RECENT RESULTS OF LATTICE QCD SIMULATIONS[1]

The LANL Collaboration[2]

ABSTRACT

We describe recent progress in numerical computations of the properties of strongly interacting elementary particles. On the 1024 node Connection Machine-5 (CM-5) at Los Alamos National Laboratory, we are calculating the spectrum of light hadrons, scattering amplitudes and a variety of electroweak matrix elements. On the Cray C-90 at NERSC we are studying topology and calculating the kaon B-parameter, B_K. By working on a large lattice ($32 \times 32 \times 32 \times 64$), and collecting a large sample of gauge configurations, we are able to substantially reduce the statistical errors compared to previous work. The level of precision is such that, combined with existing and future experimental data on weak decays, these results are beginning to provide significant tests of the Standard Model of particle physics.

Our largest scale computations are on the CM-5. By coding the computationally intensive routines in CDPEAC, we attain node speeds of 80-100 MFlops, close to the theoretical maximum. For the production code, including i/o and communications, the sustained speed is 25-35 MFlops per node.

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1 Introduction

This document describes the recent results of the LANL collaboration, a group centered at Los Alamos National Laboratory. We have been carrying out large scale simulations of quantum chromodynamics (QCD) on the 1024 node Connection Machine-5 (CM-5) at the Advanced Computer Laboratory (ACL) at Los Alamos, and on the C-90 and other Cray machines at NERSC. The former work is as part of the QCD Grand Challenge Applications Group, a designation shared with the MILC collaboration, whose recent work is described here by Claude Bernard.

2 Scientific Objectives

QCD is a theory of quarks (up, down, strange, charm, bottom and top) interacting with gluons. The gluons bind the quarks into the strongly interacting particles, the hadrons, that we observe in nature. The binding is so strong that the quarks and gluons cannot be isolated as free particles but are observed only as bound states—this is the phenomenon of "confinement". The structure of the resulting hadrons is very complicated, and has not so far been amenable to study using analytic methods. In particular, low order perturbation theory is not useful, because the expansion parameter is of order unity. Non-perturbative techniques are required, and the only method available is to simulate the theory numerically, after discretizing space-time into a lattice. In our calculations, we use lattices of size up to $32^3 \times 64$, i.e. 32 points in the spatial directions and 64 in the (imaginary) time direction.

There are three major aims of our calculations. First, we wish to calculate the masses and other properties of the hadrons, in order to compare them to experimental results and test that QCD is indeed the correct theory. Because of various approximations that have to be made, this goal has yet to be attained. Second, we want to gain insight into the physics behind confinement. This might open up the possibility of semi-analytic calculations in QCD, or allow us to understand the behavior of other strongly coupled theories, such as technicolor or chiral theories. And, finally, we wish to use lattice methods to allow us to isolate the effects of QCD which obscure the underlying electroweak decays of hadrons. This work is the most advanced, and thus we explain the motivation for it in some detail.

In addition to feeling the strong force, through interactions with gluons, the quarks also interact through the weak and electromagnetic interactions, which form collectively the electroweak interactions. For example consider a D^- meson, composed of a d quark and an anti-c quark. This meson decays some of the time through the quark-level weak interaction process shown in Fig. 1: $\overline{c} \to \overline{s} e^- \overline{\nu}$. The theory of weak interactions predicts the decay rate of the quarks, up to an overall factor associated with the $\overline{c} W \overline{s}$ vertex, $|V_{cs}|^2$. Because the

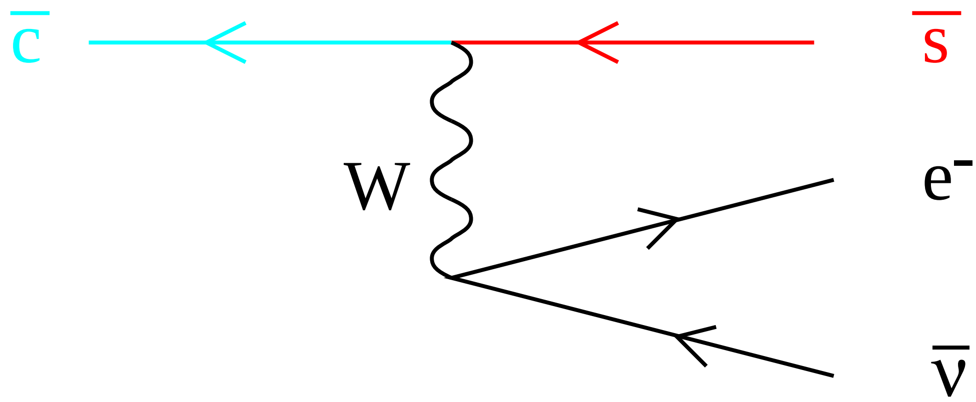

Figure 1: Feynman diagram for semi-leptonic weak decay of a quark.

