RECENT PROGRESS ON LATTICE QCD WITH MIMD PARALLEL COMPUTERS[1]

The MILC Collaboration[2]

ABSTRACT

We describe recent progress in numerical computations of the properties of strongly interacting elementary particles. On the 512 node Intel Paragon at Oak Ridge National Laboratory, we are calculating the parameter "f_B," which is needed in order to extract weak interaction properties of the B meson. We are also studying the "deconfining" phase transition, the thermodynamics of the quark-gluon plasma, and the spectrum and wave functions of hadrons at low energy.

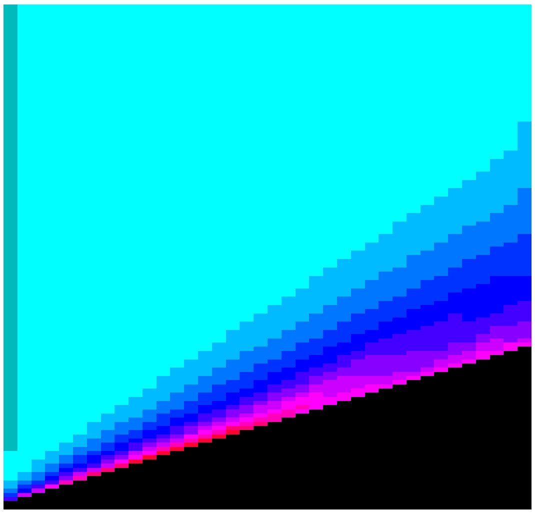

Figure 1: Convergence of the "effective mass" of the lattice B meson propagator in the hopping expansion. The x axis is time, the y axis is iteration number. The y-independence at the top of the figure indicates convergence of the algorithm; the x-independence, that a pure B meson has been extracted. ($24^3 \times 80$ lattice, $\beta = 6.3$)

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The theory which describes the strong force between quarks and between nucleons is Quantum Chromodynamics (QCD). Because the QCD coupling is large at low energy, there is no natural small parameter in which to expand, and the theory must be treated nonperturbatively. Large scale numerical simulations, using the techniques of lattice gauge theory, provide the only known method to compute from first principles the properties of quark bound states (hadrons). Fig. 2, for example, shows the wave function of the rho meson, obtained from such a simulation by our collaboration.

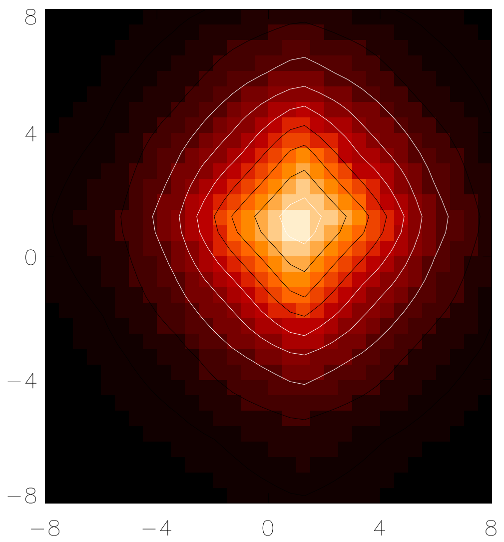

Figure 2: The wavefunction as a function of the separation between the quark and the antiquark in a rho meson. The simulation is on a $16^3 \times 24$ lattice at $\beta = 5.445$, with dynamical quarks of mass $ma = .025$.

QCD computations are also crucial to the study of the weak interactions. In order to use the hard-won experimental information on hadronic weak interactions to test the "Standard Model" of particle physics at its most vulnerable points, one needs to remove the QCD effects. In particular, the elements of the so-called "CKM matrix" can only be determined if certain hadronic parameters are computed in QCD.

One such parameter is the decay constant of the B meson, "f_B." If f_B is known, the experimental measurement of the mixing of B and $\bar{B}$ mesons can be used to fix the CKM element V_{td}. A major goal of our DOE Grand Challenge Applications Group is the determination of f_B (and related constants f_{B_s}, f_D, and f_{D_s}) from lattice QCD.

