J. Phys. G: Nucl. Phys. **10** (1984) L45–L49. Printed in Great Britain

LETTER TO THE EDITOR

Microcanonical Monte-Carlo simulation of SU(3) gauge theory in four dimensions

Michael Creutz and K J M Moriarty†

Brookhaven National Laboratory, Upton, Long Island, New York 11973, USA

Received 22 November 1983

Abstract. We apply a microcanonical algorithm developed recently to the Monte-Carlo simulation of pure SU(3) gauge theory on a 6^4 space–time lattice. The results are compared with the standard Monte-Carlo simulation method.

In a recent paper by one of the authors (Creutz 1983), a microcanonical Monte-Carlo simulation method for carrying out gauge field calculations on the lattice was introduced and applied to the SU(2) gauge group. However, the gauge group for quantum chromodynamics (QCD) is SU(3). It therefore seems reasonable to apply this new technique to SU(3). The microcanonical algorithm is applied to SU(3) using both systematic and random sweeps through a 6^4 lattice. The results are compared with results obtained using the standard method of Metropolis *et al* (1953).

We worked with a hypercubical lattice in four space–time dimensions. We joined nearest-neighbour 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

$$U_{ij} = (U_{ji})^{-1}.$$

We define our partition function as

$$Z = \sum_{\mathrm{C}} \sum_{E_{\mathrm{D}}} \delta(S(\mathrm{C}) + E_{\mathrm{D}} - E)$$

where $S(\mathrm{C})$ 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

$$\beta = \langle E_{\mathrm{D}} \rangle^{-1}.$$

Periodic boundary conditions were 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. There are two methods of achieving an iteration or sweep through the lattice: first, the traditional sequential sweep and second, the random sweep, In all cases, our initial

† Permanent address: Department of Mathematics, Royal Holloway College, Englefield Green, Surrey TW20 0EX, UK.

