The successes of the standard model of electromagnetic, weak, and strong interactions have been remarkable. Nevertheless, this model contains many assumptions and undetermined parameters that are displeasing aesthetically. Also, the model has not yet produced a satisfying route to unifying gravity with the other three fundamental forces.

The goal of particle physicists now is to discover where the standard model fails and so to find clues to a better theory, perhaps ultimately achieving Einstein’s dream of unifying all forces including gravity. It is hoped that the clues will emerge from highly sophisticated experiments in which particles are accelerated and smashed together at very high energies. To date, however, no deviations from the standard model have been found, and so the search for new clues must be performed at even higher energies—such as those that will be achieved at the Superconducting Super Collider (SSC) now under construction in Texas.

Much theoretical analysis is still needed to interpret the results of these extraordinary and expensive experiments. The strong-interaction part of the standard model—quantum chromodynamics, or QCD—presents the major computational stumbling block. Qualitatively, QCD has all the right properties, but so far theoretical physicists have not been able to extract accurate predictions from this precise mathematical model with the traditional tools of the theoretical physicist—pencil and paper. To obtain reliable self-consistent results when dealing with the strong force between, say, two protons requires calculating many subprocesses involving quarks and gluons. In fact, the number of subprocesses is so large that the calculation far exceeds the scope of analytical techniques.

The solution is to turn to a new tool: the supercomputer. Large-scale numerical simulations of QCD are the most promising technique for analyzing the strong interactions. In order to solve QCD on a computer one has to approximate space and time by a four-dimensional grid, or lattice, of points. The discretized version of the theory is called lattice QCD. Experimentally measurable quantities (such as the particle masses and the probabilities of specific transitions) are determined from a statistical average over quantum fluctuations in the quark and gluon fields. The fluctuations at each position in the lattice are simulated by a Monte Carlo procedure, so each Monte Carlo calculation determines one state in a statistical sample of possible states of a system. Monte Carlo methods are an efficient way of sampling the important states, that is, states that give the dominant contributions to the process. The best Monte Carlo calculations to date have used lattices of size up to $32^4 \times 48$ and generated only a small statistical sample (twenty to fifty of the possible states). The three sources of errors in such simulations are the lattice size, the lattice spacing, and the limited statistical sample. These errors can be systematically reduced by making the lattice size larger, the statistical sample larger, and the lattice spacing smaller.

To reduce statistical and systematic errors to the level of a few percent requires a computer with a very large memory and a very high operating speed, over 1000 billions of arithmetic operations per second. For comparison, a typical state-of-the-art home computer has a few million bytes of memory and runs at a few million operations per second. The required technology is just beginning to appear in the form of the parallel supercomputer. In fact, scientists interested in solving the riddle of QCD have played a significant role in the development of parallel supercomputers. The basic principle of these new machines is simple—thousands of
small but powerful computers work simultaneously to solve one big problem.

The first large-scale simulations of lattice QCD were performed around 1980. Because in those days the fastest computer generally available had the same power as today’s desktop workstation, the simulations involved so many approximations that the results were not realistic.

To overcome this limitation, physicists turned to parallel computers, often building them themselves. Though the capabilities of the earlier versions of such computers were quite limited, a start had been made, and scientists in other fields became excited by the potential of parallel computation.

A watershed for parallel computing came in 1988. In that year Thinking Machines Corporation introduced the first commercial parallel supercomputer, the Connection Machine 2 (CM-2), and DOE announced its first “Grand Challenges” program, which allocated large grants of supercomputer time to scientists working on key computationally intensive problems. The Los Alamos QCD collaboration was one such recipient. Build-
ing on the cruder calculations of 1980–88, we demonstrated, using the most powerful Crays and the CM-2, the viability of numerical methods for QCD. We obtained many new results with an accuracy comparing favorably with the best analytical estimates, though the computational power was still too limited to make definitive predictions. The Los Alamos QCD collaboration also played a key role in technology transfer by pioneering the use of the CM-2 and showing other scientists at the Laboratory and around the world how to use this machine as a production supercomputer.

The revolutionary nature of parallel computing poses new challenges beyond the design of faster hardware: We also need to develop software paradigms for parallel supercomputers that simplify their use for a wider variety of problems and fully exploit the advantages of parallelism. Progress requires close collaboration between scientists, computer engineers, and applied mathematicians. A successful collaboration of this type has begun between our Los Alamos QCD group, the Advanced Computing Laboratory (a DOE High Performance Computing and Research Center at Los Alamos), and Thinking Machines Corporation. This collaboration has received a Grand Challenge grant from the DOE to perform the next generation of QCD calculations on the 1024-node CM-5 located at Los Alamos National Laboratory.

Compared with the computing power of the Cray computers and the CM-2 used in our previous Grand Challenge calculation, the available memory in the CM-5 will be more than an order of magnitude greater, and the available computer speed will be at least two orders of magnitude greater. We plan to use these improvements in computer hardware in three ways. First, we will exploit the increased speed to generate much larger statistical samples for the processes we have already calculated. These simulations will be done on lattices of the size we used previously, $32^3 \times 64$. Second, once the new computers become stable and the proposed hardware upgrades are in place, we will begin simulations on much larger lattices of size $64^3 \times 128$. Finally, we will exploit the larger memory to undertake more complex calculations than have been feasible so far.

Our calculations will yield predictions for a large number of observables affected by strong interactions. The theoretical uncertainties in these quantities will be as low as a few percent. An illustrative and important example concerns the violation of “CP” symmetry. All interactions except the weak are unaffected if one simultaneously interchanges particles and antiparticles (charge conjugation, or C) and takes the mirror image of space (parity transformation, or P). The only experimentally established violation of CP symmetry occurs in the transmutation of a neutral strange meson ($K^0$) into its antiparticle ($\bar{K}^0$). This discovery was made more than twenty-five years ago and was rewarded with the 1980 Nobel Prize. To test the standard model against this long-standing experimental result requires calculating a parameter called $B_K$. The more accurately we can determine this quantity, the more precisely we can probe the validity of the standard model. Prior to numerical calculations, the uncertainty in $B_K$ was at least 50 percent. Our present Grand Challenge calculation has reduced this error to about 15 percent. We expect that the planned calculation will further reduce the level of uncertainty to a few percent.

To search for physics beyond or in contradiction to the standard model, one must combine experimental and theoretical knowledge of many quantities. Our calculations will provide theoretical results for a number of the standard-model observables with an accuracy of 10 to 25 percent, small enough to put meaningful constraints on the unknown parameters of the model. Thus, over the next few years, theoretical predictions combined with new experimental results will provide stringent tests of the standard model.

Further Reading


Rajan Gupta was awarded an M.S. by the University of Delhi, India, and a Ph.D. by the California Institute of Technology in 1982. In 1985 he became an Oppenheimer Fellow at the Laboratory and three years later joined the staff of the Elementary Particles and Field Theory Group. Among his scientific interests are the development of non-perturbative methods to solve QCD, using lattice QCD to constrain the standard model, and studying the critical behavior of statistical-mechanics models by means of Monte Carlo renormalization-group methods.