GLOBAL DEMONS IN FIELD THEORY:
CRITICAL SLOWING DOWN IN THE XY MODEL

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ABSTRACT

We investigate the use of global demons, a ‘canonical dynamics’, as an approach to simulating lattice regularized field theories. This deterministically chaotic dynamics is non-local and non-Hamiltonian, and preserves the canonical measure rather than \( \delta(H - E) \). We apply this inexact dynamics to the 2D XY model, comparing to various implementations of hybrid Monte Carlo, focusing on critical exponents and critical slowing down. In addition, we discuss a scheme for making energy non-conserving dynamical algorithms exact without the use of a Metropolis hit.
1. Introduction

One traditional dynamical approach to simulating ensemble averages has been molecular dynamics (MD) algorithms. In the simplest of these, micro-canonical simulations, conjugate momenta are introduced for each degree of freedom in the ensemble, and the resulting system is time-evolved according to Hamilton’s equations of motion. The reversibility of Hamiltonian evolution then ensures detailed balance, i.e. that the simulation is a Markov process. If the system is sufficiently large, and the interactions sufficiently complex, one usually imposes the quasi-ergodic hypothesis, and hopes that the simulation will explore the desired ensemble. Unfortunately, it is known that Hamiltonian evolution conserves energy, and is therefore not ergodic. In fact, microcanonical simulations introduce an explicit factor of $\delta(H - E)$ into the measure of the ensemble being simulated. In order to use an MD algorithm to obtain the correct ensemble, some additional method must be introduced to integrate over the different energy surfaces $E$.

One method of dealing with this difficulty is embodied in the hybrid molecular dynamics (HMD) and hybrid Monte Carlo (HMC) algorithms[1]–[3]. In these algorithms, the micro-canonical equations of motion are integrated along a ‘trajectory’ for a time $T$, after which the momenta are touched with a heat bath, changing the energy of the system. As with any numerical integration of Hamilton’s equations, finite step size errors will build up along the micro-canonical trajectories, leading to systematic errors in the ensemble generated by HMD. Although these errors can be controlled by making the step size sufficiently small, this can become costly. The HMC algorithm is designed to correct for these $dt$ errors. It does this by treating the configuration at the end of a micro-canonical trajectory as a proposal for a global update of the system, which is then accepted or rejected according to a Metropolis hit. If the equations of motion are reversible, this sequence of configurations is then a Markov chain which, given ergodicity, is guaranteed to produce the correct ensemble. The HMC and HMD algorithms are currently widely used in lattice gauge theory simulations, especially in systems involving dynamical fermions. Typically, HMC is used in theories where the action can be expressed as the volume integral of a local function, while HMD is used when it cannot.

Although these algorithms are generally quite robust, they do have one weakness, related to critical slowing down. Associated with any observable $O$ is an autocorrelation ‘time’ $\tau_O$, the time scale required for the simulation to produce a statistically independent measurement of $O$. This autocorrelation time will generally depend on the correlation length of the system as a power law[4],

$$\tau_O = A \xi^z.$$  \hspace{1cm} (1)

where $z$ is the dynamical critical exponent, and $A$ and $z$ will depend on $O$. Critical slowing down occurs whenever $z > 0$. $\tau_O$ represents the typical amount of simulation time it takes for a local change in $O$ to propagate across a correlated cluster. For multi-scale algorithms, such as cluster algorithms, one can hope to obtain $z = 0$, since these algorithms are designed to change an entire correlated cluster simultaneously. Unfortunately, these algorithms are not easily generalized from one model to another, and have not yet
have been implemented for most lattice gauge theory models. At the other extreme, it is danger-
ously easy to obtain \( z = 2 \) with an algorithm which involves only local updates. This just cor-
responds to diffusive transport of fluctuations through the correlated cluster. In prin-
ciple, one should be able to do no better than \( z = 1 \) with a local algorithm, since the local
algorithm will restrict fluctuations to a finite propagation speed. One can obtain \( z = 1 \)\(^4\) in HMC and HMD, but to do so requires a correlation length dependant tuning of the trajectory length. If the trajectories are too short, then the frequent randomization of
the momenta causes the motion of the system through phase space to be diffusive (resulting in a \( z \) of 2), while if the trajectories are too long the quality of statistics goes down because energy
conservation correlates the measurements along each trajectory. In addition, the optimum trajectory
length is likely to differ for different observables, forcing an inefficient trajectory length for some of
t hem. (This problem is especially severe for HMC, where only one measurement is allowed per
trajectory. Running with trajectories twice as long as is necessary is therefore equivalent to a factor of two slow-down in the code.)

We would like to contrast these hybrid algorithms based on micro-canonical evolution to a purely dynamical approach we term global demons. Like the hybrid algorithms, global demons are an easily implemented, very general approach to simulating ensemble averages. Unlike the hybrid algorithms, the global demon formulation has nothing to do with Hamiltonian dynamics. For example, it can be defined completely in terms of coordinates alone if so desired: the presence or absence of a symplectic structure is irrelevant. This should be contrasted to the MD based algorithms, where a partition function whose action depends only on coordinates is usually augmented to include fictitious conjugate momenta in order to define a Hamiltonian or Poisson structure. Another way to say this is that while evolution using Hamiltonian dynamics generates a microcanonical ensemble, evolution in the global demon system generates a canonical ensemble. The global demon equations of motion are deterministic and time reversal invariant, and are designed to evolve through the physically accessible regions of configuration space (it is not a phase space) such that the trajectory fills configuration space with a density reproducing the correct ensemble. Consider, as an illustration, 1000 points in a phase space \((q,p)\) which lie equally spaced on a unit circle, as shown in the left column of Fig. 1, at \( t = 0 \). The points are connected in order to see how neighboring points behave. Under microcanonical evolution of the 1-d harmonic oscillator equations of motion \((t = 1\) is the natural time scale of the dynamics),

\[
\dot{q} = p, \quad \dot{p} = -q ,
\]

this circle will be preserved, and the points will rotate, preserving the figure at all later times. In contrast to Hamilton’s dynamics, global demon dynamics will result in a rapid dissemination of neighboring points through the space. The time evolution of the circle for a 1-d harmonic oscillator Hamiltonian \( H = \left(p^2 + q^2\right)/2 \) is shown at time \( t = 10 \) and \( t = 20 \), in our canonical dynamics. What is striking is the speed at which neighboring points on the circle evolve to opposite sides of the the space. Even at \( t = 20 \), one can see that the phase space density is nearing the desired ensemble \( \exp(-\beta H) \). In the right column of Fig. 1, we have the same situation for an \( SU(2) \) Hamiltonian \( H = J_z^2/2 \), whose phase space, parameterized by \( (J_x, J_y, J_z) \), is the unit sphere. Here an initial condition of a circle at \( J_z = 0.5 \) is evolved in a similar manner. Again, the rapid divergence of neighboring
points is striking. Since global demons generate a deterministic chaotic dynamics, the danger of diffusive motion through phase space present in the hybrid and other stochastic algorithms is absent here. The one drawback to the global demons approach is that we have been unable to determine a way of making it exact, i.e. removing the $dt$ errors in the ensemble arising from finite step size.

