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SUPERCOMPUTERS AND QUANTUM FIELD THEORY

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ABSTRACT

I review why recent simulations of lattice gauge theories have resulted in substantial demands from particle theorists for supercomputer time. These calculations have yielded first principle results on non-perturbative aspects of the strong interactions. An algorithm for simulating dynamical quark fields is discussed.

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In the last few years particle theorists have become extensive users of supercomputers. Although theorists have traditionally used computers for diverse tasks from algebraic manipulation to numerical evaluation of Feynman integrals, the total amount of computer time involved was usually rather small. This has changed markedly with the application of Monte Carlo simulation to lattice gauge theory.

The most dramatic consequence of these calculations has been rather convincing numerical evidence that the standard Yang-Mills theory of the strong interactions can simultaneously display quark confinement and asymptotic freedom. Calculations are now concentrating on first principles calculations of hadronic properties.

These simulations use the lattice formulation of gauge theory as a nonperturbative cutoff scheme. Unlike most conventional procedures for removing field theoretical divergences, the lattice prescription is applied at the outset, and the theory becomes a well defined mathematical system before any further approximations. The lattice is, however, only a mathematical trick, and an extrapolation to the continuum limit of vanishing lattice spacing is a necessary precursor to the extraction of physical results.

Let me begin this talk with a brief review of Wilson's rather elegant formulation of gauge fields on a lattice[1]. His approach is based on the concept of a gauge theory as a theory of phases. When an electron travels along some world line in space-time, its interaction with the electromagnetic field can be described in terms of its wave function acquiring a phase given by the exponential of the integral of the vector potential along its path C

$$\psi \to \psi \exp\left(i\, e \int_C A_\mu \, dx_\mu\right) \tag{1}$$

This phase is easily understood in the rest frame, where the frequency or energy of the electron is increased by the product of the scalar potential and the electron charge. Equation (1) just generalizes this to an arbitrary Lorentz frame.

To formulate this idea on a lattice, we replace continuous world lines with sequences of discrete steps between nearest neighbor sites on a hypercubic lattice. The fundamental gauge variables become phase factors associated with each of the bonds connecting nearest neighbor sites. A particularly nice feature of this formulation is the generalization to a non-Abelian theory; the phases are just replaced with matrices in the appropriate group. Thus, for the SU(3) theory of the strong interactions the elementary gauge variables are 3 by 3 unitary unimodular matrices U_{ij}, one such associated with each nearest neighbor bond (ij) on a four dimensional hypercubic lattice.

To formulate a dynamics for these variables we need an action. Motivated by the definition of field strengths as a generalized curl of the vector potential, we consider the phase factors associated with the smallest closed loops on the lattice, i.e. elementary squares or "plaquettes." A simple form which in the classical continuum limit is proportional, up to an irrelevant additive constant, to the usual gauge theory action is

$$S = - \sum_{\square} \mathrm{Re}\left(\mathrm{Tr} \prod_{\square} U_{ij}\right) \qquad (2)$$

where the sum is over all the plaquettes of the lattice and the product is an ordered group product of the elements surrounding the given square.

To quantize the theory, we use the Feynman path integral approach. Thus we exponentiate our action and integrate over all fields and consider

$$Z = \int (dU)\ e^{-\beta S(U)}$$

Here the parameter β is proportional to the inverse of the bare gauge coupling squared, and the integration over group elements uses the invariant measure.

The use of a space time lattice emphasizes the close connections between particle and condensed matter physics. Equation (3) is equivalent to a partition function. Indeed, the field theory becomes a statistical mechanics problem where the temperature corresponds directly to the coupling constant. This enables the particle physicist to borrow Monte Carlo simulation methods directly from the solid state physicist.

A lattice gauge simulation begins with some initial configuration of the field, stored as an array in a computer memory. The computer then loops through the lattice, making pseudo-random changes which mimic thermal fluctuations. After thermal equilibrium is established, Green's functions of the field theory are extracted as correlation functions of the statistical system.

Such calculations have made some particle theorists avid users of super-computers. The fastest computing machines available are necessary to overcome certain inherent problems. In a Monte Carlo calculation fluctuations are always present and give rise to statistical errors which only decrease with the square root of the computer time. A one order of magnitude improvement in accuracy requires a two order of magnitude increase in computation. In addition to high speed, large computer memories are necessary. As space-time is four dimensional, the linear sizes of lattices which are practical for simulation on modern supercomputers are quite limited, with 10 to 20 sites on a side being typical.

Despite these limitations, lattice gauge simulations have produced rather remarkable quantitative non-perturbative results on the characteristics of the strong interaction. Before discussing some of these results, let me review the

parameters of the non-Abelian gauge theory of the hadronic forces. First are the quark masses. These are presumably determined by a higher level unification of all interactions, and the values are arbitrary in our simulations. One of the most remarkable features of the continuum gauge theory is that these are the only parameters. In particular, if we consider the chiral limit where the quark masses vanish, then we have a theory with nothing to adjust to fit experiment. Indeed, any dimensionless quantity, such as the ratio of the rho mass to the nucleon mass, or the pion nucleon coupling constant, is in principle uniquely determined.

