Embedded Dynamics for ϕ^4 Theory

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A new Monte Carlo dynamics is proposed for ϕ^4 field theory that reduces critical slowing down. Discrete Ising variables are embedded into the field theory, so that large-scale tunneling events can be induced via a modified Swendsen-Wang algorithm with fluctuating site-bond percolation probabilities. The measured dynamical critical exponents $z_{\mathrm{ED}}=0.07\pm0.07$, 0.29 ± 0.09, and 0.87 ± 0.20 in one, two, and three dimensions, respectively, are consistent with our conjecture that this embedded dynamics lies in the same universality class as the Swendsen-Wang Ising dynamics.

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Monte Carlo simulations have become increasingly important as a tool in studying complex statistical systems and fundamental properties of quantum field theory. Also they provide a pseudodynamics to probe quasiequilibrium processes crucial in nucleation, domain formation, and phase stability. Greater insight into the dynamics of algorithms is fundamental both to the underlying physics and to finding faster algorithms. In particular, all local algorithms suffer from critical slowing down as one approaches a phase transition. To avoid it one must define appropriate nonlocal (or collective) variables and a new dynamics for driving them.

Progress has been made recently with some nonlocal algorithms for discrete spin models. Swendsen and Wang[1] have used the Fortuin-Kastelyn[2] (FK) percolation map for the Potts model to define collective coordinates that allow domains to be inverted with zero free-energy cost. Further improvements are possible by introducing multigrid methods.[3]

However, ϕ^4 theory presents new opportunities and challenges. It is an obvious starting point for developing new algorithms viewed either as a prototype for the quantum field theory of Higgs particles or as the standard Landau-Ginzburg-Wilson effective free energy for phase separation. But existing techniques such as Fourier acceleration[4] and multigrid[5,6] methods, while offering significant speedup in the regions where the fluctuations are dominately Gaussian, so far have been demonstrated to reduce the exponent z, controlling critical slowing down, below the Glauber value.[7]

Here we propose a scheme that succeeds in reducing this dynamic exponent. Our idea is to embed discrete variables, which are responsible for the dynamical critical properties, into the continuous field theory. In ϕ^4 theory, we know that the critical point is caused by the condensation of instantons (or kinks in the one-dimensional double-well potential). The instantons are not well approximated by harmonic fluctuations. Therefore, we introduce discrete variables s_x,

$$\phi_x = s_x\,|\phi_x|\,, \tag{1}$$

that label the two vacua. At fixed values of $|\phi(x)|$ a ferromagnetic Ising model is embedded into the ϕ^4 field theory and a modified nonlocal Swendsen-Wang dynamics drives instanton formation. This substantially accelerates the dynamics.

Consider the Euclidean action for the ϕ^4 theory,

$$S(\phi)=\tfrac{1}{2}\sum_{\langle x,x'\rangle}(\phi_x-\phi_{x'})^2+\sum_x(\tfrac{1}{2}\mu\phi_x^2+\lambda\phi_x^4)\,, \tag{2}$$

on a d-dimensional hypercubic lattice with L^d sites and periodic boundary conditions, where the sum runs over nearest-neighbor link, $\langle x,x'\rangle$. The probability density is

$$dP(\phi)=Z^{-1}e^{-S(\phi)}\prod_x d\phi_x\,, \tag{3}$$

where the partition function is

$$Z=\prod_x\int_{-\infty}^{+\infty}d\phi_x\,e^{-S(\phi)}\,. \tag{4}$$

A Monte Carlo dynamics approximates the L^d integrations over ϕ_x by a selection of configurations chosen with frequency given by the probability distribution $dP(\phi)$. The difficulty with critical slowing down is encountered when one chooses a Markov process $W(\phi'\leftarrow\phi)$ which makes only local changes in the variables. As you approach the phase transition, coherent domains develop and the correlation length diverges ($\xi\rightarrow\infty$). The local changes move the domain walls by diffusion resulting in autocorrelations that increase like ξ^z with $z\simeq2$.