quarks are confined into hadrons, however, the actual decay is, for example, $D^- \to K_0 e^- \overline{\nu}$, where the K_0 is a meson composed of an anti-s quark and a d quark. An example of the Feynman diagrams contributing to this decay is shown in Fig. 2. The binding of the quarks into mesons changes the decay rate, so that one cannot directly determine $|V_{cs}|^2$ from the experimentally observed rate of the decay process. In order to make the connection one needs to do a non-perturbative calculation of the so-called "semi-leptonic form factor", and it is for this that the lattice is required.

There are many examples of such "electroweak matrix elements" that are required to extract underlying parameters from existing, or future, experimental results. Researchers at Fermilab are studying the mixing and decays of K^0 mesons, and the future B-factory at SLAC will study many decays of the B mesons, which consist of a b-quark (or anti-quark) and a light anti-quark (or quark). Lattice calculations are required to interpret most of the experimental results. The hope is that we will be able to determine the parameters of the electroweak interactions (such as $|V_{cs}|^2$) in several ways, and thus test the theory in detail. Any discrepancies would indicated phenomena beyond the "Standard Model" of particle physics (SM).

3 Resources

For the 1993-4 fiscal year, we have been allocated 10% of the time on the CM-5 at LANL (6.1×10^6 node Megabyte hours per quarter), as part of the Grand Challenge Applications Group grant. In addition we share, with a group led by A. Soni, roughly 13000 SU's at NERSC on the C-90 and other Crays.

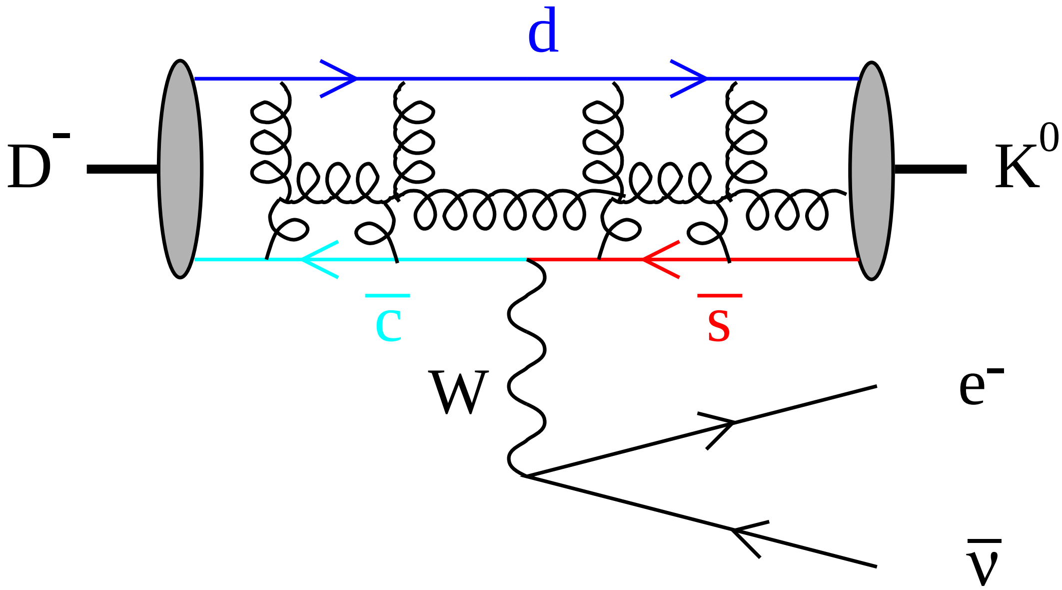

Figure 2: Feynman diagram for semi-leptonic weak decay of a meson.

4 Results from the CM-5

We proposed that, during the 1993-4 fiscal year, we would use the time on the CM-5 to generate about 100 lattices of size $32^3 \times 64$ at a coupling $\beta = 6$, and do a large scale analysis on them. This involves calculating quark propagators at five different masses, and then using these to extract hadron masses, decay constants, scattering amplitudes and various matrix elements. We are on target for completing this work, with about 80 lattices finished at present. In the following we present some highlights of our results for weak matrix elements. All results are preliminary.

