Multigrid Acceleration for Asymptotically Free Theories

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We present a multigrid Monte Carlo algorithm with piecewise-linear interpolation operator for nonlinear σ models with global chiral $SU(N)\times SU(N)$ symmetry or CP^{N-1} manifold. We demonstrate its efficiency in the two-dimensional $SU(3)\times SU(3)$ chiral model and the CP^3 nonlinear σ model for correlation length up to 77 in lattice units. On lattices up to size 512×512 we achieve almost complete elimination of critical slowing down in the CP^3 case, with a dynamical critical exponent $z_{MGMC}=0.2\pm 0.1$. Asymptotic scaling with the bare coupling does not appear to set in for the standard action of both models in the range of parameters studied.

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1. Introduction.—The development of nonlocal Monte Carlo algorithms which avoid critical slowing down has opened a new field of interest in computational physics. On the one hand, cluster algorithms for discrete [1] and continuous [2] spin models have proven to be extremely effective in reducing critical slowing down. However, it is not clear whether these methods can be extended effectively to continuous-spin models other than N-vector models, e.g., to general σ models or lattice gauge theories [3]. On the other hand, a second promising approach to overcoming critical slowing down is the implementation of multigrid ideas for Monte Carlo simulations [4-6].

Two-dimensional nonlinear σ models with a non-Abelian global symmetry group are asymptotically free and share many properties with four-dimensional gauge theories [7]. Besides the $O(N)$-invariant vector models, the principal chiral models with global $SU(N)\times SU(N)$ invariance and the CP^{N-1} models have been studied on the lattice for the last decade.

In this Letter we present a multigrid Monte Carlo algorithm for general nonlinear σ models and apply it to some two-dimensional σ models. A first test of this multigrid algorithm for the asymptotically free two-dimensional $O(3)$ nonlinear σ model was very promising: The dynamical critical exponent z was reduced to $z_{MGMC}=0.2\pm 0.1$ [8]. Here we apply this algorithm to the two-dimensional $SU(3)\times SU(3)$ chiral model and to the CP^3 model, for which cluster algorithms are believed [3] to be ineffective.

2. $SU(N)\times SU(N)$ and CP^{N-1} σ models.—A class of nonlinear σ models of great interest are the principal chiral models with global $SU(N)\times SU(N)$ invariance. For the color group $SU(3)$ they share the type of variables with QCD and in four dimensions they turn out to be an effective field theory of light mesons. Within the Migdal recursion relation the 2D models have the same renormalization-group trajectories as pure $SU(N)$ lattice gauge theories in four dimensions [9]. The existence of non-Abelian vortices is an interesting nonperturbative aspect of these models.

The chiral $SU(N)\times SU(N)$ models are defined on a two-dimensional square lattice $L\times L$ with periodic boundary conditions by the action

$$S=-\tfrac{1}{2}\beta\sum_{\langle i,j\rangle}(\mathrm{tr}U_iU_j^\dagger+\mathrm{H.c.})\,, \tag{1}$$

where U_i is a $SU(N)$ matrix in the fundamental representation, the sum runs over all nearest-neighbor pairs, and β is the coupling constant. The theory is in a disordered phase for all β and finite $N\geq 2$ with susceptibility χ defined by $\chi=(1/L^2)\sum_{i,j}\mathrm{Re\,tr}(U_iU_j^\dagger)$.

σ models which have a topological structure are very similar to $SU(N)$ gauge theories in four dimensions [10]. The CP^{N-1} manifold is a $(2N-1)$-dimensional sphere, where points related by a $U(1)$ transformation are identified. A simple choice of the lattice action for the CP^{N-1} model, which preserves this local $U(1)$ gauge invariance, is given by

$$S=2\beta\sum_{\langle i,j\rangle}(1-|\bar{z}_i\cdot z_j|^2)\,, \tag{2}$$

where z_i is a N-component complex unit vector and β is the coupling constant. The CP^{N-1} models are in a disordered phase for all finite values of N—the CP^1 model is equivalent to the $O(3)$ nonlinear σ model—and for all inverse temperatures β. The correlation length is obtained from the exponential decay of the invariant connected two-point function $G(i,j)=\langle|\bar{z}_iz_j|^2\rangle-1/N$, while the magnetic susceptibility χ is given by $\chi=(1/L^2)\sum_{i,j}G(i,j)$.

The critical behavior for $\beta\to\infty$ of all nonlinear σ models is governed by the perturbative renormalization group, which implies asymptotic freedom, and the correlation length should scale with the first two universal coefficients [11] of the renormalization-group β function.

