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**Improved Numerical Methods
for Quantum Field Theory
(Outstanding Junior Investigator Award)**

Final Report
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Alan D. Sokal

Department of Physics
New York University
4 Washington Place
New York, NY 10003 USA
SOKAL@ACF4.NYU.EDU

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Abstract

We are developing new and more efficient numerical methods for problems in quantum field theory. Our principal goal is to achieve radical reductions in critical slowing-down. We are concentrating at present on three new families of algorithms: multi-grid Monte Carlo (MGMC), Swendsen-Wang (SW) and generalized Wolff-type embedding algorithms. In addition, we are making a high-precision numerical study of the hyperscaling conjecture for the self-avoiding walk, which is closely related to the triviality problem for φ^4 quantum field theory.

During the contract period (7/15/90 – 7/14/93), the principal investigator and his collaborators pursued the following investigations into new numerical methods for quantum field theory:

1) *Multi-grid Monte Carlo.* We implemented the multi-grid Monte Carlo (MGMC) algorithm for the two-dimensional $O(4)$ -symmetric σ -model [= $SU(2)$ principal chiral model], including vectorization yielding 100 MFlops on a single-processor Cray Y-MP. Production runs on lattices up to 256×256 were completed in spring 1991 and analyzed during the summer. We found a dynamic critical exponent $z_{int, \mathcal{M}^2} = 0.60 \pm 0.07$ for the W-cycle and $z_{int, \mathcal{M}^2} = 1.13 \pm 0.11$ for the V-cycle, compared to $z_{int, \mathcal{M}^2} = 2.0 \pm 0.15$ for the single-site heat-bath algorithm (subjective 68% confidence intervals). Thus, for this asymptotically free model, critical slowing-down is greatly reduced compared to the $z \approx 2$ of the traditional local algorithms, but not completely eliminated. (For a 256×256 lattice, W-cycle MGMC is about 35 times as efficient as a single-site heat-bath algorithm.) We are able to explain this behavior as arising from the logarithmic violations of scaling characteristic of asymptotically-free theories; but unfortunately our theory is unable to make a quantitative prediction for the dynamic critical exponent z . Obviously some interesting nonperturbative physics is at work here, which bears further investigation. To test our theory, a graduate student (Tereza Mendes) has modified our MGMC program to study the *one*-dimensional $O(4)$ model, which is superrenormalizable and hence has *power-law* (rather than logarithmic) violations of scaling. If our theory is correct, this model should exhibit dynamic critical exponent $z = 0$. Production runs are planned for the near future.

We have recently invented a new and more flexible approach to multi-grid Monte Carlo, based on an embedding of XY spins into the original σ -model; the

induced XY model is then updated by our standard MGMC algorithm. With this approach, the program can be almost trivially adapted to any σ -model. We are currently beginning production runs on the two-dimensional $O(3)$ - and $O(4)$ -symmetric σ -models as well as on the $SU(3)$ principal chiral model.

[Work in collaboration with Robert Edwards, Sabino Ferreira, Jonathan Goodman, Tereza Mendes and Andrea Pelissetto.]

2) *Generalized Wolff-type embedding algorithms.* We have studied a class of Monte Carlo algorithms for the nonlinear σ -model, based on a Wolff-type embedding of Ising spins into the target manifold M . We have argued heuristically that such an algorithm can have dynamic critical exponent $z \ll 2$ only if the embedding is based on an involutive isometry of M whose fixed-point manifold has codimension 1. Such an isometry exists only if the manifold is a discrete quotient of a product of spheres. We first tested our theory by studying the codimension-2 algorithm for the two-dimensional $O(4)$ -symmetric σ -model, for which we predict $z \approx 2$; numerical simulations yield $z_{int, \mathcal{M}^2} = 1.5 \pm 0.5$ (subjective 68% confidence interval), in reasonable agreement with our heuristic argument.

Our next test was to study the codimension-1 algorithm for the two-dimensional RP^2 and RP^3 σ -models, for which we predict $z \approx 0$ in spite of the frustration in the induced Ising model. Data analysis is still in progress, but our preliminary estimates are $z \approx 0$ for the “idealized” embedding algorithm and $z \approx 1$ for the “practical” embedding algorithm with one Swendsen-Wang hit per iteration. If these data hold up, they would indicate that our heuristic theory is qualitatively correct (codimension is important) but quantitatively incomplete (z for the *practical* algorithm is not simply ≈ 2 or ≈ 0). If so, interesting new nonperturbative questions are opened up.

Very interesting dynamical behavior also occurs in the mixed isovector/isotensor model described in #3 below.