In this article, we investigate an application of the global demon algorithm to a lattice field theory. We are interested in understanding the critical properties of the dynamics near phase transitions, and how tuning the dynamics can improve convergence. We also want to examine the correctness of measurements in this inexact dynamics, as well as ways to make it exact without recourse to stochastic techniques. We choose the 2D XY model, since it has been well studied in the past in a variety of algorithms, and has an infinite order phase transition around which we can investigate the manifestations of critical slowing down. In section 2, we present the global demon dynamics for unconstrained systems. The implementation of this dynamics for the XY model in section 3 explores the behavior of simulations as various parameters of the algorithm are tuned. We find that the algorithm is quite robust, obtaining good results with little tuning. In addition, we compare the critical behavior of the algorithm to several implementations of HMC. We conclude in section 4. Finally, in an appendix, we present a scheme which, in principle, should remove the finite $dt$ errors from the algorithm dynamically. Although our present implementation of the global demon algorithm is not exact, we have chosen to compare our results to HMC, rather than HMD. The main reason for this choice is that we are treating the HMC results as a control, and would like them to be as free of systematic errors as possible. Since the HMC and HMD algorithms are so similar, however, it is quite likely that qualitative conclusions about the critical behavior of HMC will also be correct for HMD.

2. Global Demon Dynamics

Let us consider a system characterized by an action $S(x)$ and coordinates $x = (x_1, ..., x_n)$. The ensemble averages of this system will have the generic form

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\mu(x) \, e^{-\beta S(x)} \mathcal{O},$$

(3)

where

$$Z = \int \mathcal{D}\mu(x) \, e^{-\beta S(x)},$$

(4)

is the normalization, and the measure $\mathcal{D}\mu(x)$ might include constraints (for example, symmetries associated with a Lie algebra). In this article, we are only concerned with the situation when the measure is trivial, $\mathcal{D}x$. If the variables $x = (q, p)$ include canonically conjugate coordinates and momenta, $S(x)$ can be taken as a Hamiltonian: $H(p, q) = S(x)$. Otherwise, in what is more or less standard practice, conjugate momenta are introduced.
and added to $S(x)$ to make the exponent in Eq. (3) resemble a Hamiltonian

$$H(p, x) = \frac{1}{2} \sum_{i=1}^{n} p_i^2 + S(x),$$

(5)

and the measure is modified to $\mathcal{D}x \mathcal{D}p \exp(-\beta H)$, with appropriate normalization. Molecular dynamics is now easily implemented, leading to the equation of motion

$$\dot{x}_i = p_i, \quad \dot{p}_i = -\frac{\partial S(x)}{\partial x_i}, \quad (i = 1, \ldots, n).$$

(6)

This dynamics, combined with momentum refreshes and global metropolis hits, produce the HMD and HMC algorithms.

Let us now pass to the canonical dynamics for such a system[7]–[9]. In contrast to the microcanonical dynamics, the energy and the symplectic structure are no longer preserved. Rather, the measure itself is preserved directly by the dynamics. We can define such dynamics in many ways. For instance, instead of Eq. (6), we could take

$$\dot{x}_i = -\kappa \frac{\beta}{n} \frac{dG(w)}{dw} F_i(x), \quad (i = 1, \ldots, n).$$

(7a)

Here $G(w)$ and $F_i(x)$ are arbitrary functions of a global demon variable $w$ and coordinates $x$, respectively, and $\kappa$ is a coupling constant. The number of global demon interactions (the right hand side of (7a)) is unrestricted. In this example we have used 1, while 2 or 3 are usually sufficient, regardless of $n$. This type of treatment can be viewed as a deterministic version of Parisi and Wu’s stochastic quantization[10, 8]. An alternative formulation of the $x$ dynamics which includes a relic of the underlying Hamiltonian $H(p, x)$ is

$$\dot{x}_i = p_i - \kappa_1 \frac{\beta}{n} \frac{dG_1}{dw_1} F_{1i}(x), \quad (i = 1, \ldots, n).$$

(7b)

$$\dot{p}_i = -\frac{\partial S(x)}{\partial x_i} - \kappa_2 \frac{\beta}{n} \frac{dG_2}{dw_2} F_{2i}(p).$$

(7c)

An important observation here is that while we can retain a Hamiltonian sub-structure to the dynamics, it is not responsible for the ergodicity in the full configuration space, and can be retained or altogether removed. This will have some effect on the convergence, since the Hamiltonian forces can provide additional decorrelation. In non-equilibrium simulations, it is more convenient to use (7b-c) since there is a closer link to the thermodynamics of $H(p, x)$[11]. Eqs. (7b-c) also have a microcanonical limit when $\kappa_\alpha = 0$. Since we are going to compare the global demon approach to HMC, we retain the momenta to have a greater parity between the two algorithms.

With the introduction of the global demons $w_\alpha$, a larger configuration space $\{\phi\}$ must be defined, where $\phi = (x_1, \ldots, p_n, w_1, \ldots w_m)$. In $\phi$–space we can define a new action $f$, which is determined by the equations of motion (7) in the following way:

$$f(x, p, w) = S(x) + \frac{1}{2} \sum_{i=1}^{n} p_i^2 + \sum_{\alpha=1}^{m} G_\alpha(w_\alpha), \quad \rho_f = e^{-\beta f}.$$  

(8)
Unlike $H(p, x)$ in molecular dynamics, $f$ is not preserved by the equations of motion. While the definition of $f$ is not unique (in the sense that the measure for the variables $w$ is arbitrary), it is natural as well as convenient in determining the dynamics of the global demons, by providing a particular solution to the continuity equation below. Eq. (8) defines the $\phi-$space measure as $DxDPDw \exp(-\beta f) = \rho_f D\phi$. The global demon dynamics can then be determined by requiring that $\rho_f$ be a stationary solution of a generalized Liouville (continuity) equation in configuration space:

$$0 = \frac{\partial \rho_f}{\partial t} + \sum_{i=1}^{n+m} \frac{\partial (\dot{\phi}_i \rho_f)}{\partial \phi_i}.$$  (9)

This is equivalent to requiring that the master equation, enforcing conservation of probability under evolution of the ensemble, be satisfied.

The equations of motion for the demons are now found by requiring that they, combined with the generalized dynamics of (7), satisfy Eq. (9). A direct substitution of $\rho_f$ and $\dot{\phi}_i$ (Eqs. (7b-c)) into Eq. (9) allows one to solve for $\dot{w}$:

$$\dot{w}_1 = \frac{\kappa_1}{n} \left( \beta F_{1i} \frac{\partial S}{\partial x_i} - \frac{\partial F_{1i}}{\partial x_i} \right),$$  (10)

$$\dot{w}_2 = \frac{\kappa_2}{n} \left( \beta F_{2i} p_i - \frac{\partial F_{2i}}{\partial p_i} \right).$$

If we had chosen to neglect the momenta and used (7a), the form of Eq. (10) would be unchanged. Eqs. (7) and (10) define a dynamics which by construction preserves the measure Eq. (8). (It is worth noting that while we have taken an exponential form for the density, in general we can take an arbitrary function $\rho$ and still use this same procedure.)