3. Multigrid algorithm.—Updates on the various levels of a multigrid system can be viewed as nonlocal updates on the corresponding fundamental system. This unigrid point of view needs less formalism to describe the algorithm, and furthermore it is more general in the sense that not all nonlocal changes of the fundamental field configuration can be interpreted as single site changes on a multigrid system.

We use a Metropolis algorithm to update the system. But the proposals for a new field configuration are in general nonlocal. They are given by

$$U_j' = \exp(-i\Psi A_j \lambda_l) U_j \quad (3)$$

for the chiral $SU(N)\times SU(N)$ symmetric models, where λ_l is a generator of the $SU(N)$ group and

$$z_j' = \exp(-i\Psi A_j \lambda_l) z_j \quad (4)$$

for the CP^{N-1} model, where λ_l is a generator of the $U(N)$ group. Ψ is a random number with an even probability distribution.

The kernels A_j determine the relative amplitude of the change of the fields at the sites j. The A_j are chosen such that they are only nonzero within $L_B \times L_B$ blocks and the average over the block is normalized to 1. In the spin-wave approximation one can exactly calculate the mean step size $\langle\Psi\rangle$ of the heat bath version of this algorithm [12]. In two dimensions for at least piecewise linear kernels the mean step size $\langle\Psi\rangle$ is constant for increasing block sizes L_B, while it decreases like $1/L_B^{1/2}$ for kernel A_j = const within a block. In our numerical work we used kernels with a pyramidal shape.

These elementary updates build whole cycles. First we sweep through the fundamental lattice with a local Metropolis update, next over all disjoint blocks $L_B = 2, 4, \ldots$ and so on up to the maximum block size $L_{B_{\max}} = L/2$, and then start the new cycle again with a local Metropolis sweep. The computational effort for such a V cycle grows roughly like $L^d \ln L$ [6].

In order to reduce the computational effort of the algorithm we use the same generator λ_l, which is randomly selected, for all updates within one cycle. The updates with this single generator can be interpreted as updates of an embedded two-dimensional XY model with the action

$$S = -\tfrac{1}{2}\beta \sum_{\langle i,j\rangle} \{\mathrm{tr}\exp[-i(\phi_i-\phi_j)\lambda_l] U_i U_j^\dagger + \mathrm{H.c.}\} \quad (5)$$

for the chiral $SU(N)\times SU(N)$ models and

$$S = 2\beta \sum_{\langle i,j\rangle} [1 - |\overline{\exp(-i\phi_i\lambda_l) z_i} \exp(-i\phi_j\lambda_l) z_j|^2] \quad (6)$$

for the CP^{N-1} models, where we set the real variables $\phi_i = 0$ at the beginning of each cycle. After one cycle the original fields are changed according to

$$U_i' = \exp(-i\phi_i\lambda_l) U_i \quad (7)$$

in the case of the chiral $SU(N)\times SU(N)$ models and

$$z_i' = \exp(-i\phi_i\lambda_l) z_i \quad (8)$$

in the case of the CP^{N-1} models. Test runs on small lattices showed that the block updates need overlap. We satisfied this demand by translating the fields after each cycle by a randomly chosen distance.

In order to reduce the dependence of the Markov chain on the special properties of our Metropolis implementation, we use a 10-hit Metropolis update for the simulations discussed in the following.

4. Numerical results.—We did numerical studies of the performance of this multigrid Monte Carlo algorithm with piecewise linear kernels for the 2D chiral $SU(3)\times SU(3)$ and the CP^3 nonlinear σ models.

The autocorrelation time τ is used to measure the speed with which statistically independent configurations are generated. Its dependence on the correlation length ξ is parametrized by the dynamical critical exponent $\tau \propto \xi^z$.

We calculated integrated autocorrelation times τ_{int} from the normalized autocorrelation function $\rho(t)$ with a self-consistent truncation window of width $4\tau_{\mathrm{int}}$ [13] for the energy E and the magnetic susceptibility χ.

For both models we find $\tau_{\mathrm{int}}^E < \tau_{\mathrm{int}}^\chi$ and an exponential falloff with a single decay constant in all our runs. We determine the correlation length ξ by fitting the invariant zero-momentum correlation functions to

$$G(x) \propto \exp\left(-\frac{x}{\xi}\right) + \exp\left(-\frac{L-x}{\xi}\right) \quad (9)$$

in the interval ξ–3ξ and checked the stability and significance of these fits by comparing with further fits in the intervals $\frac{1}{2}\xi$–$\frac{3}{2}\xi$, ξ–2ξ, up to as large a distance as a fit can be obtained. The error is estimated by a jack knife analysis. In Fig. 1 the zero-momentum correlation function of the CP^3 model on a $L=512$ lattice and a coupling $\beta=3.3$ is plotted together with the fit Eq. (9) with $\xi=77.7$. For distances x smaller than ξ contributions of states of higher energy are not negligible, but for larger distances the fit is quite satisfying. The results for the chiral $SU(3)\times SU(3)$ and the CP^3 model of these fits are gathered in Table I.