Another interesting aspect of QCD is that it predicts a transition between ordinary strongly interacting hadronic matter and a high temperature quark–gluon plasma. A quantitative understanding of this transition is important for interpreting heavy ion collision experiments presently being planned by nuclear physicists for facilities such as the Relativistic Heavy Ion Collider. We are studying the transition and the properties of the high temperature phase with lattice QCD simulations.

Lattice gauge theory is widely recognized as one of the grand challenges of high performance computing. The new generation of massively parallel computers offers the possibility of making significant progress in this field. The MILC (MIMD Lattice Computations) Collaboration has been awarded Grand Challenge time on the Intel Paragons at the Center for Computational Sciences (CCS) at Oak Ridge National Laboratory (ORNL); we began the development of MIMD code for the study of lattice gauge theory under an earlier grant. This MIMD code is highly portable, running on a large number of parallel machines, but is specially tuned for the Intel line of parallel computers.

By the time we obtained access to the 66 node Paragon XPS5 at ORNL in May, 1993, we had already ported our code and developed the specialized software needed to carry out the first large project planned for ORNL using Paragons at the San Diego Supercomputer Center (SDSC) and Indiana University. Our codes provide stress tests of all key features of parallel computers: integer and floating-point operations, inter-node communications, and I/O. We were able to uncover several problems with the Intel iPSC/860 and Intel Paragon which had not been detected by Intel diagnostic software or by other users. For example, we recently helped Intel to identify a bug in the Paragon's global sum routine under version R1.1 of the operating system. Large sections of our code are being incorporated in standard Intel diagnostic software.

The MILC Collaboration consists of a group of geographically distributed physicists with a broad range of research interests. We felt it important to design a flexible computing environment in which collaboration members could easily develop and test new ideas and new algorithms, focusing their attention on the science while using the computing resources efficiently. We have developed a portable, flexible MIMD code. It is designed especially for the Intel machines, but it runs efficiently on a large number of parallel machines, including the Intel iPSC/860 and Paragon, the nCUBE 2, the Connection Machine CM-5, the Cray T3D, the IBM SP1, clusters of RS6000/560 and DEC ALPHA workstations running under PVM, and uniprocessor computers. Table 1 shows some benchmarks for our code.

The bulk of our code is written in C. All of the physical variables associated with a lattice site are stored together in a single structure. This organization of the data is advantageous for a processor with a data cache, such as the Intel i860. Pointers to the structures at neighboring sites and pointers set by the communications routines are stored in separate lists. This turns out to optimize the cache hits since these lists are usually scanned sequentially.

Our calculations are carried out on four dimensional space-time lattices. It is natural to divide the computation among the processors by assigning each of them a piece of the lattice.

Machine	Nodes	Lattice Size	MF per node
Intel iPSC/860	1	$8^3 \times 4$	24.0
	64	$16^2 \times 32^2$	17.8
Intel Paragon	1	8^4	27.7
OSF/1	64	$16^2 \times 32^2$	21.2
	256	32^4	19.0
Intel Paragon	1	8^4	29.5
SUNMOS	64	$16^2 \times 32^2$	25.1
	256	$32^3 \times 64$	25.3
	1024	32×64^3	24.4
CM5 (Conjugate gradient)	128	$24^3 \times 12$	40.0
CM5 (Full code)	128	$24^3 \times 12$	22.5
Cray T3D	1	8^4	26.9
	64	$16^2 \times 32^2$	20.5
IBM SP1/MPLp	1	$12^3 \times 6$	30.0
	8	$12^3 \times 6$	20.0
nCUBE-2	1	$8^3 \times 4$	1.2
	128	$16^3 \times 32$	0.9
RS6000/560 Cluster (PVM)	1	$8^3 \times 20$	26.0
	4	$8^3 \times 20$	12.0
Alpha 500 Cluster	1	8^4	23.0
(Gigaswitch)	2	$8^3 \times 16$	16.0

Table 1: MIMD QCD code performance in Megaflops (MF) per node.

In thinking about the computation we imagine that computing is done at each lattice site by whichever processor is in charge of that site. To calculate the updated value of a field at a site we need to know the variables at other lattice sites. In thinking about the physics we do not want to worry about whether these other lattice sites are on the same processor as the variable we are updating. Our solution is to hide the details of accessing variables. This is feasible because of the simplifying features of the access to variables at other lattice sites in QCD simulations: they are homogeneous, mostly local and predictable.