Microcanonical dynamics preserve the phase space volume exactly, since the divergence of the equations of motion,

$$\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i},$$  (11)

trivially vanishes by Hamilton’s equations of motion. The global demon equations of motion (7), (10), on the other hand, do allow for fluctuations in the $\phi-$space volume, which can be quite large. Writing these equations as $\dot{\phi}_i = \mathcal{F}_i(\phi)$, the divergence is explicitly

$$\frac{\partial \dot{\phi}_i}{\partial \phi_i} = -\frac{\beta}{n} \left( \kappa_1 \frac{dG_1}{dw_1} \frac{\partial F_{1i}}{\partial x_i} + \kappa_2 \frac{dG_2}{dw_2} \frac{\partial F_{2i}}{\partial p_i} \right).$$  (12)

This local ‘breathing’ of $\phi-$space is controlled by the arbitrary functions $G$ and $F$. Although this behavior is not microcanonical, there is nevertheless an invariant quantity, called the pseudoenergy $\mathcal{E}$, which is preserved:

$$\mathcal{E} = f(x, p, w) + \frac{1}{\beta} \int_{0}^{t} dt' \frac{\partial \dot{\phi}_i}{\partial \phi_i}.$$  (13)

One can check directly that $\dot{\mathcal{E}} = 0$. 

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There is clearly some freedom in defining the dynamics: the functions $G$ and $F_i$ and the coupling strength $\kappa$. The only restriction on $G(w)$ is that the measure Eq. (8) is normalizable; in general the auxiliary variables $w$ can have any desired measure. In practice, highly non-linear functions are impractical since they will require small integration time steps. For these reasons, it is convenient to take $G = w^2/2$ or $G = w^4/4$. A necessary condition for $F_i$ is for it to be at least linear in its argument, the minimal requirement for the existence of the fluctuations in the volume $\langle 12 \rangle$. The precise relation to the fluctuations in a volume $V$, or equivalently, the instantaneous $\phi$–space compressibility, can be found using the divergence theorem

$$\frac{dV}{dt} = -\frac{\beta}{n} \int_V \mathcal{D}\phi \left( \kappa_1 \frac{dG_1}{dw_1} \frac{\partial F_{1i}}{\partial x_i} + \kappa_2 \frac{dG_2}{dw_2} \frac{\partial F_{2i}}{\partial p_i} \right). \quad (14)$$

In this paper, we do not explore the effect of different choices of $G_i$, $F_i$. Such studies have been done on smaller systems\[7\]–\[9\].

Finally, we observe that the equations of motion (7), $\langle 14 \rangle$ will have no stable fixed points\[12\]. This is the case since the sum of the Lyapunov exponents is related to the average rate of change of total volume of $\phi$–space. By the Liouville equation, this will necessarily vanish\[13\]:

$$\sum_{i=1}^{n+m} \lambda_i = \left\langle \frac{\partial \phi_i}{\partial \phi_i} \right\rangle = 0. \quad (15)$$

3. Implementation for the 2D XY Model

The 2D XY model consists of spins located on the sites of a two dimensional square lattice, which are free to rotate in the plane. The action is given by

$$V(\theta) = -\sum_{<ij>} ReU_i U_j^\dagger = -\sum_{<ij>} \cos (\theta_i - \theta_j), \quad (16)$$

where the sum is over nearest neighbors, and the $U_j = e^{i\theta_j}$ are elements of $U(1)$ located at each lattice site $j$. In two dimensions, this model exhibits a Kosterliz-Thouless phase transition near $\beta \sim 1\langle 14 \rangle$–\[17\]. Above the phase transition, the dynamics is dominated by dissociated vortex-antivortex pairs. These pairs become tightly bound below the phase transition, where the dynamics is dominated by spin waves. The K-T phase transition is infinite order, characterized by an exponentially diverging correlation length ($\xi$):

$$\xi = a_\xi \exp(b_\xi (T - T_c)^{-\nu}). \quad (17)$$

Numerical simulations indicate similar critical behavior for finite lattices\[16, 17\]. Near the critical temperature, the system experiences an exponential increase in the correlation length $\xi$, which can lead to critical slowing down in simulations by virtue of Eq. $\langle 1 \rangle$. 

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3.1 Equations of Motion

The implementation of global demons to the XY model is straightforward. Following the equations of motion (7b-c) and (10), we have

\[
\begin{align*}
\dot{\theta}_i &= p_i - \frac{\kappa_2}{n} w_2 \sin^3 \theta_i, \quad (i = 1, \ldots, n), \\
\dot{p}_i &= -\frac{\partial V(\theta)}{\partial \theta_i} - \frac{\kappa_1 \beta}{n} w_1^3 p_i.
\end{align*}
\]

\(F_i(\theta) = \sin^3 \theta_i\) is chosen to respect the periodicity in \(\theta\), while \(G_i(p) = p_i\) has no such restriction. This choice was motivated only by simplicity, and in general, we could take more complicated interactions, and include additional global demons. The corresponding equations for the global demons are then

\[
\begin{align*}
\dot{w}_1 &= \kappa_1 \left[ \beta \sum_i p_i^2 - 1 \right], \\
\dot{w}_2 &= \frac{\kappa_2}{n} \left[ \beta \sum_i \frac{\partial V(\theta_i)}{\partial \theta_i} \sin^3 \theta_i - 3 \sum_i \sin^3 \theta_i \cos \theta_i \right].
\end{align*}
\]

We used leapfrog integration, which included a Taylor expansion so that the \(O(dt^2)\) errors in a time step cancel. The pairs \(q, w_1\) and \(p, w_2\) were updated in alternate steps. \(w_1\) was taken with \(q\) since they both involve momenta, and \(w_2\) with \(p\) since they both involve coordinates. Our general studies of the systematics of the model under tuning of parameters were performed on a \(16^2\) lattice, while the studies of the critical exponents were done on a \(64^2\) lattice, to allow longer correlation lengths. The particular choice of functions \(F\) leads to a small non-ergodicity for this particular system: the momentum zero mode cannot change sign. (We have corrected for this by occasionally (every 64 trajectories) refreshing the momenta, using the same procedure as in HMD. In general, this is probably a good idea, to ensure that the evolution is ergodic. This particular non-ergodicity could also have been corrected by a small modification of the equations of motion.) We have verified that the equations of motion are correct to \(O(dt^3)\) on a time step, leading to \(O(dt^2)\) systematic errors in observables, by computing the \(dt\) behavior of several observables in Fig. 2, demonstrating the quadratic behavior of the systematic error.