The coupling constant $\beta = 6$ corresponds to a physical lattice spacing of about $a \approx 0.1 fm$, small enough that lattice artifacts are a relatively small correction to most quantities. We have previously undertaken exploratory studies at this lattice spacing on a sample of 35 small ($16^3 \times 40$) lattices, the major aim of which was the development of techniques [1]. In particular, we found that using extended ("smeared") sources we could significantly improve the signal to noise ratio. The idea is that mesons and baryons are extended objects, of typical size $0.5 - 1.0$fm, and so an operator which can efficiently create them should be of similar size.

The new calculations are in large part a production run using the methods we had developed. By working on a lattice having eight times the spatial volume, we (a) improve the signal, since this is almost equivalent to an eight-fold increase in statistics, (b) halve the minimum non-zero spatial momentum, since $p_{\min} = 2\pi/N_s a$, where N_s is the number of spatial points, and (c) allow the study of smaller quark masses. The latter improvement is very important since it allows more reliable extrapolations to the physical up and down quark masses. An additional improvement is that we are using about three times as many lattices (100 versus 35), which further decreases the statistical errors.

All our calculations are carried out in the so-called "quenched" approximation. Mesons and baryons contain, in addition to the "valence" quarks which determine the quantum numbers of the states, a complicated cloud of gluons and quark-antiquark pairs. In the quenched approximation the quark-antiquark component of this cloud is ignored. This approximation is made in order that the large systems can be studied with present computer resources: the cost of removing the approximation is roughly two to four orders of magnitude. Properties of hadrons that are not particularly dependent on the quark-antiquark component, for example the masses, decay constants, and form factors, will not be changed substantially by quenching. In some cases one can estimate the changes; for the masses they are in the 10-30% range [2]. Other properties are crucially dependent on the quark-antiquark component, are will be radically effected by quenching. Examples are the matrix elements of $\tilde{F}F$ discussed in Ref. [3].

Our aim in the calculations is to reduce other sources of error—statistics, finite lattice spacing, finite volume, extrapolation in quark masses—to the point where quenching is likely to be the dominant error.

4.1 Semileptonic form factors

Semileptonic decays of charmed mesons, such as that illustrated in Fig. 2, can be directly simulated on present lattices. The main decays of interest are

$$D \to \pi e\nu \; ; \quad D \to K e\nu \; ; \quad D \to \rho e\nu \; ; \quad D \to K^* e\nu \; . \tag{1}$$

These decays are amenable to lattice calculations as they only involve a single strongly interacting particle in both initial and final states. The unknown part of the decay amplitude is a matrix element such as

$$\langle K^*(p')|J^\mu(q)|D(p)\rangle \; . \tag{2}$$

$q = p - p'$ is the four-momentum carried by the weak current J^μ, and is the sum of the momenta of the e and ν in the actual decay. If we could calculate these matrix elements from first principles, for the physical range of q, then we could predict all aspects of the decay process in terms of a single unknown constant, the appropriate weak coupling constant for the underlying quark decay. This element is V_{cd} for $D \to (\rho,\pi)e\nu$ and V_{cs} for $D \to K^{(*)}e\nu$.

In fact, within the standard model, if there are only three generations, we can use other results to predict V_{cd} and V_{cs} to good accuracy. The lattice calculations thus allow a test of the consistency of the SM. In addition, experiments have not yet fully measured all aspects of the angular distribution of the decays, allowing the opportunity for lattice calculations to predict these distributions.

In practice, lattice calculations cannot access the full physical range of q. Instead they work in a small range of q^2 around zero, and assume pole-dominance to extrapolate to larger q^2. This restriction arises because the lattice results have small errors only for small spatial momenta. In our calculations we set $\vec{p} = \vec{0}$, while $\vec{q}/(2\pi/N_s) = (0,0,0)$, $(1,0,0)$, $(1,1,0)$, $(1,1,1)$ and $(2,0,0)$, where N_s is the number of spatial lattice points. Using a larger N_s decreases the step size in $\vec{q}$, and thus increases the number of usable momenta.