All of the routines which involve internode communications, as well as various "housekeeping" routines such as the function that returns the node number of a processor, are isolated in one file. A different version of this file exists for each of the computers on which our code runs.

We have done extensive production work with this code on the Intel iPSC/860 and Paragon, the Thinking Machines CM-5, and the Cray T3D. We have made an effort to optimize our code for these machines. In the case of the iPSC/860, Paragon and CM-5 this has meant writing selected subroutines in assembler language, and in the case of the T3D, rewriting some of the assembler output of the compiler. We have put the largest effort into the Intel machines.

We have been disappointed in the performance and stability of the ORNL Paragon, but both appear to be improving. Up to now the instability of the machine has severely hampered our ability, and that of other users, to make progress on our research. Under the OSF/1 operating system with which we are carrying out our production runs, it is only very recently that we have obtained performance significantly better (23%) than that of the iPSC/860.

The i860 chips that are supposed to be dedicated to communications have only just been made functional in latest update to the OSF/1 operating system. This update is not yet running reliably; however, as expected, it has significantly improved the performance of our code.

Finally, our work has been hampered by the lack of an archival storage system at ORNL. Much of the time, lattice configurations have had to be moved over the Internet and stored on tape at our workstations. An archival system has very recently been brought up at ORNL. Our lives should now become a lot easier, and we may be able to expand our project to do significantly more physics without an increase in the "CPU" time required.

We obtained access to the 512 node Paragon XPS35 at the end of November, 1993, and immediately began work on a calculation of heavy-light meson decay constants, in particular, f_B. (A "heavy-light meson" has one heavy quark, such as a b, and one light quark, such as a d.) In the first stage of this project, we are working on $24^3 \times 80$ lattices, which means that 319 Mbytes data sets (gauge configurations) must be read into and out of memory at the beginning and end of each run. An even more daunting I/O problem was posed by the larger size (1.27 Gbytes) of the quark propagators. The only solution was to make use of the "hopping parameter" computation of the heavy quark propagator [1], which allows the calculations to be done "on the fly." One first computes the light quark propagator, and then uses an iterative scheme to compute the heavy quark propagator. At each order in the latter computation, "meson" propagators are formed and stored. Later on, the terms can be put together (assuming the scheme converges) to form a meson with arbitrary heavy-quark mass.

Fig. 1 shows the convergence of the hopping algorithm. The colors show different ranges of the "effective mass" (m_{eff}) of a lattice B meson as a function of time from the source (x axis) and iteration number (y axis). Since the algorithm is local, it takes proportionately more iterations for the points further from the source to begin to be updated; this explains the black triangle at the bottom of the picture. A converged m_{eff} which is independent of time is an indication that a pure lattice B mesons has been extracted: the higher energy excitations of the state have died away. This is the case at top of the picture (with the exception of small times at the left).

The effective mass of the lattice B meson after convergence is shown more precisely in Fig. 3. Note that, in the current work, m_{eff} is approximately constant from time $t = 3$ through time $t = 36$. This is a very large region of pure B meson propagation: indeed the propagator falls like a pure exponential over more than 15 decades! (The increase in m_{eff} near $t = 40$ is just the result of periodic boundary conditions on our length 80 lattice.) Where m_{eff} is constant in both the new and old [2] work, the results agree. However, the much poorer sources and larger boundary effects in Ref. [2] led to a much smaller region of constant m_{eff} and therefore considerably larger systematic errors associated with extracting f_B.

