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PROGRESS REPORT OF A RESEARCH PROGRAM
IN COMPUTATIONAL PHYSICS

Task D
Progress Report
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ABSTRACT

Task D's research is focused on the understanding of elementary particle physics through the techniques of quantum field theory. We make intensive use of computers to aid our research. During the last year we have made significant progress in understanding the weak interactions through the use of Monte Carlo methods as applied to the equations of quenched lattice QCD. We have launched a program to understand full (not quenched) lattice QCD on relatively large lattices using massively parallel computers. Because of our awareness that Monte Carlo methods might not be able to give a good solution to field theories with the computer power likely to be available to us for the foreseeable future we have launched an entirely different numerical approach to study these problems. This "Source Galerkin" method is based on an algebraic approach to the field theoretic equations of motion and is (somewhat) related to variational and finite element techniques applied to a source rather than a coordinate space. The results for relatively simple problems are sensationally good. In particular, fermions can be treated in a way which allows them to retain their status as independent dynamical entities in the theory.

Progress Report for a Research Program in Computational Physics

General

Task D supports two physicists at Brown University: Professor Gerald Guralnik and Research Assistant Professor Gregory Kilcup, who work in the area of lattice gauge theory. This work has been going on for several years and has encompassed many aspects of the field, including algorithms, machines, theoretical studies and large scale simulations. We also have two graduate students: Santiago Garcia and John Lawson who have, until now, been supported by the Physics Department. This last year we made progress in the following areas: studies of QCD including the effects of dynamical fermions, large scale simulations (in particular the calculation of matrix elements for hadronic weak interactions), and in new algorithms. We describe these in turn.

The Weak Interaction Matrix Element Grand Challenge

The payoff from studying lattice QCD will be more than merely showing that QCD is the correct theory of the strong interactions. Once we are satisfied that the lattice gives a reasonable picture of hadrons, we can compute the strong interaction corrections to weak processes, which then allows us to test the whole standard model. One of the most promising systems to study is the weak decay $K \rightarrow \pi\pi$, where we can ask (1) do strong interaction corrections give an adequate account of the $\Delta I = \frac{1}{2}$ rule, and (2) how much CP violation does the standard model predict? Another quantity we would like to know is the kaon B parameter, which give the strength of the $K \leftrightarrow \bar{K}$ transition.

For the past two years, Kilcup (together with Sharpe, Gupta, Bernard and Soni) has been granted a large chunk of computer time (about 8000 hours per year on the Cray-2's at NERSC) to pursue these questions, under the DOE's "Grand Challenge" Program. In the first phase of the project, we generated two sets of quenched lattices ($16^3 \times 40$ and $24^3 \times 40$), which are then analyzed using Wilson fermions and staggered fermions. Having two lattice sizes enabled us to make a direct comparison and study finite volume effects on the matrix elements. Kilcup worked on the staggered fermions part of the calculation, the first results from which were published in Ref. [1]. The results have been superb, in that we now know the kaon B parameter (at a certain scale, and within the quenched approximation), with only a couple of percent statistical error, and no discernible finite volume error. Results for other matrix elements (such as the ones relevant for ϵ'/ϵ) have not been formally published, but have been presented in several talks, e.g. Refs. [2] and [3].

The remaining systematic errors in the matrix element program are due to (1) the finite lattice spacing, and (2) the quenched approximation. Accordingly, we have begun two new runs this year.

One run addresses issue (1) by using a $32^3 \times 48$ quenched lattice, with half the lattice spacing of the older $16^3 \times 40$ system. This is the largest system run anywhere to date, and has once again involved substantially rewriting our programs to make everything fit into the memory of the Cray-2. The results will enable us to compare systems with similar physical volumes and look for finite lattice spacing effects. The first phase of this project should be completed by the fall of 1990.

