JOURNAL OF COMPUTATIONAL PHYSICS 80, 472–479 (1989)

Note

Combining Renormalization Group and Multigrid Methods*

1. INTRODUCTION

At this conference it is hardly necessary to remind you that faster computers by themselves are unlikely to satisfy our needs for improved methods to simulate quantum field theory. Similarly in statistical physics and optimization theory even "simple" problems such as the Ising spin glass and the travelling salesman defy massive simulations. Brute force is not only unaesthetic, it is inadequate. On the other hand, it is necessary to consider new algorithms that are compatible with the architecture of the new generation of vector supercomputers and massively parallel arrays. The fastest and most efficient computing machinery will require codes with large numbers of independent concurrent computations.

For the solution of PDEs, multigrid methods [1] yield dramatically increased speeds while at the same time being well suited to the architecture of parallel processors. Here we consider adapting such techniques to simulations in statistical mechanics and quantum field theory. Three crucial issues we present are (i) the role of the renormalization group, (ii) the exact preservation of detailed balance, and (iii) the exact preservation of gauge invariance. Tests of the resulting algorithms are being developed in simulations on the IBM 3090 with vector facility, the CDC Cyber 205, the ETA-10, and the Connection Machine.

Let us begin by reminding ourselves of why Monte Carlo algorithms (or any other local iterative algorithm, for that matter) are so time consuming. There are several causes, but the principle one is that we introduce a fictitious small length scale a (the lattice spacing) into problems when the interesting physics takes place at a much larger scale ξ (the "correlation" length). Generally, simulations take place in a space–time volume of sites ($V > \xi^d$) via a local relaxation algorithm on these sites. Almost all local relaxation algorithms (for example, heat bath Monte Carlo or Gauss–Seidel matrix inversion) converge by sending information via a random walk throughout the lattice. The result is a relaxation time τ which increases as ξ^2, or more precisely like ξ^z, where the dynamical critical exponent includes small non-gaussian corrections [2]. Consequently, useful results require a simulation time that increases as the product of volume effects and the relaxation time τ,

$$\text{unit simulation time} = \text{const} \times V^\lambda \times \xi^z.$$

* Based on a talk given by R. C. Brower at the Conference on "Gauge Theory on the Lattice," Seillac, France, Sept. 28–Oct. 2, 1987.

0021-9991/89 $3.00

The power of volume factor λ is 1 for bosonic theories and perhaps as large as 2 for internal fermions in QCD [3]. Here we address the question of how to avoid this additional factor of ξ^z which is referred to as **critical slowing down** in the literature [3] on dynamical critical phenomena.

Obviously the general answer to the problem is to somehow avoid simulating the physics of the longer length scales $O(\xi)$ as an accumulation of effects on the shortest length scale $O(a)$. Renormalization group and multigrid relaxation methods are two approaches that seek to use iterations on a logarithmic series of scales between the lattice length a and the physical length ξ. Here we present some of our attempts to build algorithms by bringing these two approaches together.

At this stage, we have identified the role of the renormalization group in multigrid and given a rather general framework for its implementation which we refer to as the renormalization group multigrid (RGM) method. Eventually efficient algorithms require that we learn enough about the physics to identify the relevant collective coordinates on each scale and their appropriately renormalized dynamics at that scale. The black box of Monte Carlo simulations must be illuminated a bit by the physics. It is too early to know whether our approach will succeed.

2.1D Examples of RG Multigrid

An easy way to see the connection between multigrid speedup and the renormalization group is to look at several trivial one-dimensional examples. Our formulation of the RGM method is a generalization of these simple examples.

2.1. *Renormalized Multigrid Solver*

We wish to set up a multigrid PDE solver by starting with the Green's or correlation function for a gaussian theory. This will allow us to easily extend our discussion to Monte Carlo for non-gaussian theories in Section 2.2. Imagine a set of coordinates ϕ_x on a periodic lattice with N sites $x = 0, 1, 2, ..., N-1$. Green's function $\Phi(x)$ for a fixed source at $x = 0$ is