This lack of parameters seems rather peculiar because on the lattice it looks like we do have further variables. For instance, we have the bare coupling constant and the lattice spacing. It is in taking the continuum limit that these quantities "eat" each other via a mechanism given the marvelous name "dimensional transmutation" by S. Coleman and E. Weinberg[2]. I will now describe this phenomenon in lattice language.

When the lattice cutoff is in place, the lattice spacing a forms a natural unit in which to measure dimensionful quantities. For example, the mass m of some physical particle measured in lattice units is an inverse correlation length

$$m\,a = \xi^{-1} \tag{4}$$

Non-particle physicists may wish to put appropriate factors of Planck's constant and c into this equation. For a continuum limit we wish to take a to zero while m goes to its physical value. This will give a divergent correlation length and is the reason for the statement that one must take a statistical system to a critical point to obtain a continuum field theory.

Now for an asymptotically free gauge theory we know something about how the bare coupling behaves as we approach the continuum limit. The coupling is an effective coupling at the scale of the lattice spacing, and therefore it should decrease logarithmically with decreasing scale

$$g_0^2 = 1/\left(\gamma_0 \log\left(a^{-2}\Lambda_0^{-2}\right) + (\gamma_1/\gamma_0)\log\left(\log\left(a^{-2}\Lambda_0^{-2}\right)\right) + O(g_0^2)\right) \quad (5)$$

Here γ_0 and γ_1 are the first two coefficients in the Gell-Mann Low renormalization group function and Λ_0 is an integration constant. We now invert this well known relation to obtain the cutoff a as a function of the coupling. Putting this in eq. (4) gives an explicit formula for how the correlation length diverges as the coupling is taken to zero

$$m\,a = (m/\Lambda_0)\left(g_0^2\gamma_0\right)^{-\gamma_1/(2\gamma_0^2)} \exp\left(-1/(2\gamma_0 g_0^2)\right)\left(1+O(g_0^2)\right) \quad (6)$$

Note the essential singularity at vanishing coupling; dimensional transmutation is inherently non-perturbative.

We can use this equation to determine m. If by Monte Carlo simulation or some other means one can obtain the correlation length as a function of the bare coupling, it should display the essential singularity of equation (6). The coefficient of this singularity is the mass in units of Λ_0. The important point here is that Λ_0 is independent of the particular mass being measured. By performing the above procedure for two different masses, one can divide the results to eliminate Λ_0 and obtain the ratio of the corresponding masses, with no parameters remaining to adjust.

As a first application, consider the quark-antiquark potential. We first put external sources with quark quantum numbers into our lattice and measure the resultant energy. We then extract the linear part of long range potential

associated with confinement. In lattice units, this gives a dimensionless number a^2K, where K is the coefficient of this linear behavior or the so called "string tension." The empirical Regge trajectories give us an experimental value of about $(400\ \text{MeV})^2$ for K. Looking for the essential singularity in a^2K as above then gives a relation between K and Λ_0. A recent calculation for pure SU(3) fields gave[3]

$$\Lambda_0 = 9.6 \times 10^{-3}\ \sqrt{K} \tag{7}$$

Using the perturbative relation[4] between Λ_0 and a somewhat more conventional parameter Λ_{mom} gives the experimentally acceptable result

$$\Lambda_{mom} = 320\ \text{MeV}. \tag{8}$$

This calculation is particularly remarkable in that it relates the short distance behavior of asymptotic freedom to the long distance scale of confinement.

The next physical number to come from lattice calculations was the temperature of a real phase transition between a vacuum well described by thermal excitations of a few hadrons and a high temperature phase best characterized as a black body gas of quarks and gluons. In the pure glue theory this transition appears to occur at a temperature of about 200 MeV and to be first order with a rather large latent heat[5]. Calculations including light quarks still indicate a rather abrupt change, but there is some controversy whether the transition remains first order or if a true thermodynamic singularity remains[6].

Another observable that has received considerable attention is the glueball mass. Ignoring the quarks, there should exist particles which are bound states of gluons alone. Lattice simulations[7] suggest a very rich spectrum below 2 GeV

beginning with a state of $J^{PC} = 0^{++}$ and a mass in the range 700-1000 MeV. This is somewhat awkward experimentally, but the present calculations ignore mixing with quark states and say nothing about the width of this particle.

Including dynamical effects of quark fields in lattice simulations is an area of intense ongoing research. Here there is an approximation which has generated considerable interest. This "valence" or "quenched" approximation takes gauge field configurations obtained via conventional Monte Carlo simulations of the gluon part of the action alone, and then the Dirac equation is solved in these fields. Various combinations of quark propagators then represent propagation of different mesonic states. In terms of Feynman diagrams, this approximation includes all gluonic exchanges between the valence quarks, but neglects virtual production of quark pairs from vacuum fluctuations. As the simple quark model has had many successes, one might hope that this approximation is reasonable. Indeed, the results on hadronic spectra have been remarkably good; a recent calculation[8] which input the pion and rho masses gave, among other results,

particle	calculated mass (MeV)	experimental mass
A_1	1497+/-162	1275
S	1063+/-79	975
N	1073+/-91	939

A remarkable feature of this approximation is that it gives rise to a light pion, consistent with spontaneous breaking of chiral symmetry.