3.2 Hybrid Monte Carlo

We have used the critical properties of HMC as a benchmark for comparison of our global demon approach, studying three of its variations[6]. The equations of motion are the same as those used for global demons, except with \(\kappa_i = 0\). By modifying the length of the HMC trajectory between momentum refreshes, we modify the decorrelation time[4]. The first variation, denoted HMC-1, has trajectories of length 1, where the highest frequency of the free theory is \((2\pi)^{-1}\). While this ‘standard’ choice is easy to implement, it suffers from severe critical slowing down, with \(z = 2\) in Eq. (1). The critical behavior should be improved by choosing the trajectory length proportional to the spatial correlation length.
ξ of the system[4]. The two variations we consider are denoted HMC-S, for $T = \xi$, and HMC-L, for $T = 2\pi\xi$. Again we point out that, in order to make this choice, we require the very information which we are attempting to measure. We were fortunate to have previous results for ξ available to us[17], but in general this is not likely to be the case.

The integration time step was kept fixed at $dt = .1$ along trajectories of length $T$. This value of $dt$ was chosen so that the acceptance rate of the global Metropolis hit in the HMC algorithm was approximately 80%. For HMC, it is necessary to use random trajectory lengths for optimum relaxation[2]: we chose $T$ uniformly distributed on the interval $(.5\langle T \rangle, 1.5\langle T \rangle)$, with $\langle T \rangle = 1$ for HMC-1, and $\langle T \rangle \approx \xi, 2\pi\xi$ for HMC-S,L. We also made several runs of HMC-L using exponentially distributed random trajectory lengths. We found that this does not lead to any improvement over the runs with uniformly distributed trajectories, and may even have resulted in slightly noisier measurements.

One interesting difference between HMC and global demons is that, for global demons, $T$ simply denotes time between measurements along a single trajectory - the evolution of the simulation is completely unaffected by the choice of $T$. At the end of a HMC trajectory we performed a global metropolis hit, after which we performed measurements and refreshed the momenta by choosing new, gaussian distributed $p_i$.

### 3.3 Coupling Strength Dependence

In the micro-canonical algorithms HMC and HMD, the rate at which the simulation covers phase space in the non-ergodic directions (i.e., changes energy) is controlled by the time between momentum refreshes. If the trajectories are too long, the system changes total energy very slowly, leading to autocorrelations on timescales proportional to the trajectory length. If the trajectories are too short, on the other hand, the motion between energy shells is rapid, but motion in the micro-canonical directions is diffusive, leading to a dynamical critical exponent of 2. This means that, for large correlation lengths, the efficiency of the algorithm can vary as a power of $T/T_{opt}$, where $T_{opt}$ is the optimum trajectory length. As shown in Refs. [2, 4], $T_{opt}$ should be proportional to the correlation length of the system, which is not known a priori. Thus it is necessary to perform a sensitive tuning which depends on a parameter measured in the simulation.

In the global demon algorithm, on the other hand, the parameter which controls energy (or action) non-conservation is just the coupling $\kappa$ of the demons to the system. In the limit $\kappa \to 0$, the demons decouple and ergodicity is lost. If $\kappa$ becomes too large, the equations of motion will suffer the characteristic instabilities of discretized dynamics. In contrast to the HMC and HMD algorithms, however, we can make an a priori choice of $\kappa$ which works quite well at all values of the correlation length. To do this, consider the change in total action, $\Delta S = S(\phi_2) - S(\phi_1)$, in a single time step,

$$\Delta S \approx \Delta t \left. \frac{\partial S}{\partial \phi_i} \right|_{\phi_i}$$

(20)

where $S$ now refers to the total global demon action $f$ in Eq. (8). Using equations (7)-(10) and (20), we see that $<|dS/dt|>$ is proportional to $\kappa$, with a constant of proportionality of order one. Thus, the change in $S$ along a trajectory of length $T$ should be $\Delta S \approx \kappa T$. To
set the scale of $\Delta S$, we can compute its expectation value if two consecutive measurements are totally decorrelated:

$$\sigma = \sqrt{\langle \Delta S^2 \rangle} = \sqrt{2\langle(S(\phi))^2\rangle - \langle S(\phi) \rangle^2} = \frac{1}{\beta} \sqrt{2nC_s}, \quad (21)$$

where $C_s$ is the specific heat of the system. In order for the action to decorrelate between measurements (with $T = 1$), we conclude that the optimal choice of $\kappa$ is likely to be $\kappa \approx O(\sqrt{\beta})$. Note that this philosophy of forcing large fluctuations in energy along a trajectory is inherently different from HMC, where (in order to avoid prohibitively low acceptance rates) $\Delta S$ is $O(1)$.

To investigate the behavior of the global demons algorithm under tuning, we ran a series of simulations on a $16^2$ lattice. (Except where otherwise indicated, we used an integration time step of $dt = 0.1$ and measuring at intervals $T = 1 = 10dt$; we will call this time between measurements a trajectory length, even though no momentum refresh is performed). Along the trajectory, we determine the square of the change in action between measurements, $\Delta S^2 = [S(t) - S(t-T)]^2$, which is then averaged along the entire trajectory to obtain $\sqrt{\langle \Delta S^2 \rangle}$. The result gives a guide as to how fast the trajectory can diffuse through configuration space. In Fig. 3, we plot the quantity $\overline{\Delta S}$, which we call the diffusiveness, defined by

$$\overline{\Delta S} = \frac{\sqrt{\langle \Delta S^2 \rangle}}{\sigma}, \quad (22)$$

as a function of coupling strength $\kappa$, for simulations at representative values of $\beta$ both above and below the phase transition. In the limit $\kappa_i = 0$, the equations of motion (18)-(19) are microcanonical and $S$ is preserved, as indicated in the figure. For small couplings, the microcanonical component of the dynamics is only slightly perturbed by the canonical component, and the ergodicity is weak. The convergence times here are quite large. For $\kappa_i \sim \sqrt{2n} \sim 23$, the value of $\overline{\Delta S}$ can be seen to saturate near unity, the value expected when two consecutive measurements are uncorrelated; here the steps are quite large through configuration space. For larger values of the coupling, the change in action remains saturated. Convergence is also generally slower for larger $\kappa$, since the additional decorrelation produced by the microcanonical component to the dynamics is reduced. The reduction of $\overline{\Delta S}$ in Fig. 3 for $\beta \sim 1$ can be attributed to critical slowing down. However, while the correlation lengths become quite large, the dip in $\overline{\Delta S}$ is not so noticeable. In this respect, critical slowing down does not seem to strongly effect this measure of the dynamics as one approaches the phase transition from either side. An important result is that the couplings $\kappa$ are essentially independent of $\beta$ as well as the details of the physics of the model under study.