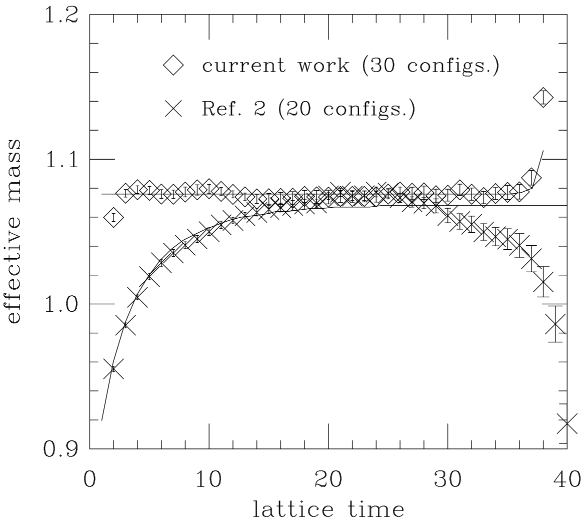

Figure 3: The effective mass of the lattice B meson propagator *vs.* time, for current and previous work. ($\beta = 6.3$, $\kappa_{\text{heavy}} = .117$, $\kappa_{\text{light}} = .149$. Current: $24^3 \times 80$ lattice; previous: $24^3 \times 55$.)

A preliminary result for the decay constant, f_P, of an arbitrary mass heavy-light meson is shown in Fig. 4. The mass of the meson is varied by adjusting the mass of the heavy quark in our simulation; the light quark mass has been extrapolated to the mass of the d or u quark. The decay constant of the B or D meson (f_B or f_D) can be easily determined from such a graph. A similar graph where the light quark has been extrapolated to the mass of the s quark can be used to determine f_{B_s} and f_{D_s}.

Our preliminary results from 40 configurations on a $24^3 \times 80$ lattice at $\beta = 6.3$ are:

$$\begin{aligned} f_B &= 174 \pm 7 \text{ MeV}; & f_D &= 204 \pm 5 \text{ MeV} \\ f_{B_s} &= 198 \pm 7 \text{ MeV}; & f_{D_s} &= 174 \pm 5 \text{ MeV} \end{aligned}$$

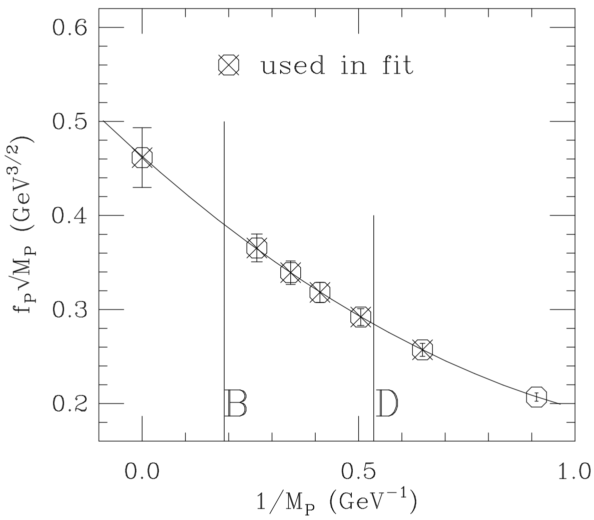

Figure 4: The decay constant, f_P, times $M_P^{\frac{1}{2}}$ as a function of $1/M_P$. M_P is the mass of the heavy-light meson. The values of $1/M_P$ for the B and D mesons are shown by the vertical lines. The point at $1/M_P = 0$ is obtained using the static approach of Eichten [3].
($\beta = 6.3$, $24^3 \times 80$ lattice, 40 configurations).

These results are consistent with those of [2], but the statistical errors are already considerably reduced. A total run of 200 configurations is planned, which should reduce the statistical errors by another factor of 2. In addition, the improved sources and the hopping parameter approach are expected, upon completion of the analysis, to diminish significantly several sources of systematic error. Planned runs on other lattices with different volumes and lattice spacings will reduce the most of the remaining sources of systematic error.

The above results represent about two-thirds of the running to date on the XPS35 Paragon at the Oak Ridge Center for Computational Sciences. Total running is about 2.6×10^5 node hours.

The study of QCD at high temperatures has been another one of the principal activities of our collaboration. Our objectives include determining the nature of the transition between ordinary matter and the high temperature quark-gluon plasma, calculating the temperature at which this transition occurs, and understanding the properties of the plasma. In a project presently in progress we are studying Kogut-Susskind quarks on $24^3 \times 12$ lattices. The lattice spacing in this work is approximately a factor of 1.5 smaller than in any previous high temperature studies that we are aware of. It should bring us to the edge of, if not into, the perturbative scaling region from which continuum results can be extracted. Our first step is to determine the position of the transition. In Fig. 5 we show a preliminary plot of the real part of the Polykov loop as a function of the gauge coupling constant for a quark mass of 0.008 in lattice units. Clearly the crossover is in the vicinity of $6/g^2 = 5.725$. Work is in progress to refine this result, to study other quark masses, and to determine detailed properties of the high temperature regime. In this project we are making use of both a TMC CM5 and a Cray T3D, showing the advantage of portable code.

