DYNAMICAL PROPERTIES OF THE HYBRID MONTE CARLO ALGORITHM*

Sourendu Gupta

Theory Division, CERN, CH-1211, Geneva 23, Switzerland.

ABSTRACT

Some aspects of the dynamical critical behaviour of the Hybrid Monte Carlo algorithm are reported. Studies with the two-dimensional XY model and $U(1)$ pure gauge theory reveal that the algorithm can be tuned to yield $z \approx 1$ at a critical point. We emphasise the importance of using long trajectories of random length. Barrier penetration takes exponential time.

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We report some results on the dynamical properties of the HMC algorithm [1]. We use a first-order leap frog with a time step Δt , and continue the trajectory for N_{md} steps between successive Metropolis questions. Measurements are made after each Metropolis choice. We study the behaviour of the integrated correlation time τ and the effort $E = \tau N_{md}$. The algorithmic parameters N_{md} and Δt must be tuned to minimise E , and thus obtain the smallest possible error estimate in a given amount of CPU time. Some of these results have been presented elsewhere [2].

It is well known [3] that for fixed N_{md} the acceptance, P_{acc} , is controlled by Δt . Also, a limiting value of P_{acc} is reached when $\Delta t N_{md} \sim 1$. We observe that for fixed N_{md} there is a shallow minimum of τ for P_{acc} between 60 and 80% (Fig. 1). In the rest of this talk we present results obtained at an acceptance of about 75%.

Figure 1: τ as a function of P_{acc} at fixed N_{md} for the magnetic susceptibility in the vortex (filled circles) and spin-wave (open circles) phases of the XY model.

At fixed Δt , E is minimised at some N_{md} . As the lattice size L increases, this optimal N_{md} , for any operator, increases linearly with L (Fig. 2). Short-distance operators are optimised at a smaller N_{md} than long-distance operators.

The linear scaling of the optimal N_{md} can be understood through a simple experiment. We take two copies of a given configuration, perturb one spin on one

Figure 2: E as a function of N_{md} for magnetic susceptibility at $\beta = 1.30$ in the XY model on 16^2 (circles), 32^2 (squares) and 64^2 (triangles) lattices.

of them, and evolve both. After each MD step we compare the two configurations. In Figure 3 we show the MD time at which the perturbation reaches a distance r from the origin. The signal propagates linearly through the lattice. The speed depends on β . The constant speed of propagation sets a typical scale for the trajectory length on a lattice of size L , and this scale increases linearly with the lattice size. The time taken for a signal to reach through the lattice seems to be related by a β -independent constant to the optimal trajectory length, which is 2π in free field theory and about 8 in the 2-d XY model.

We measured the dynamical critical index at fixed acceptance and the optimal N_{md} , and found that this index is always close to the free theory value [4] of 1. We measured

$$z = \begin{cases} 1.01 \pm 0.07 & \text{XY model vortex phase} \\ 1.36 \pm 0.07 & \text{XY model spin wave phase} \\ 1.00 \pm 0.06 & \text{U(1) pure gauge theory} \end{cases}$$

These were obtained from measurements of the magnetic susceptibility for the XY model, and the Wilson line susceptibility for the pure gauge theory. Other observables yield exponents in close agreement with these.

Figure 3: The MD time (T) taken for a perturbation to reach distance r at $\beta = 1.30$ on a 32^2 lattice for the XY model.

For free field simulations with fixed N_{md} , certain modes get locked [5] at one value. We observe similar mode locking in the spin wave phase of the XY model. This is visible on constructing the Fourier modes of fields and measuring τ for each mode. There are sharp peaks in $\tau(k)$ as a function of the mode number k . These disappear when trajectory lengths are randomised. Mode-locking seems to lead to long period oscillations in run-time histories, which are removed by choosing trajectory lengths at random (Fig. 4).

Further observing $\tau(k)$, we find that at small trajectory lengths it is a sharply falling function of k , but becomes flatter as N_{md} increases (Fig. 5). This implies that for long trajectory lengths correlation functions at different separations have equal autocorrelations. As a result, the errors on mass measurements can be brought under very good control.

Sectors with different topological charges in the two-dimensional $U(1)$ pure-gauge theory are separated by barriers of height 2β . Consequently, autocorrelations in the topological charge are dominated by barrier penetration times. In a series of runs at 75% acceptance on 16^2 lattices at β between 2 and 8 we found

Figure 4: The run-time history of the magnetic susceptibility at $\beta = 1.50$ on 64^2 lattices for the XY model with (a) fixed and (b) random N_{md} . In both cases $\langle N_{md} \rangle = 400$ and $P_{acc} = 75\%$.

that

$$\tau \sim \exp(-1.78 \pm 0.02\beta).$$

By increasing the step size in order to keep the acceptance at 50% we found that the constant in the exponent could be decreased to 1.50 ± 0.02 .

Figure 5: $\tau(k)$ in the XY model at $\beta = 0.90$ and $L = 32$ at $P_{acc}=75\%$, for runs with $N_{md}=10$ (filled circles) and $N_{md}=300$ (open circles).

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