In Fig. 4, the $\beta$ dependence of $\overline{\Delta S}$ is plotted for simulations at fixed coupling strengths. By selecting the $\kappa = 32$ curve, for instance, we see that we can study both the low and high temperature properties of the $XY$ model, as well as the phase transition, without modifying $\kappa$. While there is a small dip in the curves near $\beta \sim 1$, critical slowing down does not seem to strongly effect this measure of the dynamics as one approaches the phase transition from either side. An important result is that the couplings $\kappa$ are essentially independent of $\beta$ as well as the details of the physics of the model under study.

It should be emphasized that the runs with $\kappa \ll \sqrt{2n}$ converge slower as $\kappa$ decreases, and ultimately do not converge for the microcanonical limit $\kappa = 0$. We have checked
the convergence of the dynamics to the proper ensemble by measuring and subsequently histogramming $w_\alpha$ and $p_i$ along the trajectory and comparing them to their exact analytic distributions, finding that convergence is best above $\kappa \sim \sqrt{2n}$. We can also examine the $\kappa$ dependence of measurements at fixed $\beta$, illustrated in Fig. 5 for $\beta = 1/1.1$. What we see is that the measurements for coupling strengths roughly 5-8 times saturation do not exhibit any systematic deviation as $\kappa$ increases. For much larger $\kappa$ (at fixed $dt$), there will be the characteristic instabilities associated with difference equations. However, the value $\kappa = \sqrt{2n}$ clearly is not near this instability limit, and we can safely use it. In the low $\kappa$ limit, we are close to micro-canonical dynamics, and $S$ begins to become approximately conserved. This slow diffusion results in long time correlations and poor statistics. This figure is typical of other temperatures, above and below the phase transition.

### 3.4 Choice of Trajectory Length (i.e. Measurement Frequency)

An indication of how rapidly measurements decorrelate is shown in Fig. 6. There we plot the diffusiveness $\Delta S$ as a function of trajectory length $T$, for $\kappa_1 = \kappa_2 = 16$ and $\beta = 1$. We observe a saturation in the trajectory length near $T = 2$. Because measurements do not effect the time evolution of the global demon trajectory (they are not associated with any Metropolis hit or momentum refresh), the choice of frequency of measurements is governed by the relative costs of the time evolution and measurement routines. Because our measurement algorithm was relatively inexpensive, we chose to use $T = 1$.

### 3.5 Observables

The observables we measured include the energy $E$, lattice magnetization $M$, topological charge $Q$, defined by

$$E = -\frac{1}{n} \sum_{<ij>} ReU_i U_j^\dagger,$$

$$M = \frac{1}{n} \sum_i U_i,$$

$$Q = \frac{1}{n} \sum_p q_p.$$

The sum in $Q$ indicates the sum over all plaquettes of the number of positive topological charges occupying that plaquette. (For an exact definition of the topological charge, see e.g. [19].) Corresponding to these observables, we can define the specific heat and susceptibilities:

$$C_v = \beta^2 n (\langle E^2 \rangle - \langle E \rangle^2),$$

$$\chi_Q = n (\langle Q^2 \rangle - \langle Q \rangle^2),$$

$$\chi_M = n (\langle (ReM)^2 \rangle + \langle (ImM)^2 \rangle).$$

In both our global demon and HMC runs, we started with about 20000/$T$ trajectories for thermalization, followed by 160,000/$T$ trajectories of data, where $T$ is the trajectory length.
length. Statistical errors in observables were obtained by binning measurements in bins of size $2^n$. The errors quoted in our tables use the smallest bin larger than $8\tau_M$, where $\tau_M$ is the integrated autocorrelation time of the total magnetization. The errors in the susceptibilities were obtained from the errors in the corresponding observables by assuming gaussian fluctuations on a timescale $\tau_O$, where $O$ is the appropriate observable. A selection of our observables are indicated in Table 1. We find that the global demon results usually agree with the HMC results within a few $\sigma$, which indicates that the systematic errors are not large. They could, of course, be further reduced by extrapolating to $dt = 0$.

### 3.6 Autocorrelation Functions and Decorrelation Times

Because we have a dynamical algorithm, the trajectory has a memory, which will be reflected in the auto-correlation functions. This can be analyzed by examining autocorrelation functions of the observables $M, E, Q, \text{ and } S$. When the couplings $\kappa$ are small, the dynamics is near the microcanonical limit, and decorrelation is very poor. Typical auto-correlation functions for $\kappa_1 = \kappa_2 = 1$ are shown in Fig. 7 (dots) for $\beta = 1/1.1$. Here we define

$$\delta O(t) = O(t) - \langle O \rangle,$$

as the fluctuation from the mean. As the couplings are increased near their optimum values, the ringing disappears, and decorrelation times become better defined quantities, indicated by the solid curve with $\kappa_1 = \kappa_2 = 16$. The corresponding HMC autocorrelation functions are shown as well. Parenthetically, this type of ringing can also occur in HMC simulations if one uses a constant trajectory length. The comparison to our HMC runs at this $\beta$ is shown in Fig. 8.

A comparison of auto-correlation functions for the total lattice magnetization $M$ for global demons to the various implementations of HMC are shown in Fig. 9 for a selection of temperatures. It is clear that HMC does not significantly out perform global demons in terms of decorrelation, no matter how ‘optimal’ the trajectory length. The points in these curves indicate the actual number of data points. Hence while the number of global demon measurements is given by $t$, the optimal HMC runs have between one and two orders of magnitude smaller sampling rate in order to have similar decorrelation behavior.

### 3.7 Critical Exponents

The integrated autocorrelation times $\tau$ are defined for a given quantity $O$ as

$$\tau_O = T \left[ \frac{1}{2} + \sum_{t=1}^{\infty} \frac{\langle \delta O(0) \delta O(t) \rangle}{\langle \delta O(0) \delta O(0) \rangle} \right].$$

(26)

Note that we are measuring $\tau$ in units of total time evolved rather than number of trajectories. In Fig. 10 we present a ln-ln plot of the decorrelation times $\tau$ vs. the correlation length $\xi$ for several observables. The fit parameters are indicated in Table 2, and are only indicative of the critical behavior, since they will depend strongly on systematic effects. What is seen is that in almost every case, the global demon prefactor and critical
exponent are smaller than the HMC results. The integrated autocorrelation times are tabulated in Table 3. In Ref. [4], it was argued that the critical exponent is unity when \( T \) is proportional to the lowest frequency mode in the system for a free field theory. The results in Tables 2–3 seem to be good evidence that their results are qualitatively correct in an interacting field theory as well.