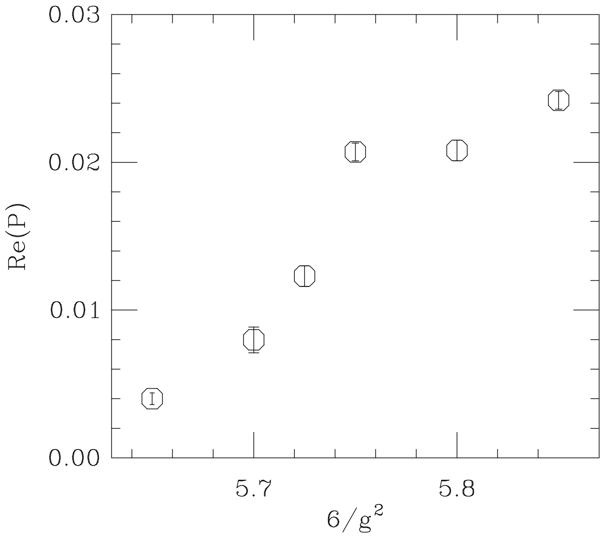

Figure 5: The real part of the Polykov loop *vs.* $6/g^2$ on a $24^3 \times 12$ lattice. Temperature increases to the right.

We have recently completed an extensive series of studies of high temperature QCD using Wilson quarks. Our primary objectives in this work were to understand the phase structure, which turns out to be richer than that for Kogut-Susskind quarks, and to see whether there are indications that the two formulations of lattice quarks yield the same continuum limit. These calculations were very computationally intensive, and once again we spread them over a variety of machines including the CM5, the iPSC/860, and the ORNL Paragon XPS5.

A subset of the MILC collaboration has begun a project to compute the equation of state, or energy and pressure versus temperature, of QCD with two light flavors of quarks. A knowledge of the equation of state is important to understanding the dynamics of the expansion and cooling of the "fireball" produced in a high energy collision of heavy ions. In Fig. 6 we show the pressure as a function of gauge coupling. Work on this project is being carried out on Paragons including the ORNL XPS5, a Cray T3D, and an Alpha cluster.

References

[1] D. Henty and R. Kenway, Phys. Lett. **B289** (1992) 109.

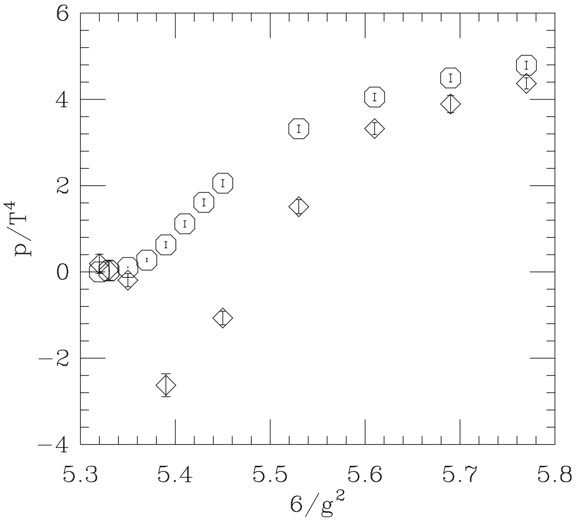

Figure 6: Pressure of QCD *vs.* $6/g^2$ for two flavors of quarks of mass 0.1 in lattice units and $N_t = 4$. The octagons are the nonperturbative results from the present study, while the diamonds are the results from operator averages and perturbative calculations.

[2] C. Bernard, J. Labrenz, and A. Soni, Phys. Rev. **D49** (1994) 2536; Nucl. Phys. B (Proc. Suppl.) **30** (1992) 465; Nucl. Phys. B (Proc. Suppl.) **26** (1992) 384.

[3] E. Eichten, Nucl. Phys. B (Proc. Suppl.) **4** (1988) 170.