0305-4616/84/030045 + 05 $02.25

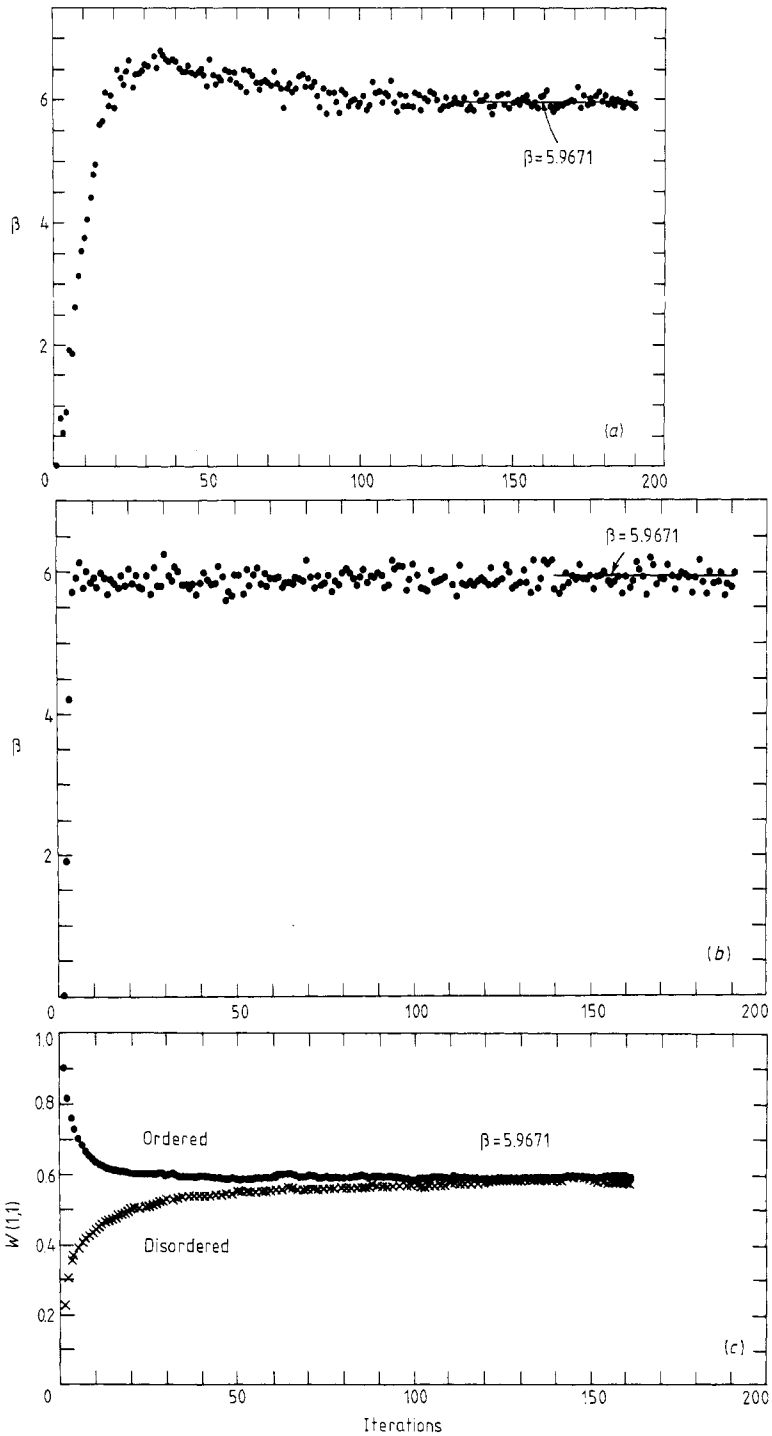

Figure 1. The evolution of the inverse coupling constant squared β for pure SU(3) gauge theory on a 6^4 lattice as a function of the number of iterations through the lattice where the microcanonical demon moves (*a*) sequentially through the lattice and (*b*) jumps randomly from site to site. In (*c*) we show the simulation of Metropolis *et al* (1953) at $\beta = 5.8$ from Creutz and Moriarty (1982).

configuration was an ordered starting lattice and the demon possessed an enormous amount of energy. A more detailed description of our calculational technique can be found in Creutz and Moriarty (1983).

In figure 1 we show the results of our simulations for pure SU(3) gauge theory on a 6^4 lattice. The evolution of the inverse coupling constant squared β as a function of the iterations through the lattice is shown for a sequential and for a random sweep through the lattice in figures 1(*a*) and (*b*), respectively. Averaging over the last 60 iterations gives a value for β of 5.9671. The amount of energy in the demon's sack gives a final average action per plaquette of

$$\langle E\rangle = \langle 1 - \tfrac{1}{3}\mathrm{Re\ Tr}\ U_{\mathrm{P}}\rangle = 0.4260$$

where U_{P} is the parallel transporter around a plaquette. In figure 1(*c*) we show the evolution of the average action per plaquette using the conventional method of Metropolis *et al* (1953) at $\beta = 5.8$ (Creutz and Moriarty 1982). All the initial conditions were the same as in figures 1(*a*) and (*b*). We can see that microcanonical algorithm with a random sweep through the lattice in figure 1(*b*) converges quickest. In figure 2 we show the distribution of the demon energies over the last ten sweeps of figure 1(*a*) after 150 iterations through the lattice. As expected, the distribution is exponential,

$$\exp(-\beta E_{\mathrm{D}}),$$

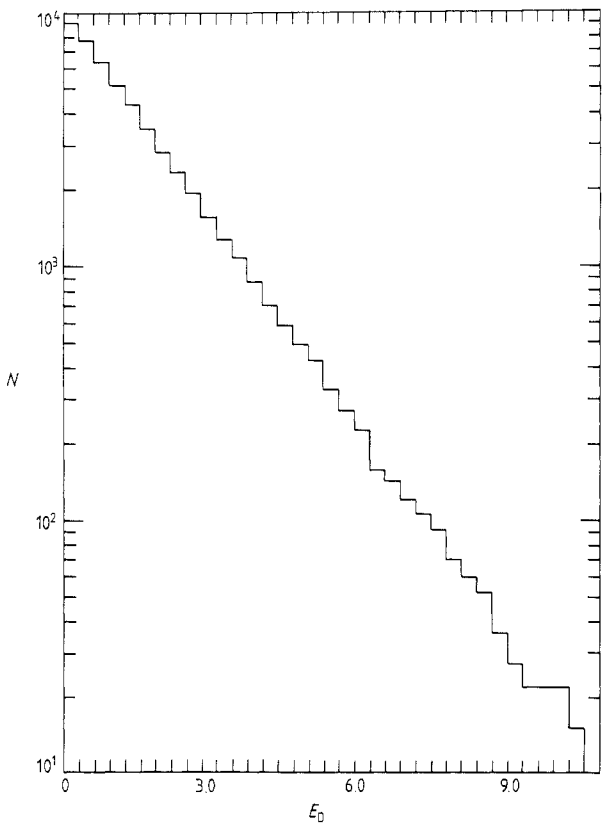

Figure 2. The number of times out of 51 840 steps that the demon is in the corresponding energy bin of width 0.1 as a function of the demon energy E_{D}.

