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IMPLEMENTATION OF THE MICROCANONICAL MONTE CARLO SIMULATION ALGORITHM FOR SU(N) LATTICE GAUGE THEORY CALCULATIONS *

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ADAPTATION SUMMARY

Title of adaptation: MICROCANONICAL DEMON

Adaption number: 0001

Programs obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Reference to original program:

Title of program: SUUNFA

Catalogue number: AAOT

Ref. in CPC: 29 (1983) 97

Authors of original program: R.W.B. Ardill, K.J.M. Moriarty and Michael Creutz

High speed store required: 47 Kwords

No. of bits in a word: 64

Additional keywords: microcanonical demon

Number of cards required to effect adaptation (including directive cards): 20

Nature of the physical problem
Recently a new algorithm for Monte Carlo simulation, called the microcanonical algorirthm [1], was introduced for lattice gauge theory calculations. We wish to apply this technique to SU(3) gauge theory.

Method of solution
We altered a previously introduced Monte Carlo simulation program [2] to implement the microcanonical algorithm for SU(3) gauge theory [3].

Restrictions on the complexity of the program
The only restriction on the complexity of the program is the size of gauge field links array. This array, called ALAT, must be adjusted to fit the memory of the computer available to the user.

Typical running time
To generate the test run output took about 1 h 23 min of CRAY-1S CPU time.

References

[1] M. Creutz, Phys. Rev. Lett. 50 (1983) 1411.
[2] R.W.B. Ardill, K.J.M. Moriarty and M. Creutz, Comput. Phys. Commun. 29 (1983) 97.
[3] M. Creutz and K.J.M. Moriarty, Microcanonical Monte Carlo Simulation of SU(3) Gauge Theory in Four Dimensions, Brookhaven National Laboratory Preprint (June 1983).

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LONG WRITE-UP

1. Introduction

The theory of strong interactions is generally believed to be Quantum Chromodynamics (QCD), which is a quantum field theory. However, as with any quantum field theory, QCD has ultraviolet divergences which have to be regularized. Because the running coupling constant of QCD increases with increasing quark separation, the theory is inherently non-perturbative which means that the Feynman expansion technique, which is so useful in Quantum Electrodynamics (QED), is not applicable. By performing a Wick rotation on our time component of our space–time and quantizing our field theory by the Feynman path integral approach, the equivalence of our quantum field theory and statistical mechanics can be shown. Wilson [1] suggested that this approach be followed with the space–time continuum being replaced by a lattice with the lattice spacing acting as a regulator. The Monte Carlo method [2] has proved to be very effective in studying statistical systems and these methods have been carried over into lattice gauge theory calculations [3]. The main Monte Carlo algorithm used up to now for gauge field calculations has been the method of Metropolis et al. [4]. In the present paper we present a simple modification of our SU(N) program [5] to permit simulation of SU(N) lattice gauge theory using the new microcanonical Monte Carlo method of ref. [6]. We present some sample results with the gauge group SU(3).

2. Outline of the theory

We work with a hypercubical lattice in four space–time dimensions. We join nearest-neighbor lattice sites, which are denoted by i and j, by a link $\{i,j\}$ on which sits an $N \times N$ unitary–unimodular matrix $U_{ij} \in \mathrm{SU}(N)$ with $U_{ij} = (U_{ji})^{-1}$.

As described in ref. [6], we consider the quantity

$$Z = \sum_{C} \sum_{E_D} \delta(S(C) + E_D - E), \qquad (1)$$

where $S(C)$ is the action for any configuration C of our gauge fields, E_D is the demon's energy and E is an initially determined total energy. The inverse coupling constant squared β is determined by

$$\beta = 1/\langle E_D \rangle.$$

Periodic boundary conditions are used throughout our calculations. The microcanonical algorithm proceeds through the demon trying to update a link variable by sampling from a randomly generated table of SU(N) matrices, where the change would be accepted providing the demon has sufficient energy. The convergence of the procedure can be accelerated by the traditional method of making N^2 hits per link before moving to the next link. In all cases, our initial configuration was an ordered starting lattice and the demon possessed the full energy of the entire system.