To emphasize this picture, the action for μ negative is expressed as

$$S(\phi)=\tfrac{1}{2}\sum_{\langle x,x'\rangle}(\phi_x-\phi_{x'})^2+\sum_x\lambda(\phi_x^2-\phi_{\min}^2)^2\,, \qquad (5)$$

with a double-well potential. In the continuum approximation the two vacua, located at $\phi_x=\pm\phi_{\min}=\mp\mu/4\lambda$, are connected by the kink solution, $\phi_x^{\text{kink}}\simeq\phi_{\min}\times\tanh(x\sqrt{-\mu})$. So we introduce discrete variables s_x to connect the two vacua and a new Swendsen-Wang dynamics to increase their mobility:

$$S(s_x,|\phi_x|)=-\sum_{\langle x,x'\rangle}\beta_{xx'}s_xs_{x'}+\sum_x[d|\phi_x|^2+\lambda(|\phi_x|^2-\phi_{\min}^2)^2]\,. \qquad (6)$$

At fixed $|\phi(x)|=s_x\phi_x$, the effective spin-spin coupling is $\beta_{xx'}=|\phi_x\phi_{x'}|$. For future reference note that as $\lambda\to\infty$ with $\phi_{\min}$ fixed, there are sharp minima in the potential at $\pm\phi_{\min}=\pm\sqrt{\beta}$, and so we expect to get nearly pure Ising dynamics with small fluctuations in the effective $\beta_{xx'}$ around the inverse Ising temperature $\beta=(\mu/4\lambda)^2=1/kT$.

The update algorithm consists basically of two parts: a conventional Monte Carlo update for the ϕ_x field and a Swendsen-Wang sweep for the embedded Ising variables s_x. The detailed procedure is as follows:

(i) Update the ϕ_x fields via a standard local Monte Carlo algorithm. For simplicity, we choose one pass of a local heat-bath algorithm implemented via multiple Gaussian random hits.

(ii) At fixed $|\phi_x|$ introduce an effective Ising-type system,

$$e^{-S_{\text{Ising}}}=\prod_{\langle x,x'\rangle}e^{\beta_{xx'}(s_xs_{x'}-1)}=\prod_{\langle x,x'\rangle}[(1-e^{-2\beta_{xx'}})\delta_{s_x,s_{x'}}+e^{-2\beta_{xx'}}]\,, \qquad (7)$$

and form site-bond percolation clusters dictated by the joint probability,

$$P(s_x,n_{xx'})=Z_{\text{Ising}}^{-1}\prod_{\langle x,x'\rangle}[(1-e^{-2\beta_{xx'}})\delta_{s_x,s_{x'}}\delta_{n_{xx'},1}+e^{-2\beta_{xx'}}\delta_{n_{xx'},0}]\,. \qquad (8)$$

Thus percolation is controlled by a variable bond probability (or edge-contraction probability in FK terminology),

$$p_{xx'}=1-e^{-\beta_{xx'}(1+s_xs_{x'})}=1-e^{-(|\phi_x||\phi_{x'}|+\phi_x\phi_{x'})}\,. \qquad (9)$$

(iii) Update the Ising variables subject to the constraint of Eq. (8) that percolation clusters are flipped coherently with 50% probability, and repeat the above cycle.

The beauty of the Swendsen-Wang update step is that the entropy of the percolated cluster formation *exactly* cancels the surface energy to give zero free-energy cost. Detailed balance is guaranteed by the condition that summing out the percolation variables, $n_{xx'}$, in the joint distribution, $P(s_x,n_{xx'})$, of Eq. (8) yields the correct Ising distribution of Eq. (7).

Arguments analogous to those advanced by Fortuin and Kasteleyn[2] and Coniglio and Klein[8] suggest that the connectedness length for percolation diverges at the critical surface of the ϕ^4 theory just as it does for the pure Ising or Potts systems, and numerical evidence given below supports this conjecture. Additional insight into the consequences of the Fortuin-Kasteleyn mapping in mean-field-theory context can be seen in the recent paper of Klein, Ray, and Tamayo.[9]

We have done a variety of simulations to compute static and dynamic exponents. We measure the autocorrelation times for four operators, the energy (or action) density, and three measures of "magnetization" by summing over the operators, ϕ_x, $\text{sgn}(\phi_x)$, and $|\phi_x|$, respectively. Since our dynamics averages over the sign of ϕ_x the most useful one is the $|\phi_x|$ magnetization measure. The measurement of autocorrelation length τ is based on an exponential fit, $\text{const}\times e^{-t/\tau}$, to the autocorrelation functions.