Despite the successes, these calculations are an approximation. There are several algorithms available to include the effects of dynamical quark loops,

but they all are extremely intensive in demands for computer time. To show that fermionic algorithms in principle do exist, I will now discuss one such[9]. This is a variation on the algorithms of refs. (10) and (11).

Because the Fermionic part of the gauge theory action is quadratic in the fermionic fields, the latter can be formally integrated out. Thus the goal of a fermionic simulation is to generate gauge configurations weighted with the distribution

$$P_E(A) \sim \left|M(A)\right| e^{-S(A)} \tag{9}$$

Here M(A) is the Dirac operator. I assume that some trick such as considering two flavors has been done to make M positive. The following three steps will take an ensemble of gauge configurations closer to the above distribution. For every initial gauge configuration A:

1. Select a trial new configuration A'. This could differ from A by, say, one link variable. The choice of A' should be done symmetrically so that the probability choosing A' given A is the same as would be the probability of chosing A as the trial if the original configuration had been A'. This is identical to the first step of the usual Metropolis algorithm for pure gauge fields.

2. Generate a complex field ϕ on the lattice sites with a Gaussian weight depending on the trial A'

$$P(\phi) \sim e^{-\phi^* M(A')\phi} \tag{10}$$

3. Conditionally accept the change A goes to A' with the probability

$$\text{Min}\,(1,[\exp(S(A)-S(A') + \phi^*(M(A')-M(A))\phi)] \tag{11}$$

Note that one factor here is exactly what one would use with the conventional

Metropolis approach for pure gauge fields. The remainder is the inverse of what one would include for bosons coupled to the gauge field.

This algorithm is easily justified by showing that it satisfies the detailed balance condition

$$P_E(A)P(A\to A') = P_E(A')P(A'\to A) \tag{12}$$

where $P(A\to A')$ is the probability for taking A to A'. This is a sufficient but not necessary condition to approach equilibrium; a necessary and sufficient condition is the sum of this equation over A'. Clearly we only need to investigate this relation when A is unequal to A'. The probability of taking A to A' involves integrating over all possible intermediate values of the auxiliary "pseudofermion" field ϕ. Thus the left hand side of the above equation for $A \neq A'$ is

$$P_E(A)P(A\to A') = P_E(A)U(A,A')\,\frac{1}{Z_\phi}\int(d\phi)\; e^{-\phi^* M(A')\phi}\,\min\left(1,\; e^{-S'+S+\phi^*(M'-M)\phi}\right) \tag{13}$$

where the integral over ϕ requires the normalization factor

$$Z_\phi = \int(d\phi)\; e^{-\phi^* M(A')\phi} \sim 1/\left|M(A')\right| \tag{14}$$

and $U(A,A') = U(A',A)$ is the probability of choosing trial A' given A. Explicitly combining eqs. (9), (13), and (14) gives

$$P_E(A)P(A\to A') \sim \left|M(A)\right|\,\left|M(A')\right|\,U(A,A')\,\times$$

$$\int d\phi\,\min\left(e^{-S(A)}\,e^{-\phi M(A')\phi},\; e^{-S(A')}\,e^{-\phi^* M(A)\phi}\right) \tag{15}$$

This form it is explicitly symmetric in A and A'; thus, detailed balance is satisfied.

Several comments on this algorithm are in order:

1. There is no need for A' to be very near A because no first order approximation in the change of A is made. The ability to make large changes

should be an advantage over both the algorithm in ref. (10) and the microcanonical approach of ref. (12).

2. Unlike the discussion in ref. (11), the acceptance requirement does not require an average over an ensemble of ϕ fields.

3. As with all known fermionic methods, there is one time consuming step deep within the main Monte Carlo loop. Here it is the generation of the Gaussian weighted field ϕ. Grady[9] is investigating whether one may be able to only partially relax the pseudofermion field at each step. This hope arises from the considerable freedom available in boson simulations.

In this talk I have discussed how the possibility of studying the solutions to nontrivial quantum field theories has made particle theorists avid users of supercomputer time. The results have been spectacular, with first principle calculations of non-perturbative hadronic properties. The main outstanding problem is the simulation of dynamical quarks, which at present strains even the most advanced facilities. The problem appears so severe that a few groups are attempting to design their own special purpose processors to obtain the needed computer cycles[13]. More research is also needed into new algorithms; for example a microcanonical Monte Carlo approach that I have recently been developing[14] is about an order of magnitude faster than conventional approaches for simulation of discrete systems such as the Ising model. Finally, in the enthusiasm for numerical methods, analytic approaches to lattice gauge theory have been somewhat neglected.

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