The critical behavior of global demon dynamics will also depend on the coupling strengths. In Fig. 11 we plot \( \tau \) as a function of \( \kappa \) for simulations at several values of \( \beta \), on a \( 16^2 \) lattice. As \( \kappa \) increases, the system tend to decorrelate faster, again generally saturating above \( \kappa \sim \sqrt{2n} \). In Fig. 12, the \( \beta \) dependence of simulations at \( \kappa = 1, 4, 16, 64 \) are indicated. The \( \kappa = 1 \) runs have the highest decorrelation times as expected, but we also observe that the high temperature phase is rather insensitive to the value of the coupling. Although convergence of the trajectory to the correct ensemble will always depend strongly on the coupling strength, the decorrelation times of both weakly ergodic and strongly ergodic trajectories are very similar. The effects of critical slowing down are particularly noticeable in \( \tau_Q \) and \( \tau_E \) near \( \beta \sim 1 \). The peak in the \( \tau_E \) is closely related to the dip in \( \overline{\Delta S} \) in Fig. 4. The reason is that the diffusiveness measures the maximum rate at which the total energy \( S \) can change, so if \( \Delta S \ll 1 \), the potential energy \( E \) will change slowly.

One might conclude from Figs. 11–12 that the coupling strength dependence is not too important, and that \( \kappa \sim 2 \) is roughly equivalent to 128. Clearly, while the decorrelation times are indicative of the dynamics, they do not provide the complete picture of the situation. For example, information such as the ringing in the autocorrelation functions (see Fig. 7) average out, and are not strongly reflected in the value of \( \tau \). We also see that simulations with very similar decorrelation times can have disparate values of the diffusiveness \( \overline{\Delta S} \). But in all these guides, the tuning is consistently optimal for \( \kappa \sim \sqrt{2n} \).

### 4. Conclusions

We have studied the global demon dynamical approach to simulating lattice regularized field theories. This method breaks away from the conventional Hamiltonian wisdom, defining a deterministically chaotic, time reversal invariant ‘canonical’ dynamics which rapidly fills configuration space with the desired ensemble. We have taken a particularly simple implementation of global demons using two coupling functions and examined its critical behavior, comparing to HMC using various trajectory lengths.

We have found that the algorithm is very stable under tuning of the various parameters. In particular, once \( \kappa \) is large enough, the quality of the results seem to be independent of \( \kappa \) until the simulation becomes unstable. It appears that \( \kappa \approx \sqrt{2n} \) is a good rule of thumb for which the simulation will perform well in all regimes. In addition we found that the systematic errors were small (a few standard deviations), and that the critical slowing down properties of the algorithm were competitive with or better than the best implementations of HMC. The main fault with the algorithm is that it is not exact, i.e.
there is a systematic error associated with the numerical integration. This problem is addressed in the appendix.

One advantage of this approach is that there is no barrier in principle to obtaining $z < 1$ (note our estimated critical exponents for $S$, $E$ and $Q$ in Table 2). In contrast, local algorithms such as HMC and HMD are limited by $z \sim 1$. In addition, the dynamical nature of the algorithm has allowed extensions to non-equilibrium situations. One possible improvement which we have not examined is Fourier acceleration. This technique improves $z$ to 0 for HMC in free field theory, and may help our approach.

The numerical computations in this work were performed on the Cray Y-MP8/864 at the Ohio Supercomputer Center. We thank Aurel Bulgac, Robert Edwards, Rajan Gupta, Bill Hoover, Tony Kennedy, Greg Kilcup, Klaus Pinn, Junko Shigemitsu and Beth Thacker for useful conversations. This work was supported under DOE grants DE-AC02-ER01545 and DE-FG02-91ER40608.
One major weakness of the global demon algorithm presented in this paper is the systematic error associated with finite step size. In HMC, this error is eliminated by performing a global metropolis hit before every measurement. Unfortunately, this technique has no hope of working for an algorithm with global demons, since the trajectories do not conserve energy. One might hope to use the pseudo-energy $E$ in this capacity, since it is conserved. However, the memory term in Eq. (13) precludes this. For Hamiltonian systems, one can implement symplectic integrators[20] to render the dynamics exact, or one can introduce a global Metropolis hit as in HMC. For our non-Hamiltonian ‘canonical’ dynamics, this procedure is not so clear. Although we have been unable to satisfactorily solve this problem, we mention here one approach which we have tried. We present this method because, although it is presently numerically impractical, it appears to be correct in principle. In addition, it should be applicable to any dynamical simulation which does not conserve energy, and is quite different from the traditional method of using metropolis hits to ensure exactness.

Consider the exact (i.e. $dt = 0$) equations of motion, $\dot{\phi} = F(\phi)$, which, by construction, preserve the measure $\rho(\phi) = \exp(-\beta f(\phi))$. When we discretize time, $\rho$ is no longer preserved exactly. Let us assume that there exists some measure, $\tilde{\rho} \neq \rho$, which is preserved by the discretized equations of motion $\phi_{n+1} = M(\phi_n)$, where $M$ is the time evolution operator. We can now define a correction factor $\alpha$ such that, up to normalization,

$$\rho(\phi) = \alpha(\phi)\tilde{\rho}(\phi). \quad (A.1)$$

If we know $\alpha$, we can obtain the exact expectation values of observables through convolution:

$$\langle O \rangle = \int O \rho d\phi = \int \frac{f(O\alpha)\tilde{\rho} d\phi}{f(\alpha)\tilde{\rho} d\phi} = \frac{\langle O\alpha' \rangle}{\langle \alpha' \rangle}, \quad (A.2)$$

where the prime indicates evaluation in the $\tilde{\rho}$ ensemble. The discretized Liouville (continuity) equation tells us that after one integration time step, we preserve the measure $\tilde{\rho}$:

$$\tilde{\rho}_{n+1} d\phi_{n+1} = \tilde{\rho}_n d\phi_n. \quad (A.3)$$

We can now use (A.1) and (A.3) to solve for the correction factor $\alpha$, through which we can measure exact observables:

$$\alpha_{n+1} = \alpha_n \frac{d\phi_{n+1}}{d\phi_n} \frac{\rho_{n+1}}{\rho_n} = \alpha_n \det \left( \frac{\partial M}{\partial \phi} \right) \frac{\rho_{n+1}}{\rho_n}, \quad (A.4)$$

where $\det(\partial M/\partial \phi)$ is just the Jacobian of the map $\phi_n \to \phi_{n+1}$. Thus, by choosing $\alpha_0 = 1$ at the initial point of the trajectory, we can compute $\alpha_n$ at all subsequent points along the trajectory.

Note that $\alpha$ should play a role very similar to the acceptance rate in HMC. When $dt$ is small, the distribution $\tilde{\rho}$ is very close to $\rho$, so $\alpha \approx 1$ and all of the configurations will be of approximately equal statistical weight. This corresponds to high acceptance rates in
HMC. When $dt$ is large, on the other hand, $\alpha$ will be large in some regions and small in others, meaning that the simulation spends significant amounts of time in regions of low statistical importance. This is similar to the rejection of many proposed configurations when the acceptance is low. Also note that, although in general it is quite difficult, for our leapfrog algorithm the calculation of $\text{det}(\partial M/\partial \phi)$ is straightforward and only $O(\text{volume})$.