$$\Phi(x) = \text{const} \times \int D\phi \phi_x \phi_0 \exp[-(\phi, L\phi)],$$

where

$$(\phi, L\phi) = \Sigma_x [Z^2(\phi_{x+1} - \phi_x)^2 + m^2 a^2 \phi_x^2]/2a.$$

In the standard multigrid approach to a PDE, the update cycle has four elements: (1) smoothing the high frequency components on the original fine lattice using the operator L; (2) introducing and initializing new collective coordinates $\hat{\phi}$ on a coarser sublattice with an appropriate projection $R: \phi(x) \to \hat{\phi}(\hat{x})$, where $\hat{x}$ refers to a subset of sites x; (3) choosing a renormalized operator $\hat{L}$ on the coarser lattice to update the collective variables $\hat{\phi} \to \hat{\phi}'$; (4) interpolating these changes onto

the fine lattice variables by an injection transform $Q: \hat{\phi}'(\hat{x}), \phi(x) \to \phi'(x)$. These steps are then applied on a fixed recursive schedule between the finest and the coarsest scales.

Now we will show how an $O(N)$ renormalization group approach solves this problem exactly for $N = 2^p$ sites in our 1D toy problem. We will refer to the levels as $w = 0, 1, 2, \ldots, p$ from top to bottom with lattice spacing

$$a_w = a \times 2^w,$$

respectively. The original lattice at the top is $w = 0$. Because of the gaussian form of the 1D problem, integrating out all the odd sites gives back the same problem on $N/2$ sites with renormalized wave function (Z) and mass (m) parameters:

$$Z_{w+1}^2 = Z_w^2/(1 + m_w a_w/2)$$
$$m_{w+1} a_{w+1} = m_w a_w \sqrt{(m_w a_w)^2 + 4}.$$

The multigrid cycle consists of going to the coarsest lattice and solving the trivial one-site problem, and then iteratively back-substituting interpolated values from the nearest-neighbor form of the linear differential equation at each finer lattice. In N algebraic steps, you have the exact answer, which in multigrid language consists of the upward half of a single V-cycle. While this is a rather simple exercise, it is also instructive. We observe that (i) we have used the full renormalization group equations to connect the lattices, (ii) our speedup of $O(N)$ is even better than an FFT algorithm of $O(N \log_2 N)$, and (iii) we can generalize this procedure to a non-gaussian Monte Carlo example—the 1D Ising model (see Section 2.2).

2.2. *Renormalized Multigrid Monte Carlo*

Let us illustrate this renormalization group multigrid (RGM) method for a Monte Carlo update by considering the 1D Ising system [4],

$$Z = \mathrm{Tr}[\exp(-\beta \Sigma_x (1 - s_x s_{x+1}))].$$

Summing out the odd spins, we get a new dynamics with renormalized coupling,

$$\beta_{w+1} = \tfrac{1}{2} \log(\cosh(2\beta_w)).$$

The following half V-cycle works in $O(N)$ steps to get an entirely uncorrelated new state. At the bottom $w = p$ level choose s_0 at random, then use the heat bath algorithm to get the spins coupled to it at $w = p - 1$, and so on up to the top $w = 0$. As we will show in Section 3 in a general argument, this algorithm satisfies detailed balance exactly.

Again we note that an ideal multiscale algorithm takes the form of a renormalization group improved multigrid method. The essential question at this point is whether or not these simple 1D examples are in any way typical of the general problem of critical slowing down in higher dimensions. We have only partial answers to this question at present.

3. RGM Methods in Higher Dimensions

We are investigating two problems in higher dimensions to see how these renormalization group multigrid (RGM) methods might be used. The first is Monte Carlo for the Ising model and the second is lattice fermions in non-abelian gauge theories. We wish to report on the progress and the remaining difficulties.

3.1. *Metropolis Formulation*

We will begin with the formulation of a general renormalization group multigrid method for Monte Carlo updates. Just as in the review talk of M. Creutz [5], we have found that most of our individual algorithms can be cast in terms of a Metropolis algorithm. However, to implement detailed balance, it is useful to superimpose the variables of all levels into a "super Hamiltonian" or "super action." For example, if we consider two levels (more will be added recursively), we define a "super Hamiltonian" H_{super} that depends on the variable for both levels ϕ and $\hat{\phi}$ as well as the level selector variable w,

$$H_{\text{super}}(\phi, \hat{\phi}, w) = \delta_{w,0} H(\phi) + \delta_{w,1} H^R_{\phi}(\hat{\phi}).$$

The renormalized Hamiltonian on the first level down ($w = 1$) H^R, may depend on fields on the fine level ϕ as in the approach of Goodman and Sokal [6].