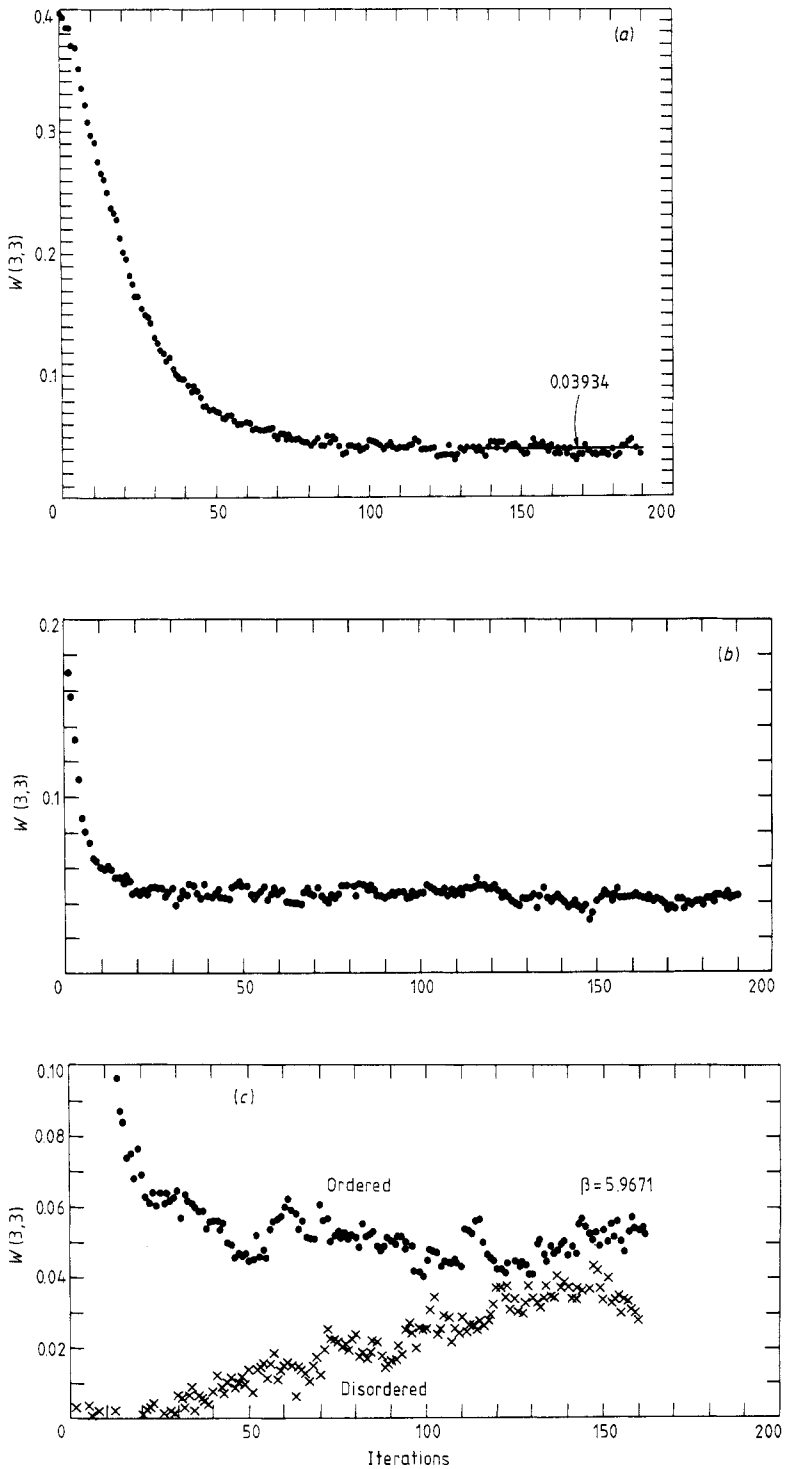

Figure 3. The evolution of the 2×2 and 3×3 Wilson loops corresponding to the three runs presented in figure 1.

with β as given above. Figure 3 shows the convergence of the 2×2 and 3×3 Wilson loops (Wilson 1974) for the runs shown in figure 1.

We conclude from figures 1 and 3 that the randomly hopping demon substantially reduces the initial relaxation time to equilibrium. This may be due to the good starting lattice created after the demon uniformly distributes his initial energy. After coming to equilibrium, this algorithm is essentially equivalent to the conventional approach because before visiting any site the demon energy becomes exponentially distributed in its wanderings through distant parts of the lattice. As most of the computation with SU(3) is spent multiplying neighbours, the computer time per link update in all these simulations is nearly the same.

We would like to thank the Science and Engineering Research Council of Great Britain for the award of research grants (Grants NG-0983.9, NG-1068.2 and NG-13300) to buy time on the CRAY-1S computer at Daresbury Laboratory where part of this calculation was carried out and the University of London Computer Centre for the granting of discretionary time on their CRAY-1S where the remainder of this calculation was performed. The calculations of the present Letter took 2.4 h on the CRAY-1S to perform. One of the authors (KJMM) would like to thank the Science and Engineering Research Council of Great Britain for the award of a Senior Visiting Fellowship (Grant NG-13928) to travel to the United States of America and the Brookhaven Directorate for the award of a Visiting Fellowship to visit Brookhaven where this work was completed. This research was also carried out in part under the auspices of the US Department of Energy under contract DE-AC02-76CH00016.

References

Creutz M 1983 *Phys. Rev. Lett.* **50** 1411
Creutz M and Moriarty K J M 1982 *Phys. Rev.* D **26** 2166
—— 1983 *Comput. Phys. Commun.* **31**
Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 *J. Chem. Phys.* **21** 1087
Wilson K G 1974 *Phys. Rev.* D **10** 2445