The correction factor can also be written as

$$
\alpha_n = \alpha_o \exp \left\{ \sum_{i=0}^{n-1} \ln \frac{\partial q_{i+1} \partial p_{i+1}}{\partial q_i \partial p_i} - \beta H_i + \beta H_0 \right\} 
$$

(A.5)

where $E_n$ is the pseudo-energy (13) evaluated at $\phi_n$.

We have implemented this algorithm for small harmonic and anharmonic oscillator systems. In all runs, we found that, along the trajectory, the magnitude of $\alpha$ would occasionally rapidly decrease several orders of magnitude and never recover. We believe that this is due to an instability in the equations of motion: if the demons become too large at fixed $\kappa$ and $dt$, they begin to grow in an unbounded manner. It is quite likely that this means that a non-zero $\tilde{\rho}$ does not exist. We have tried decreasing $dt$ and various improvements in the equations of motion, but all of these fixes only decrease the frequency of drops - they do not eliminate them.

In the scheme described above, it is not obvious how to perform a momentum refresh. This is because the absolute magnitude of $\alpha$ is not known, only its ratio to the previous alpha along the trajectory. We will now show (again, assuming the existence of $\tilde{\rho}$) that the correct procedure is to reset $\alpha$ to 1 after a gaussian momentum refresh. Assume, given $\tilde{\rho}$ and a refreshing scheme, that the probability of a trajectory beginning at $\phi$ is $P(\phi)$. In addition, let $\tilde{\alpha}(\phi)$ be the correctly normalized function $\alpha$ discussed above and $\alpha(\phi|\phi_0) = \tilde{\alpha}(\phi)/\tilde{\alpha}(\phi_0)$ be the value of alpha obtained using (A.4) along the trajectory from $\phi_0$ to $\phi$ (note that $\alpha(\phi_0|\phi_0) = 1$). Then

$$
\langle O \rangle = \frac{\int d\phi_0 P(\phi_0) \int d\phi O P(\tilde{\alpha}(\phi) \alpha(\phi|\phi_0))}{\int d\phi_0 P(\tilde{\alpha}(\phi_0)) \int d\phi P(\tilde{\alpha}(\phi) \alpha(\phi|\phi_0))} = \frac{N \langle O \tilde{\alpha}' \rangle}{\langle \tilde{\alpha}' \rangle} 
$$

(A.6)

where $N = \int d\phi_0 (P(\phi_0)/\alpha(\phi_0))$. We attempted to test this scheme on the systems discussed above, but we found that the statistical errors in the exact demon simulation tended to be larger than the systematic errors in a similar inexact simulation. Thus, it is presently more efficient to eliminate $dt$ errors by extrapolation techniques than by using the exact algorithm.
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TABLE 1. Comparison of observables between algorithms. For each $\beta$, the four rows correspond to global demons, HMC-1, HMC-S, HMC-L, respectively. Measurements were performed on a $64^2$ lattice, with 160K/T statistics.

| $\beta$ | $E$    | $C_v$  | $Q \times 100$ | $\chi_Q \times 100$ | $|M|$     | $\chi_M$ |
|--------|--------|--------|-----------------|----------------------|----------|----------|
| 0.70   | 0.8287(1)| 0.760(3)| 6.241(2)        | 4.49(2)              | 0.0484(2)| 12.2(1)  |
|        | 0.8299(1)| 0.765(5)| 6.235(2)        | 4.50(3)              | 0.0487(3)| 12.4(2)  |
|        | 0.8297(2)| 0.750(7)| 6.233(2)        | 4.40(3)              | 0.0493(3)| 12.7(1)  |
|        | 0.8300(3)| 0.686(14)| 6.231(5)    | 4.36(7)              | 0.0490(3)| 12.5(1)  |
| 0.78   | 0.9573(1)| 0.992(4)| 4.725(2)        | 3.92(2)              | 0.0683(3)| 24.3(2)  |
|        | 0.9577(2)| 0.994(8)| 4.730(3)        | 3.93(3)              | 0.0683(6)| 24.3(4)  |
|        | 0.9573(3)| 1.010(12)| 4.731(3)     | 3.94(4)              | 0.0674(4)| 23.6(3)  |
|        | 0.9582(5)| 1.061(30)| 4.722(6)    | 4.04(9)              | 0.0683(5)| 24.3(3)  |
| 0.82   | 1.0243(1)| 1.138(5)| 3.981(2)        | 3.62(2)              | 0.0848(5)| 37.2(4)  |
|        | 1.0238(2)| 1.13(1) | 3.995(3)        | 3.61(3)              | 0.0828(9)| 35.8(8)  |
|        | 1.0244(3)| 1.12(2) | 3.987(3)        | 3.61(4)              | 0.0828(7)| 35.7(6)  |
|        | 1.0234(6)| 1.09(4) | 3.996(7)        | 3.53(10)             | 0.0837(7)| 36.4(6)  |
| 1/1.1  | 1.1757(2)| 1.396(7)| 2.431(2)        | 2.73(2)              | 0.162(1) | 133(2)   |
|        | 1.1750(3)| 1.40(2) | 2.448(4)        | 2.76(4)              | 0.151(3) | 116(4)   |
|        | 1.1756(5)| 1.44(4) | 2.443(5)        | 2.80(5)              | 0.161(2) | 132(3)   |
|        | 1.1777(10)| 1.38(6)| 2.418(10)       | 2.67(11)             | 0.166(2) | 140(3)   |
| 1/1.04 | 1.2632(3)| 1.512(9)| 1.638(3)        | 2.14(2)              | 0.295(3) | 409(7)   |
|        | 1.2618(5)| 1.50(3) | 1.659(5)        | 2.14(4)              | 0.276(7) | 370(20)  |
|        | 1.2618(7)| 1.50(6) | 1.657(6)        | 2.14(6)              | 0.281(4) | 374(10)  |
|        | 1.2630(13)| 1.76(17)| 1.647(12)       | 2.33(15)             | 0.291(5) | 401(11)  |
TABLE 2. Comparison of estimated critical exponents $z$ and prefactor $A$ for global demons, HMC-1, HMC-S and HMC-L, where $\tau = A\xi^z$. Measurements were performed on a $64^2$ lattice, with 160K/T statistics.

|                | $z$ | $A$ |
|----------------|-----|-----|
| $Lattice\ Magnetization\ M:\$ |     |     |
| Global Demons  | 1.3 | 2.4 |
| HMC-1          | 2.0 | 5.7 |
| HMC-S          | 1.3 | 6.9 |
| HMC-L          | 1.05| 5.8 |

| $Single\ Spin\ S:\$ |     |     |
| Global Demons       | 0.8 | 1.0 |
| HMC-1               | 1.5 | 1.6 |
| HMC-S               | 1.0 | 1.6 |
| HMC-L               | 1.0 | 4.3 |

| $Potential\ Energy\ E:\$ |     |     |
| Global Demons         | 0.5 | 0.8 |
| HMC-1                 | 1.0 | 1.9 |
| HMC-S                 | 1.4 | 2.1 |
| HMC-L                 | 1.3 | 14  |

| $Topological\ Charge\ Q:\$ |     |     |
| Global Demons           | 0.8 | 0.8 |
| HMC-1                   | 1.0 | 1.4 |
| HMC-S                   | 1.3 | 1.6 |
| HMC-L                   | 1.3 | 8.2 |
TABLE 3. Auto-correlation times for total magnetization $M$, a single spin $S$, topological charge $Q$ and internal energy $E$, and the magnetization correlation length $\xi$. Measurements were performed on a $64^2$ lattice, with 160K/T statistics.