Knowing the corresponding values of τ for different values of the correlation length ξ allow us to compute the critical exponent z using $\tau\sim\xi^z$ or $\tau\sim L^z$ if finite-size scaling is used. Static exponents are measured from the susceptibility, the specific heat, the correlation length, and the connectedness length of percolation clusters.

The numerical results from our main simulation are summarized in Fig. 1. We simulated the $d=2$, ϕ^4 theory at $\lambda=0.1$ and varied both the size of the lattice (in order to use finite-size effects) and the mass parameter μ in the neighborhood of the critical surface $\mu\simeq-0.6$. The same value of λ was used by Goodman and Soka[6] because it was sufficiently close to the Gaussian theory ($\lambda=0$) to show considerable speedup for their multigrid approach. It is interesting that our value for $z_{\text{ED}}=0.29\pm0.09$ is clearly less than the z_G for Glauber dynamics and it is consistent with the value found for the $d=2$ Is-

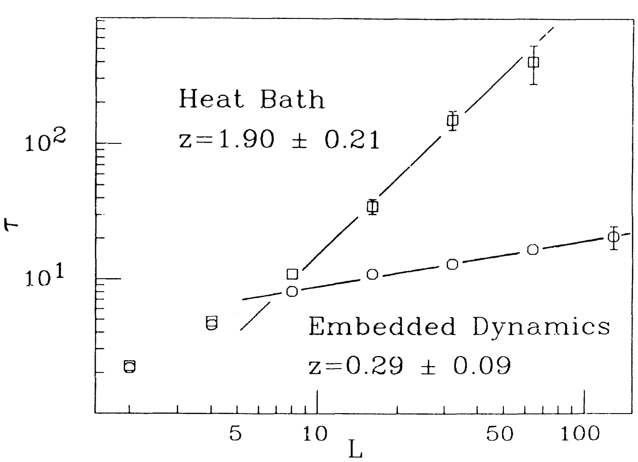

FIG. 1. Autocorrelation times τ for $d=2$ ϕ^4 theory using pure heat bath and our Swendsen-Wang embedded algorithm.

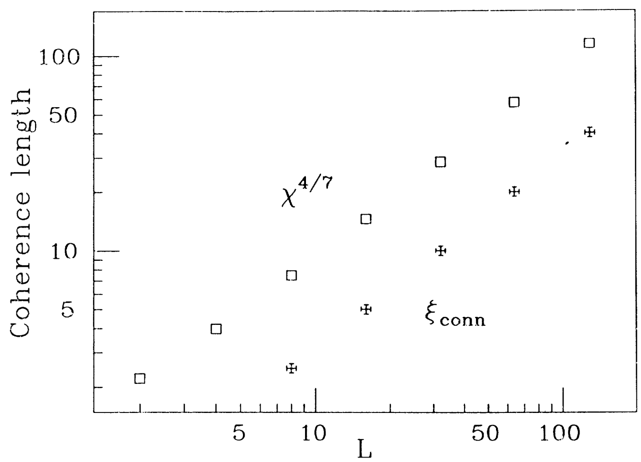

FIG. 2. Static scaling laws for $d=2$ ϕ^4 theory: susceptibility χ and the connectedness length ξ_{conn} for the associated site-bond diluted percolation.

ing model in the Swendsen-Wang dynamics. We have also checked the static exponent γ/ν and the divergence of the connectedness length to confirm that we are inside the scaling region and that we are approaching a critical point for our percolation process (see Fig. 2).

Our main observation is that up to statistical errors the values for the critical exponents z_{ED} for the ϕ^4 theory embedded dynamics are the same as the exponents z_{SW} found for the Swendsen-Wang Ising dynamics (see Tables I and II).