Using these measurements of ξ and the autocorrelation times τ_{int} we estimate the dynamical critical exponents of the conventional Metropolis updating and our multigrid algorithm. In Fig. 2 a log-log plot of τ_{int} versus the correlation length ξ for both Metropolis and multigrid updating of the CP^3 model is shown. We have two subsets of data with $L/\xi \approx 7$ (five data points) and $L/\xi \approx 14$

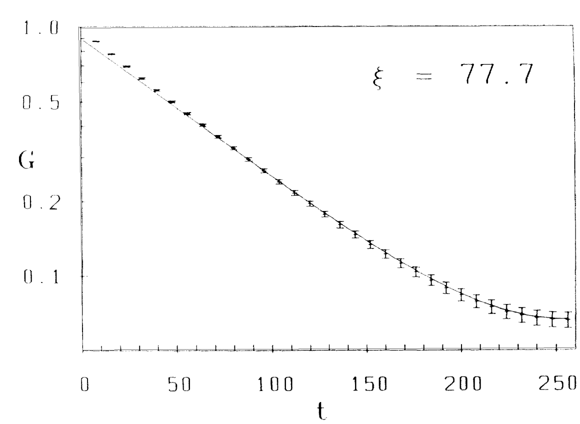

FIG. 1. The zero-momentum correlation function of the CP^3 model on a $L=512$ lattice and a coupling $\beta=3.3$ is plotted together with the fit Eq. (9) with correlation length $\xi=77.7$.

TABLE I. From top to bottom: data from Monte Carlo runs of the chiral SU(3)×SU(3) model with multigrid updating followed by CP^3 model data from local Metropolis and multigrid updating, with lattice size L, coupling β, statistics (stat), correlation length ξ, susceptibility χ, and integrated autocorrelation times τ_{int} of χ.

L	β	stat	ξ	χ	τ_{int}
16	1.4	200*k*	2.28(4)	34.1(3)	42(3)
32	1.5	100*k*	3.07(7)	57.5(5)	40(5)
64	1.5	30*k*	3.05(8)	57.5(7)	16(2)
64	1.65	50*k*	5.41(8)	145(2)	26(4)
64	1.75	60*k*	8.54(16)	307(5)	65(9)
128	1.75	40*k*	8.27(11)	297(4)	31(4)
128	1.85	70*k*	13.2(2)	629(10)	65(8)
256	1.85	20*k*	12.8(2)	619(14)	45(8)
256	1.92	40*k*	17.4(2)	1031(18)	40(5)
256	2.00	40*k*	25.3(3)	1915(36)	56(8)
256	2.10	40*k*	36.6(5)	3868(90)	72(13)
32	2.3	120*k*	2.64(5)	11.2(1)	50(3)
32	2.5	400*k*	4.4(1)	25.9(6)	172(24)
32	2.6	1200*k*	6.5(2)	45.9(5)	340(24)
32	2.5	120*k*	4.49(6)	26.2(3)	28(2)
64	2.5	40*k*	4.54(4)	26.6(3)	22(2)
32	2.6	80*k*	6.49(4)	45.8(3)	21(1)
64	2.7	40*k*	8.82(13)	79.6(1.1)	26(3)
128	2.7	28*k*	8.76(12)	79.2(1.3)	30(4)
128	2.9	28*k*	18.5(6)	273(3)	38(4)
256	2.9	28*k*	18.4(4)	276(3)	31(3)
256	3.1	40*k*	38.2(6)	933(12)	41(4)
512	3.1	28*k*	37.1(6)	922(11)	37(3)
512	3.3	40*k*	77.7(1.4)	3034(50)	48(6)

(four data points), respectively. Within these data subsets the unknown scaling function $g(\xi/L)$ of the dynamic scaling ansatz $\tau_{int}=g(\xi/L)\xi(\beta,L)^z$ varies very little. A fit to these subsets following $\tau_{int}\propto\xi^z$ gives for z_{MGMC} $=0.20(4)$ (upper line) and $z_{MGMC}=0.23(6)$ (lower line) with a χ^2/N_{DF} of order 1. For the chiral SU(3)×SU(3) model we do not have enough data yet to do this finite-size scaling analysis [14].