Now we consider a Monte Carlo algorithm that works in the combined space $\Phi = (\phi, \hat{\phi}, w)$ with the standard form for the Metropolis acceptance,

$$A(\Phi' \leftarrow \Phi) = \text{MIN}\left[1, \frac{\rho(\Phi \leftarrow \Phi') \exp(-H_{\text{super}}(\Phi'))}{\rho(\Phi' \leftarrow \Phi) \exp(-H_{\text{super}}(\Phi))}\right].$$

All update steps are required to preserve the equilibrium distribution for the super Hamiltonian, $P_{\text{super}} = \exp(-\beta H_{\text{super}})/Z_{\text{super}}$ so that the averages over any function of the fine variables will be equivalent to the averages in the distribution of the original problem with distribution function $P_{\text{equ}}(\phi) = \exp(-\beta H(\phi))/Z$.

We construct a four-step multigrid cycle very similar to the PDE case, except that for steps 1 and 3 we use horizontal Metropolis steps that keep the level parameter w fixed and for steps 2 and 4 we use vertical Metropolis steps that change the level parameter w. The multigrid cycles must consist of a fixed schedule independent of the state of the system in order to preserve detailed balance. The schedule acts recursively on many levels, alternating updates on individual levels with updates that change levels. The updates on a fixed level are the diagonal elements in $\rho(w' \leftarrow w)$ viewed as a matrix in w space and these updates can be restricted to only change coordinates ϕ on that same level as in any standard single level Monte Carlo algorithm.

To change levels, we use the off-diagonal elements, $R_w = \rho(w+1 \leftarrow w)$ and $Q_w = \rho(w \leftarrow w+1)$. It is now relatively easy to see that the 1D algorithm for the Ising model is a specific form of this RGM algorithm. In this case, R_w sets all $\hat{s}$ to

be equal to the even subset of the s variables above it and Q_w is the heat bath step itself for choosing the interpolated variables relative to the renormalized H_w^R with β_w. As in the standard heat bath this ρ function is chosen so as to exactly give you an acceptance of one.

In 2D it is, in principle, possible to use the fully renormalized hamiltonian H^R but it involves long-range couplings. Defining the fully renormalized H^R as the decimation of half the spins (say all black spins in a red–black scheme),

$$\exp(-H^R(\hat{s})) = \mathrm{Tr}_s[\delta_{\hat{s}\, s_R} \exp(-H(s))],$$

and iterating this rule to many levels involves progressively longer range couplings, as in most renormalization group schemes. At present we are doing numerical simulations of algorithms that replace the fully renormalized H^R by a Hamiltonian $\hat{H}$ which is truncated to nearest-neighbor couplings. The renormalized temperature β_m and zero-point energy E_m are allowed to be tuned parameters. The resulting acceptance depends on the change in the Hamiltonian

$$A(w+1 \leftarrow w) = \mathrm{MIN}[1, \exp(-\hat{H}_{w+1} + H^R_{w+1})]$$
$$A(w \leftarrow w+1) = \mathrm{MIN}[1, \exp(-H^R_{w+1} + \hat{H}_{w+1})].$$

Tuning the parameters to maximize the acceptance is our renormalization group prescription. Numerical calculations show us that the critical temperature is an RG invariant to high accuracy even on small lattices. However, as we feared, we find that as the lattice becomes larger the mean acceptance rate falls exponentially in the volume of the lattice like $\exp(-\varepsilon \times V)$, where ε is small **but** nonzero. When equilibrium is reached our simulations give us a value of $\varepsilon = 0.016$ at optimal values for the renormalized parameters in the 2D Ising model.

This volume effect is a major problem to which we have not yet found a satisfactory solution. With this volume term, we believe that the multigrid algorithm cannot reduce the exponent z for critical slowing down. It is not yet clear to us why on the basis of the operator product expansion [8], the volume term should not cancel to an order of some power of the inverse correlation length. Lacking such a theoretical picture, we cannot be sure whether a few more terms in the renormalized Hamiltonian might not be able to eliminate the volume term altogether. We are investigating these questions. However, as in the volume effect seen in the exact versions of the pseudo-fermion algorithms, there may be a trade-off between this rejection rate and slower or more local changes of the coarser collective coordinates. This could be achieved by a direct coupling in the renormalized Hamiltonians back to the fine lattice similar to the terms in the Goodman and Sokal approach [6].