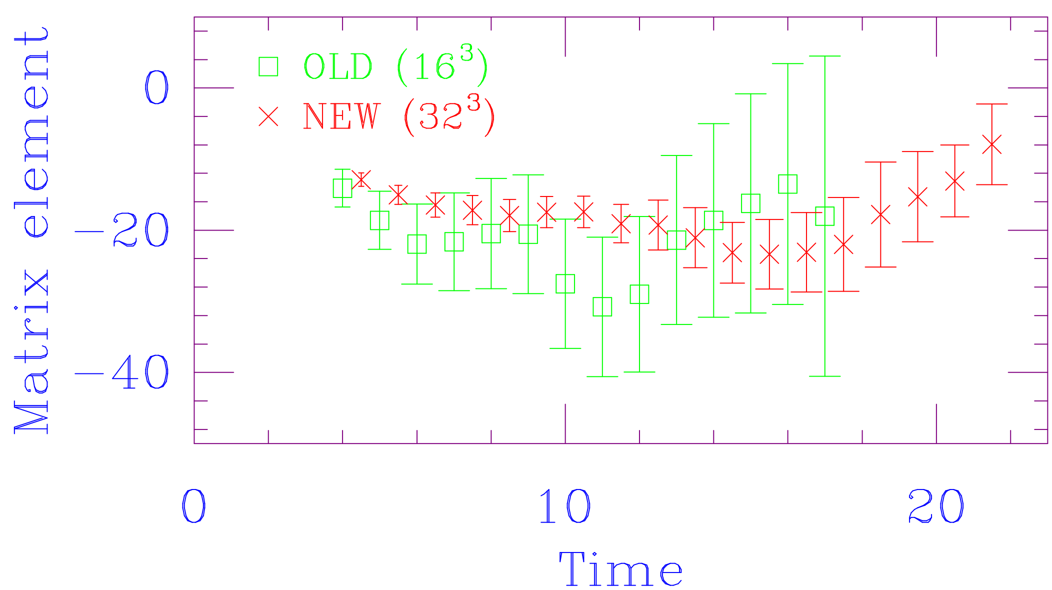

Figure 3: Comparison of new and old results for a semi-leptonic form factor.

To give an indication of the improvement in quality of the results that we have achieved with our new simulations, we compare to our old data on $16^3 \times 40$ lattices in Fig. 3. In the plot, the lattice kaon is created at $t = 0$, propagates to the Euclidean time t, where it is converted by the weak current J_μ into a D-meson, which propagates to time $t = 25$ (31) for the new (old) data. We have divided by two-point correlators in such a way that the signal should have constant magnitude. The matrix element is for the spatial part of the vector current, $J = V_i$, inserting momentum $\vec{q} = (2\pi/16, 0, 0)$. We have adjusted the overall scales so that the size of the errors can be directly compared, and we see that there has been both a substantial reduction in the errors, and a lengthening of the "plateau" region.

We have done a preliminary analysis of 50 of the new lattices. We find, for example, that

$$f_+^{D\to Ke\nu}(q^2=0) \;=\; 0.81 \pm 0.03 \pm 0.03 \ . \tag{3}$$

The first error is statistical, the second the systematic error due to extrapolation to the physical light quark masses. This form factor governs the rate for $D \to Ke\nu$ decay. The experimental result for this decay, together with the value of $|V_{cs}|$ required for consistency of the three generation SM, implies $f_+(0) = 0.77 \pm 0.04$ [4]. Typical previous lattice results are 0.65 ± 0.18 [5] and $0.90 \pm 0.08 \pm 0.21$ [6]. We see that that the errors have been substantially reduced, and are now at the point where discrepancies with the SM could appear.

The most likely source of any such discrepancy is our use of the quenched approximation. Turning this around, we can see that, for this quantity, the quenched approximation is apparently reliable to $\sim 10\%$. Assuming this accuracy applies to other form factors, we can make predictions. In particular, in the decay $D \to K^* e\nu$, we find

$$\frac{A_2(0)}{A_1(0)} = 0.93 \pm 0.27 \pm 0.09 \ . \tag{4}$$

This should compared to the previous results 0.7 ± 0.4 [5] and $0.70 \pm 0.16^{+0.20}_{-0.15}$ [6]. One early experiment found a ratio consistent with zero (with large errors), whereas the latest result is $0.82 \pm 0.23 \pm 0.11$.

5 Results from NERSC

We have used the Cray-2's and the C-90 extensively for the last several years. While slower than the CM-5, these machines have the advantages of stability, user-friendliness, and large storage capacity. We have collected a large database of lattices and quark propagators using which we have repeated calculations with refined methods, and tested new techniques.