The effort to address issue (2) involves major assistance from the Columbia lattice group (Norman Christ, Frank Brown and others), who have built themselves the world's fastest QCD computer. The Columbia machine has a relatively small memory considering its power, and though it is well suited to generating gauge configurations including dynamical fermions, it would be hard for them to do weak interaction matrix elements. The Columbia group is therefore making their gauge configurations available to Kilcup, who then analyzes them on the Cray-2's at NERSC. The first results indicate that quenching is not such a bad approximation after all, being at most a 10% effect for the kaon B parameter.

Kilcup has also taken some time this year to write some more generally accessible articles describing the physics which is being done in the Grand Challenge. These are listed as Refs. [4], [5] and [6].

QCD with Dynamical Fermions

One of the biggest obstacles to doing fully realistic simulations in lattice QCD is the problem of going beyond the quenched approximation and including dynamical fermion loops. The computer power available has now increased to the point where one can begin to simulate moderate size systems. In particular this past year saw the placement of Thinking Machines Inc.'s CM-2 computers at several sites across the country. Kilcup was part of the first group to implement a QCD code on the CM-2, which has then been in a good position to use the newly installed machines. Using time on machines at Los Alamos, Syracuse, Argonne and at Thinking Machines itself, we have begun production running of systems of size 16^4 with dynamical Wilson fermions. The algorithm used was Hybrid Monte Carlo, with the refinements we described in Ref. [7]. The first physics results from these CM-2 runs were presented at the APS meeting in Houston [8], and as a first step we were able to confirm some results obtained by other groups using the uncorrected Langevin algorithm. We are continuing these production runs, and have drafted a longer paper giving the first results for the QCD spectrum.

Source Galerkin Method

The above discussion suggests how difficult it is to extract physics results through numerical techniques. That some success has been achieved reflects our persistence and the vast amount of the existing research allocated computational resources that have been dedicated to Lattice QCD. Despite the hard reality, the solution of a path integral representation of a quantum field theory by Monte Carlo integration is in principle a straightforward procedure. One develops a sampling technique to find contributions from the most significant regions of integration and repeatedly applies this procedure to obtain an approximation to the exact answer. In practice the problem is so difficult because the systems considered must have a huge number of degrees of freedom if they are to correspond to the physical world and the iteration number must be correspondingly large in order to get a reasonable approximation to the exact answer. Fermions add immense additional complication and computational demand. They are represented in the path integral through integrals over exponentials involving anti - commuting objects. It is not known how to develop an appropriate sampling technique involving such non-numeric objects. Consequently fermions are dealt with by modifying (if need be) the action to make it bilinear in the fermi fields and then using an ansatz which makes it possible to explicitly integrate out fermionic degrees of freedom in the path integrals of such actions. After this procedure, it is possible to perform Monte Carlo integrations on the remaining integrand. This has become very complicated in structure because it now contains the infamous fermion determinant. The determinant contains all information about the fermionic interactions and involves every site on the lattice so for this object the nearest neighbor interaction structure of the original action is concealed. Most of the effort in lattice gauge theories has been associated with dealing with the vast computational power needs imposed by the situation outlined above.

The Monte Carlo method was the first serious attempt to numerically solve quantum field theory. This method, while powerful, has no intrinsic subtlety. In particular very little of the symmetry of space - time is exploited in even the most sophisticated analysis that currently exists. It seems very likely that there is the possibility for basic algorithmic improvement. Guralnik, with his students, has devoted his entire effort during the past year to developing an alternative to the Monte Carlo techniques. It is emphasized that the method he has constructed is entirely different in philosophy and execution from all existing numerical techniques in quantum field theory and quantum mechanics. It is (somewhat) related to variational and finite element techniques of other disciplines. It has zero relationship to any previous method which has been associated with finite elements in quantum field theory. The analysis begins by deriving the space time lattice differential equations for the quantum field theory under consideration. The vacuum expectation value of these equations is evaluated in the presence of appropriate external sources. These exact