3. Description of the code

The microcanonical Monte Carlo simulation algorithm [5] can be implemented in our previous program [6] by the following changes.

(1) Add the variable DEMON to the COMMON BLOCK VARL in lines 0195, 0334, 0396, 0729,

(2) Delete statements 0315 to 0323 and replace with the statements

```
DEMON = NGROUP * NLINKS/B
CALL MONTE (190)
```

We normalize DEMON to be NGROUP times E_D of eq. (1).

(3) Insert after the statement 0499 the statement

```
TEMP = 0.
```

(4) Replace the statements 0651 to 0655 with the statements

```
IF (ATEST.GT.DEMON) GO TO 151
DEMON = DEMON-ATEST
```

(5) Insert after statement 0678 the statement

```
TEMP = TEMP + DEMON
```

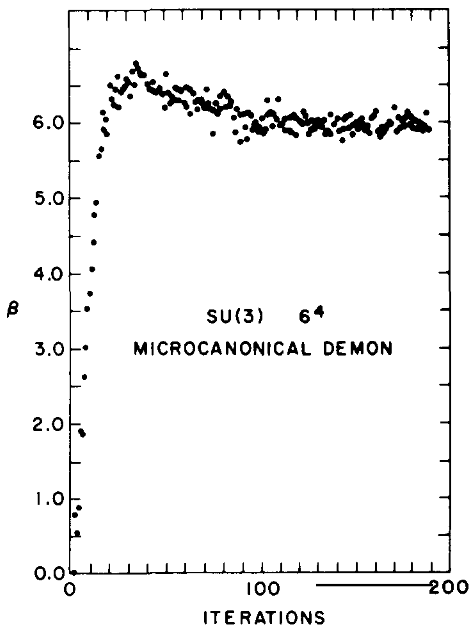

Fig. 1. The evolution of the inverse coupling constant squared β for pure SU(3) gauge theory on a 6^4 lattice as a function of the number of iterations through the lattice where the microcanonical demon moves sequentially through the lattice.

(6) Insert after statement 0704 the statement

B = NGROUP * NLINKS/TEMP

With these alterations to program SUUNFA the microcanonical demon is ready to run. For the test run we set

NDIM = 4
ISIZE = 6
NTMAX = 9
NTPASS = 200
B = 1.6
BA = 0.001
STYPE = *U*
NGROUP = 3.

In fig. 1 we show the results [7] of our simulations for pure SU(3) gauge theory on a 6^4 lattice using these parameters. The evolution of the inverse coupling constant square β as a function of the interations through the lattice is shown for a sequential sweep through the lattice in fig. 1. The amount of energy in the demon's sack gives a final average action per plaquette of

$$\langle E \rangle = \langle 1 - \tfrac{1}{3}\mathrm{Re}\,\mathrm{Tr}\,U_{\mathrm{P}} \rangle = 0.4166,$$

where U_{p} is the parallel transporter around a plaquette. This corresponds to a value of the inverse coupling constant squared of

$$\beta = 5.9671$$

which was found by averaging β over 60 iterations after iteration 130.

Acknowledgements

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References

[1] K.G. Wilson, Phys. Rev. D10 (1974) 2445.
[2] Monte Carlo Methods in Statistical Physics, ed. K. Binder (Springer-Verlag, Berlin, 1979).
[3] M. Creutz, L. Jacobs and C. Rebbi, Phys. Rep. 95 (1983) 201.
[4] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.
[5] R.W.B. Ardill, K.J.M. Moriarty and M. Creutz, Comput. Phys. Commun. 29 (1983) 97.
[6] M. Creutz, Phys. Rev. Lett. 50 (1983) 1411.
[7] M. Creutz and K.J.M. Moriarty, Microcanonical Monte Carlo Simulation of SU(3) Gauge Theory in Four Dimensions, Brookhaven National Laboratory Preprint (June 1983).