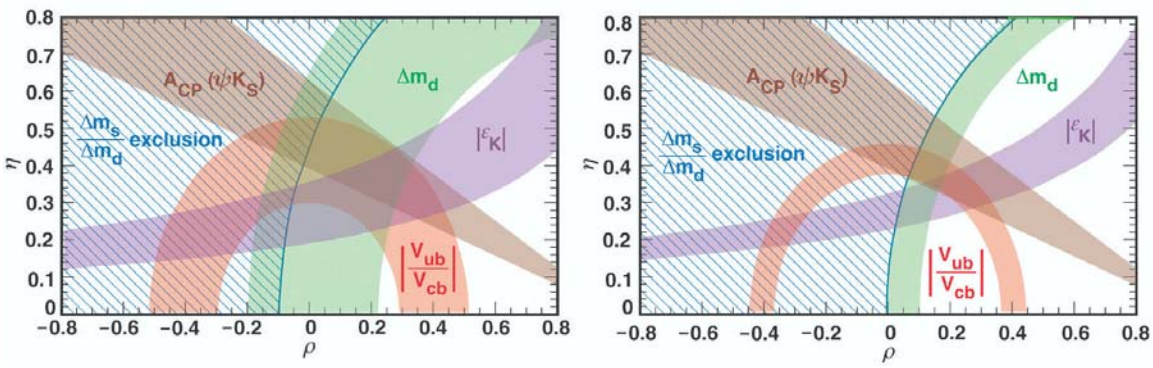

Figure 1. Constraints on the Standard Model parameters ρ and η, the least well known elements of the CKM matrix. For the Standard Model to be correct, they must be restricted to the region of overlap of all the solidly colored bands. The figure on the left shows the constraints as they exist today. The figure on the right shows the constraints as they would exist with no improvement in the experimental errors, but with all lattice gauge theory uncertainties reduced to 3%.

gluons. That subtraction is easier said than done, because within each hadron is a dynamic "sea" of gluons exchanging gluons among themselves, as well as quark-antiquark pairs popping in and out of existence. The effect of all this frenetic strong-force activity is called "quark vacuum polarization," and it has been one of the most difficult quantities to include in lattice QCD calculations.

Quark vacuum polarization is the most computationally expensive ingredient in a QCD simulation because moving quarks from real space into lattice space increases the number of quarks by a factor of 16. In the past, most QCD simulations have either omitted quark vacuum polarization altogether ("quenched QCD") or inflated the lightest quark masses by a factor of 10 to 20, reducing both the computational effort and the accuracy of the results.

The "Symanzik-improved staggered-quark discretization" of the lattice, developed by the MILC Collaboration and others, includes the vacuum polarization effects of all three light quark flavors (up, down, and strange) and allows QCD simulations with much smaller and more realistic quark masses than previously possible. This algorithm improves on an older method called "staggering" — spreading each quark over four neighboring lattice points.

Including quark vacuum polarization has dramatically improved the accuracy of lattice QCD calculations. Figure 1 graphically depicts the impact of improved lattice calculations on constraints to the Standard Model. "In this study, we chose to calculate quantities whose values are well known experimentally," says MILC collaborator Bob Sugar of the University of California, Santa Barbara. "This allowed us to verify that we have control over all sources of systematic errors." Now that lattice QCD has accurately reproduced a range of well known quantities, researchers will have more confidence in the calculation of other quantities that experiments cannot determine.

Describing the MILC Collaboration's computations at NERSC, Sugar says, "The bulk of our allocation goes into the generation of lattices — snapshots of the systems we are simulating — using the improved discretization. These lattices are saved, and then used to calculate a wide variety of physical quantities." The MILC collaborators produced the gluon configurations, as well as the raw simulation data for pions and kaons, that were used in the "QCD confronts experiment" paper.

QCD theory and computation are now poised to fulfill their role as an equal partners with experiment. Sugar comments, "The importance of this can be seen from the fact that a significant fraction of the $750 million per year that the United States spends on experimental high energy physics is devoted to the study of the weak decays of strongly interacting particles. To fully capitalize on this investment, the lattice calculations must keep pace with the experimental measurements."

Publications:

C. T. H. Davies et al. (the HPQCD, UKQCD, MILC, and Fermilab Lattice Collaborations), "High-precision lattice QCD confronts experiment," Phys. Rev. Lett. **92**, 022001 (2004).

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