| $\beta$ | $\tau_M$ | $\tau_S$ | $\tau_E$ | $\tau_Q$ | $\xi$ |
|---------|---------|---------|---------|---------|------|
| Global Demons : | | | | | |
| 0.70 | 6.5 | 1.86 | 1.14 | 1.53 | 2.2 |
| 0.78 | 11.8 | 2.6 | 1.38 | 1.97 | 3.4 |
| 0.82 | 16.8 | 3.2 | 1.57 | 2.5 | 4.3 |
| 1/1.1 | 47. | 5.9 | 2.2 | 4.5 | 9.4 |
| 1/1.07 | 62. | 7.8 | 2.4 | 5.5 | 12.8 |
| 1/1.04 | 106. | 10.3 | 3.1 | 8.8 | 18.4 |
| 1.0 | 124. | 22. | 2.8 | 9.5 | 31. |

| HMC-1 : | | | | | |
| 0.70 | 27. | 5.1 | 4.1 | 3.2 | 2.2 |
| 0.78 | 62. | 9.2 | 5.9 | 4.8 | 3.3 |
| 0.82 | 106. | 12.1 | 7.9 | 6.2 | 4.3 |
| 1/1.1 | 380 | 36. | 15.7 | 13.5 | 8.9 |
| 1/1.04 | 1620 | 99. | 30. | 26. | 17.1 |

| HMC-S : | | | | | |
| 0.70 | 17.9 | 3.7 | 6.2 | 4.0 | 2.2 |
| 0.78 | 32. | 5.5 | 12.6 | 8.0 | 3.3 |
| 0.82 | 44. | 7.4 | 18. | 10.5 | 4.3 |
| 1/1.1 | 126. | 14. | 50. | 31. | 9.3 |
| 1/1.04 | 240 | 32. | 132. | 59. | 17.5 |

| HMC-L : | | | | | |
| 0.70 | 12.7 | 9.3 | 36. | 22. | 2.2 |
| 0.78 | 21. | 15.5 | 66. | 38. | 3.4 |
| 0.82 | 29. | 20. | 136. | 61. | 4.3 |
| 1/1.1 | 64. | 40. | 144. | 132. | 9.5 |
| 1/1.04 | 114. | 84. | 760 | 350 | 17.7 |
FIGURES

1. Time evolution of $10^3$ connected points evolving according to ‘canonical’ rather than microcanonical dynamics for (a) the 1-d harmonic oscillator $H = (p^2 + q^2)/2$ (left column; $t = 0$ points lie on the unit circle), and (b) the $SU(2)$ Hamiltonian $H = J_z^2/2$ (right column; $t = 0$ points lie on the circle $J_z = 0.5$), both at $\beta = 1$. The phase space in (a) is $(q, p)$ and in (b) it is the sphere parameterized by $(J_x, J_y, J_z)$. The rapid spreading of neighboring points is characteristic of global demon dynamics. The characteristic time scale is $t \sim 1$.

2. Finite time step extrapolations, demonstrating the global $O(dt^2)$ leapfrog error for (a) potential energy, (b) topological charge and (c) magnetization.

3. Diffusiveness of a global demon trajectory versus the coupling strength, for selected values of $\beta$. $\Delta S$ is measured at intervals of $T = 1$. The ‘optimal’ value of $\sqrt{\langle \Delta S^2 \rangle} = \sigma$ is indicated by the dashed line. As can be seen, the dynamics is not strongly affected by critical slowing down. Saturation occurs when $\kappa_\alpha \sim O(\sqrt{2n}) \sim 23$. The optimal coupling can be seen to be independent of both $\beta$ and the phase transition.

4. Diffusiveness of the global demons versus $\beta$. The dip at $\beta \sim 1$ is a result of the Kosterlitz-Thouless phase transition and critical slowing down. The dynamics is not strongly effected by the transition, so no additional tuning is required, and $\kappa$ can be taken as fixed for all $\beta$.

5. Measurement dependence on the coupling $\kappa$ at $\beta = 1/1.1$.

6. Diffusiveness of a global demon trajectory a function of the trajectory length $T$, at $\beta = 1$, $\kappa_1 = \kappa_2 = 16$. Saturation can be seen, indicating an optimal trajectory length of $T \sim O(1)$.

7. Autocorrelation functions for potential energy, topological charge, magnetization and spin, at $\beta = 1/1.1$ with $\kappa_1 = \kappa_2 = 1$ (dots) and $\kappa_1 = \kappa_2 = 16$ (solid). As can be seen, the ringing vanishes as the coupling increases.

8. Autocorrelation functions for potential energy, topological charge, magnetization and spin, at $\beta = 1/1.1$ for global demons with $\kappa_1 = \kappa_2 = 16$ (solid), HMC-1 (dots), HMC-S (crosses) and HMC-L (boxes). For global demons and HMC-1, measurements are made every $t = 1$, while for HMC-S,L, the boxes and crosses indicate the actual number of data points.

9. Lattice magnetization auto-correlation function at selected temperatures for global demons (solid), HMC-1 (dots), HMC-S (dashes) and HMC-L (boxes). The time axis for $\beta = 0.7$ has been scaled by a factor of 0.1 to magnify the short time behavior.

10. The behavior of $\tau = a \xi^z$ is plotted near the phase transition on a $64^2$ lattice for (a) total magnetization, (b) the spin at the origin, (c) topological charge and (d) potential energy. In each figure, we indicate the results for HMC (boxes), HMC-$s$ (diamonds), HMC-$l$ (crosses) and global demons (circles). Critical exponents can
be extracted from a linear fit. The results of the numerical fits are given in Table 2. Results are on a $64^2$ lattice with $160K/T$ statistics.

11. Decorrelation times versus coupling strength for $\beta = 0.5$ (squares), 0.7 (diagonal crosses), 1/1.1 (diamonds), 2.0 (vertical crosses) and 4.0 (circles) for (a) total magnetization, (b) a single spin, (c) topological charge and (d) potential energy.

12. Decorrelation times versus $\beta$ for couplings $\kappa_1 = \kappa_2 = 1$ (crosses), 4 (diamonds), 16 (squares) and 64 (circles) for (a) total magnetization, (b) a single spin, (c) topological charge and (d) potential energy. The rise at $\beta \sim 1$ is critical slowing down, and is especially evident for the energy and topological charge.