We can now use our simulation data to look for asymptotic scaling with the bare coupling constant. The defect δ_m of the mass gap $m=1/\xi$ is obtained by dividing the inverse correlation length by the universal two-loop result, and the renormalization group predicts that δ_m should go to a constant as $\beta\to\infty$. But Figs. 3(a) and 3(b) show that this behavior does not describe our data for both models. In the chiral SU(3)×SU(3) model our last two data points may indicate an approach to a constant. We are presently performing simulations on $L=512$ lattices to check for finite-size effects at these two couplings [14].

But the mass-gap defect data in the CP^3 model, shown in Fig. 3(b), indicate substantial scaling violations. This effect seems even more pronounced than in the O(3) nonlinear σ model [15,16].

Our results are consistent with previous numerical studies of the chiral SU(3)×SU(3) model [17–20] and the CP^3 model [21–23]. But we would like to mention

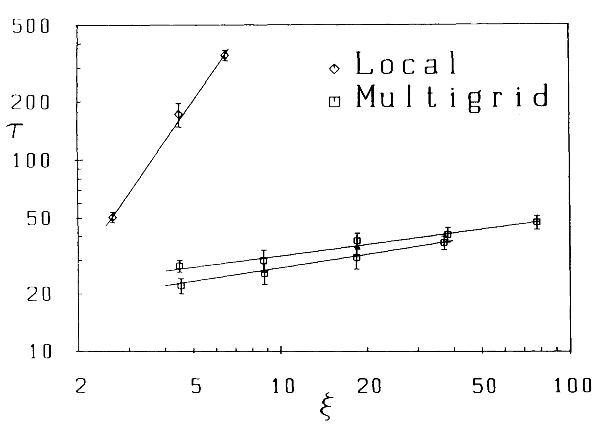

FIG. 2. Log-log plot of autocorrelation time τ_{int} vs the correlation length ξ for Metropolis and multigrid updating of the CP^3 model. The straight lines are fits with dynamical critical exponents $z_{Met}=2.15\pm0.10$ and $z_{MGMC}=0.20\pm0.04$ (upper line) and $z_{MGMC}=0.23\pm0.06$ (lower line).

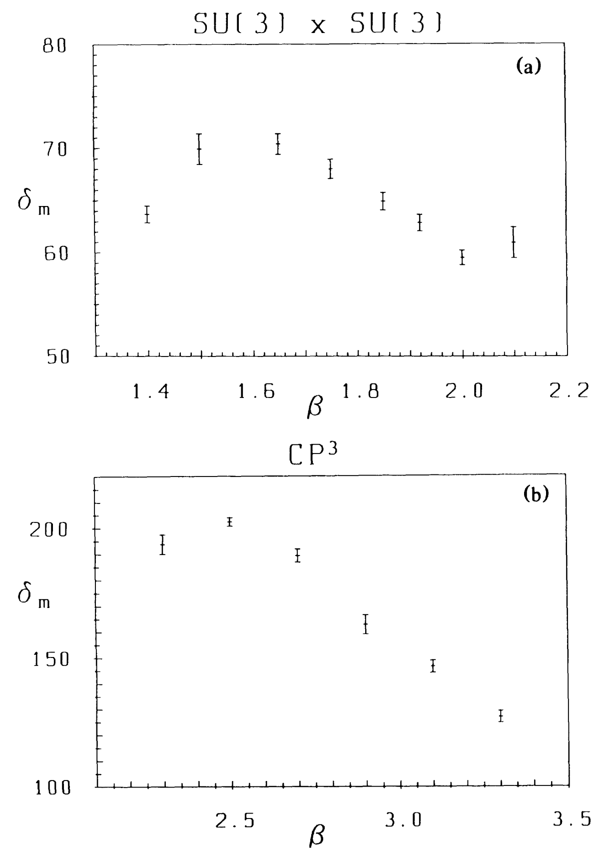

FIG. 3. (a) The mass-gap defect $\delta_m=m(4\pi\beta/3)^{-1/2}e^{4\pi\beta/3}$ vs the coupling β for the chiral SU(3)×SU(3) model. (b) The mass-gap defect $\delta_m=m(\pi\beta)^{-1/2}e^{\pi\beta}$ vs the coupling β for the CP^3 model.

that only Ref. [20] uses an accelerated algorithm and that the largest correlation length in the chiral SU(3)×SU(3) model is $\xi=10$ and in the CP^3 model is $\xi=38$, but typically with an error of 25%. Further details of our simulation including measurements of the topological susceptibility will be published elsewhere [14].

We have demonstrated that the multigrid Monte Carlo algorithm with piecewise linear interpolation almost completely eliminates critical slowing down for nonlinear σ models with a general global symmetry group. The substantial improvement in efficiency allows us to study the chiral SU(3)×SU(3) and the CP^3 much closer to criticality than previous studies.

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