[Work in collaboration with Sergio Caracciolo, Robert Edwards and Andrea Pelissetto.]

3) *New universality classes of two-dimensional σ -models.* Our studies of generalized Wolff-type embedding algorithms, described above, have led us to reconsider some questions regarding the phase diagram and universality classes for two-dimensional σ -models. The conventional wisdom holds that two-dimensional lattice σ -models with a non-Abelian symmetry group are asymptotically free — i.e. the theory has a mass gap for all $\beta < \infty$ — and that the asymptotic behavior as $\beta \rightarrow \infty$ can be deduced from the lattice Hamiltonian simply by noting its symmetries and computing its perturbative expansion around an ordered state. We have found, instead, that there are *new universality classes* which cannot be seen in conventional perturbation theory. The simplest example is the mixed

isovector/isotensor model

$$\mathcal{H}(\sigma) = -\beta_V \sum_{\langle xy \rangle} \sigma_x \cdot \sigma_y - \frac{\beta_T}{2} \sum_{\langle xy \rangle} (\sigma_x \cdot \sigma_y)^2, \quad (1)$$

which interpolates between the standard N -vector and RP^{N-1} models. We argue that there is a one-parameter family of continuum-limit theories, labelled by a parameter λ_{ren} , only one of which ($\lambda_{ren} = +\infty$) is the continuum σ -model constructed by conventional perturbation theory. We support this contention by analytic arguments as well as by a detailed Monte Carlo study (using the Wolff-type embedding algorithm).

[Work in collaboration with Sergio Caracciolo, Robert Edwards and Andrea Pelissetto.]

4) *Swendsen-Wang algorithms for Potts models.* We are endeavoring to understand better the dynamic critical behavior of the Swendsen-Wang (SW) algorithm, which plays a key role in practical implementations of the embedding algorithms. This research has several parts:

- (a) Rigorous analytical proof of lower bounds on the autocorrelation time, both for the original SW algorithm and for the Kandel *et al.* multi-level SW algorithm.
- (b) High-precision numerical studies of the dynamic critical behavior.
- (c) Numerical and analytical investigation of the Curie-Weiss (mean-field) case.
- (d) Attempts to generalize the SW algorithm to mixed ferromagnetic/antiferromagnetic Ising models. This work has important applications to generalized Wolff-type embedding algorithms, as well as to spin glasses.

We succeeded in proving rigorously that a large class of multi-level SW algorithms (including the Kandel *et al.* algorithm) has nonzero (and in some cases quite severe) critical slowing-down, contrary to the original claims of Kandel *et al.* Indeed, we showed that these algorithms obey the same lower bound $z \geq \alpha/\nu$ as the original SW algorithm. We conjecture that their dynamic critical exponent z is equal to that of the original SW algorithm. [Work in collaboration with former graduate student Xiao-Jian Li.]

5) *Hyperscaling in the self-avoiding walk.* We have employed the pivot algorithm to make a high-precision test of the hyperscaling conjecture for the self-avoiding walk [equivalent to the $N = 0$ $O(N)$ -symmetric nonlinear σ -model] in space dimensions 2, 3 and 4. This problem is closely related to the triviality problem for φ^4 quantum field theory. Preliminary results on the 3-dimensional

case, based on walks of length up to 80000, indicate that hyperscaling is obeyed, with a critical exponent $\nu = 0.588 \pm 0.001$ and an interpenetration ratio $\Psi = 0.248 \pm 0.001$. Both of these quantities are universal and experimentally measurable; we are currently investigating possible collaborations with polymer experimentalists. [Work in collaboration with Neal Madras and former graduate student Bin Li.]

In addition, the principal investigator delivered an invited lecture series at the Winter College on "Multilevel Techniques in Computational Physics" (International Centre for Theoretical Physics, Trieste, January–February 1991) and an invited plenary lecture at the 1991 Italian national conference on Current Problems of Theoretical Particle Physics (Isola d'Elba, May–June 1991); and he has written an invited review on Bosonic Algorithms for the book *Quantum Field Theory on the Computer* (edited by Michael Creutz, to be published 1992 by World Scientific).

We are in compliance with all requirements of the project agreement. Approximately 75% of the principal investigator's time since the beginning of this agreement (7/15/90) has been devoted to the investigations outlined above.

Technical reports, preprints and articles prepared for publication

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12. S. Caracciolo, R.G. Edwards, A. Pelissetto and A.D. Sokal, New universality classes for two-dimensional σ -models, preprint (July 1993).
13. S. Caracciolo, A. Pelissetto and A.D. Sokal, A general limitation on Monte Carlo algorithms of Metropolis type, preprint (July 1993).

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