equations are then approximated by a truncated Taylor series expansion in the complete set of sources (one to several at each point of space time depending on the number of field degrees of freedom). While the truncation is an approximation, it makes sense since the final results are to be calculated in the limit of vanishing external sources. The truncation corresponds to neglecting the effect of high order fluctuations in the theory. Note that it is in general possible to choose sources so as to make this truncation appropriately respect any symmetries the theory might process. This process has nothing to do with the space time structure of the theory which is entirely specified by the initial choice of space time lattice. The resulting equations have a high degree of symmetry because of the translational invariance of the underlying periodic lattice as well as reflection symmetries associated with this structure. This greatly reduces the number of equations to be considered. In addition, a further remarkable symmetry between lattices of different size is apparent because of the nearest neighbor interaction. Indeed, any point on the lattice satisfies the same differential equation as the corresponding point on a larger lattice. Differences in the solutions correspond to changes in the boundary conditions imposed by the periodicity length of the lattice. This is sort of generalized renormalization group behavior. The next problem is to solve these equations. If they are regarded as given algebraic equations in the usual sense they are, not surprisingly, inconsistent as they are approximations. Any solution technique must be consistent with the approximation. The method chosen is to generate a set of independent polynomials in the sources by any number of methods. These methods can take into account the symmetries of the problem or simply follow from identifying the appropriate coefficients of the source derivatives of the vacuum functional associated with the truncation approximation. The results produced by any choice are identical to the accuracy of the approximation. The equations are multiplied by each independent member of this polynomial set with the process stopping after the number of new equations generated is equal to the number of unknowns contained in this set. The new equations are integrated (this is easy because only polynomials in the sources appear) over a range of values of each source which includes the zero value. The resulting linear equations are then solved for the unknown coefficients in terms of ranges of integration. Finally, the limit of vanishing range of integration is taken to obtain the coefficients of the truncated series. This limit must be taken with care since the matrix that is inverted is singular in the limit of zero integration length because of the effect of disconnected graphs. There are some beautiful subtleties of boundary conditions which turn out to work automatically. That these are obeyed insure that the solutions obtained from the differential equations correspond to the evaluation of the path integral formulation of the theory. These boundary conditions might not be the ones of physical interest but to our knowledge are the ones always used in physics.

We have explicitly applied this method to three problems at this stage (unpublished-a preprint will be released in the fall):

Free scalar field theory - any dimension space time - arbitrary lattice size

The free scalar field has the same space time symmetry structure as the interacting cases and consequently is very informative about these cases. The results obtained are exact. The convergence is essentially instant so the computer time required is negligible. Consequently, convergence and accuracy are much better than in the Monte Carlo case. The computer time is vastly less but the time required to set up the problem for the computer (getting the algebra straight) is considerable. To obtain arbitrary size lattices requires doing more pure algebra than is possible with an interacting theory.

Quartic interacting scalar field theory - one dimension (anharmonic oscillator)- current maximum lattice length 24

This case and a corresponding zero dimensional case have been studied in great detail. The many energy eigenvalues obtained are extremely accurate and the computer time required is negligible (after spending an embarrassingly large number of Cray hours getting it right). The size of the lattice will be increased many fold latter this summer by application of multiple element methods which we have just understood. The algebra gets very cumbersome and too near the machines limit for larger single element calculations. Round-off errors become a problem even with 64 bit precision. There is no intrinsic problem in considering four dimensional scalar field theory. Very little additional difficulty is involved. We have limited our studies until now to one dimension in order to take advantage of the vast collection of information available on the behavior of the anharmonic oscillator.

Free two dimensional spin "spin 1/2" fermi field theory - arbitrary lattice size

What is particularly interesting about this case is that in Monte Carlo methods there is no such thing as a free fermi field calculation. This is because the integrations of Grassman algebra variables can not be handled by Monte Carlo. This is not an issue for us and if anything free fermi fields are simpler (aside from the usual "doubling problems" as compared to the continuum) than free bosons. Because of this, we can treat bosons and fermions relatively symmetrically and are not forced to solve the fermi problem exactly and then subject the remaining boson problem to a Monte Carlo treatment. We believe this will result in considerable time savings at increased accuracy for "real" problems.

We believe that the results to date make the Source Galerkin Method a possible candidate to replace the current Monte Carlo methods. The next year should verify or refute this possibility.

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