The critical region forms a surface (line) in the λ-μ plane with an infrared unstable Gaussian point at $\lambda=0$, $\mu=0+$ and a nontrivial ir-stable fixed point at $\lambda=\infty$, $\mu=-\infty$. For fixed λ the correlation length diverges as $|\mu-\mu_{crt}|^{-\nu}$. Although universality requires that the divergence of static quantities and hence the static exponents be the same independent of where you approach the critical surface between the two fixed points, the universality for z in our nonlocal dynamics is not guaranteed. However, on the basis of numerical evidence, we conjecture that embedded dynamics lies in the same universality class as the Swendsen-Wang so-called "nonuniversal" Ising dynamics.[1]

Further evidence of this equivalence was sought by running our algorithm at other values of λ in $d=2$ and in other dimensions. Since we know that there has to be a crossover to $z_{ED}=z_{SW}$ at infinite λ the important thing to check is the λ independence of our exponent z_{ED} at small λ.

We also note that for smaller λ in $d=2$ as we vary the lattice size the crossover from heat-bath dynamics to accelerated dynamics is delayed. We are investigating the possibility that this is due to the critical slowing caused by purely Gaussian fluctuations. If this is the case, by introducing multiscale dynamics that give $z=0$ in the pure Gaussian case we expect to "expose" the accelerated dynamics at shorter length scales.

For $d=1$, we can show analytically that the Swendsen-Wang dynamics gives $z=0$, and so our numerical agreement is especially significant here.[12] Our computation consists of finding the eigenvectors of the transition matrix $W(s_x' \leftarrow s_x)$ for the Swendsen-Wang dynamics in $d=1$. The eigenvalues are integer powers of $e^{-1/\tau}$, where $1/\tau = \ln[(1-e^{-2\beta})/2]$. As you approach the fixed point $\beta\rightarrow\infty$ the critical slowing down never sets in, in contrast with Glauber dynamics with $z=2$. Similarly, we can also show that z_{SW} vanishes as q goes to zero in the Swendsen-Wang q-state Potts model.[13] For ϕ^4 theory, a similar computation can be performed in the limit of a gas of kinks, yielding

$$1/\tau \simeq \ln[(1-e^{-E_{kink}})/2] ,$$

where $E_{kink}=\mu^{3/2}/3\sqrt{2}\lambda$.

More simulations are being pursued, particularly in the physical interesting dimension of $d=4$ for the quantum field theory of scalar particles.

In conclusion, we have shown how the instanton coordinates of the Fortuin-Kasteleyn percolation clusters can be used to accelerate the simulations of ϕ^4 field theory. We are also looking at faster algorithms for the "small" fluctuations cycle to replace our heat-bath algorithm. In fact, if you think of the system as combining solitons and Gaussian fluctuations, an obvious idea is to combine the Swendsen-Wang cycle with a multigrid or Fourier-acceleration cycle.

Finally, we are investigating applications of our embedded dynamics to other field theories: the xy model, complex ϕ^4 field theory, the nonlinear σ models, and Abelian and non-Abelian gauge models. Various embed-

TABLE I. Critical exponents for the ϕ^4 embedded dynamics.

Dimension	z_{ED}	γ/ν	ν_{conn}
1	0.07 ± 0.07	1.01 ± 0.02	0.87 ± 0.10
2	0.29 ± 0.09	1.75 ± 0.01	1.01 ± 0.01
3[a]	0.87 ± 0.20	...	...

[a]Reference 10.

TABLE II. Critical exponents for the Swendsen-Wang Ising dynamics.

Dimension	z_{SW}	γ/ν[a]
1	0.06 ± 0.06[b]	1
2	0.35 ± 0.01[c]	7/4
3	0.75 ± 0.01[c]	1.953

[a]Reference 11.
[b]Reference 12.
[c]Reference 1.

ding schemes can be found that respect detailed balance, and algorithms are being tested.[14] However, since the essence of our approach is to express the dynamics in terms of the appropriate excitations and collective modes, we will not hazard a prediction of success for these new systems. The peculiar physics of each phase transition can be crucial. Just as there are universality classes for static properties of phase transitions, we expect new universality classes of efficient embedded schemes.

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[10]Our current simulations do not give a reliable static exponent in three dimensions, but we are planning a much longer run on the connection machine in three and four dimensions to be presented in a more detailed followup article on embedded dynamics.

[11]Data from tabulation in D. J. Amit, *Field Theory, the Renormalization Group, and Critical Phenomena* (World Scientific, Singapore, 1984), 2nd ed.

[12]Our numerical result is consistent with Swendsen's (private communication) and our theoretical value of $z_{SW}=0$ in $d=1$.

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