5.1 The kaon B-parameter B_K

The most significant result to emerge from our work at NERSC is that for the kaon B-parameter

$$B_K(a) = \frac{\langle \overline{K} | \bar{s}\gamma_\mu(1+\gamma_5)d \ \bar{s}\gamma_\mu(1+\gamma_5)d | K\rangle}{\frac{8}{3}\langle \overline{K} | \bar{s}\gamma_\mu\gamma_5 d|0\rangle\langle 0|\bar{s}\gamma_\mu\gamma_5 d|K\rangle} \ . \tag{5}$$

Knowledge of this quantity is essential to extract a value for V_{td} (the coupling of the W-boson to the t and d quarks) from the experimentally measured CP-violating part of the $K_0 - \bar{K}_0$ mixing amplitude, and the lattice offers the only first principles method of calculation.

We have gradually learned to control the systematic errors in the calculation of B_K, using a combination of theoretical analysis and numerical improvements. Our result for the scale invariant B-parameter is [7]

$$\widehat{B}_K = 0.825 \pm 0.027(\text{stat.}) \pm 0.025(\text{syst.}) \ . \tag{6}$$

The systematic error does not include that due to quenching, or our use of degenerate quarks, but there is evidence that the additional errors are not larger than the quoted errors. B_K is thus one of the most reliably determined lattice quantities, and, furthermore, the lattice determination is more accurate than those using other methods. This result is now being used in analyses of the constraints on the consistency of the standard model.

5.2 Topology

In our most recent work at NERSC we have been studying the topological charge and the distribution of charge density on our gauge configurations. Our overall aim is to gain insight into the role of instantons in the physics of confinement, and in particular to make detailed comparisons with the instanton liquid model of Shuryak. Previous studies have used various definitions of the density, and we have undertaken a careful comparison of these methods, paying particular attention to numerical difficulties [8].

6 Computational issues

The most computationally challenging part of our work is that on the CM-5. Lattice QCD is naturally parallel, since the same operations must be performed at each space-time point. These operations involve exchanging information with adjacent sites on the hypertorus, and performing computations at each site (e.g. 3×3 complex matrix multiplies). Our basic code is written in CM-Fortran (CMF), including the communication, which is done using the command CSHIFT. To use the machine efficiently, we have found it necessary to write the computationally intensive on-node routines in the C-like assembly language CDPEAC. With the present compiler this gives speed ups of $1.5 - 3$. This arrangement also makes our code quickly adaptable to new versions of the Connection Machine, since the small modules can be developed quickly for a new processor.

Our CDPEAC codes sustain node speeds of between 80 and 100 MFlops, the latter being close to the theoretical maximum, as long as the particular computation allows chaining of adds and multiplies. The overall speed of our codes is significantly slower, mainly because of necessary internode communication. Our gauge update code sustains 25 MFlops/node. For a $32^3 \times 64$ lattice it requires 3 GigaBytes of memory, and thus runs on partitions of 256 nodes or larger. On a 256 node partition it takes 9 hours to generate an independent lattice (2000 overrelaxed and 400 Metropolis sweeps). Our propagator code for Wilson fermions requires 6 GigaBytes of memory, and sustains a node speed of 35 MFlops on a 256 node partition. It takes 16 hours to calculate propagators at 5 different masses with and without a meson source. Finally, we need to combine the propagators into the various meson correlators we use to extract masses, form factors, etc. This code spends roughly 60% of its time doing i/o from the 25 GigaBytes of data (lattices and propagators) stored on the scalable disk array. It requires the equivalent of 16 hours on a 256 node partition, although in practice we use five separate runs, two of which require a 512 node partition.

We save the configurations and the three light quark propagators on exabyte tapes, so that as we develop further analysis ideas we can test them out with relatively small cost in computer time.

Our code is very demanding of the CM-5. On various occasions it has found problems which the standard diagnostics did not uncover. In a recent example, the machine was reporting single bit memory errors, which should have been corrected in hardware, but which were causing our code to crash unreproducibly. This suggested an intermittent hardware problem. Further investigation by Thinking Machines Corporation led to the discovery of memory errors related to fluctuations in voltage and temperature. An overhaul of the entire CM-5 will be undertaken in July 1994 to correct this problem. Parts of our code are now used as diagnostics by TMC.

7 Future Plans

In the remainder of this fiscal year, we intend to complete the analysis on our proposed sample of 100 lattices at $\beta = 6.0$. We have only mentioned the highlights above—we are calculating a large number of quantities, and in all almost all cases have better statistical control than that of previous calculations.

We propose to extend this work in fiscal year 1994-5 in several ways:

- Reduce lattice spacing errors either by using a smaller lattice spacing or an improved action.
- Include non-relativistic quarks so as to directly study B mesons.

- Implement staggered fermions.

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