It may be helpful to contrast these suggestions of Goodman and Sokal with our formulation. They have suggested the use of collective coordinates for their multigrid Monte Carlo (MGMC) method. For example, in the ϕ^4 theory, their MGMC update shifts all the coordinates in a 2^d block of sites by a uniform amount (for all

x in block associated with $\hat{x}$, $\phi(x) \to \phi(x) + \Delta\hat{\phi}(\hat{x})$). However, as they are careful to point out, the dynamics for the new $\hat{\phi}$ is **not** renormalized. They use exactly the same fine distribution with the update rule satisfying the conditional probability of the changed variable in the presence of all the other fixed variables. The result is a degenerate case of our Metropolis form with acceptance always equal to one.

In contrast, we are recommending the use of renormalized actions on each level. Also as is typical in multigrid methods, we advocate that the new lattice sites be a subset of the old lattice. This is a different kind of blocking not usually used in real-space RG transformations. As our examples show, it is akin to naive decimation where the cells share some of their boundary sites with their neighboring cells. As we note below, this blocking scheme is particularly natural in applications to gauge theories.

3.2. *Swendsen and Wang Multilevel Method*

There is one method of doing multilevel updates on the Ising model that does maintain exact detailed balance, avoid any volume term in the acceptance rate, and reduces z dramatically to $z \simeq 0.3$. The method also serves to underline the tremendous advantage to a deeper insight into the proper selection of collective coordinates. Swendsen and Wang [9] consider a super partition function, inspired by the work of Fortuin and Kasteleyn [10], for the Ising model that has bond percolation variables (n).

$$P_{\text{super}}(s, n) = \Pi_{\text{bonds}}[(1 - e^{-2\beta})\, \delta_{s_x, s_y}\, \delta n_{x, y, 1} + e^{-2\beta}\, \delta n_{x, y, 0}].$$

In analogy with our partition functions with the super Hamiltonian, summing over the "coarse" variables n gives back the original partition function. However, their algorithm based on **this** clever trick adaptively finds its new collective variable every cycle by percolating the bonds inside the current Ising clusters. The resultant clusters are then decoupled by the broken bonds and can be flipped with 50% likelihood. We are currently modifying this Swendsen and Wang algorithm to operate on a series of cluster sizes from the smallest at a single lattice spacing up to the largest at the Ising correlation length by varying the percolation strength. In collaboration with Swendsen, we are running this code for Ising and spin glass models on the Connection Machine.

3.3. *Gauge Invariance*

As was shown in our recent formulation of the multigrid algorithm for Wilson fermions in lattice QCD, gauge invariance can be incorporated nicely into multigrid schemes [11].

In collaboration with Claudio Rebbi, we are investigating the proper renormalization of the effective operator for the lattice Dirac equation on the coarser lattices to maximally accelerate the multigrid convergence. Numerical evidence will be reported elsewhere. In the present discussion of RGM Monte Carlo, we have found ways to apply the general framework discussed above to gauge theories. The

constraint of gauge invariance is nicely satisfied by choosing the R and Q functions as probability distributions which connect the two lattices by Wilson loops that respect simultaneous gauge transformations on the fine and coarse lattices (i.e., lattice sites that are shared between the lattices are gauge transformed together). If, in addition, the distributions are symmetric with respect to new and old variables, they disappear from the acceptance rate. This amounts to a rather intricate, but algorithmically simple, use of gauge invariance to accomplish the smoothing and interpolation steps 2 and 4 in changing levels which is analogous to the methods we introduced for the lattice fermions [10, 11].

In summary, the extension of RGM techniques to lattice gauge theory is not a technically formidable step. However, the physics of each new application can be quite different. As reported in the summary talk by Creutz [5], the present algorithmic alternatives used for lattice QCD are, for the most part, closely related and beautifully summarized in terms of various strategies for maximizing the Metropolis acceptance. We have formulated multigrid algorithms in an analogous fashion in a larger space that combines the original and the collective coordinates into a super-partition function. We have found over the last year that almost all of our attempts to find multilevel algorithms can be expressed in this way. However, the number of possibilities is enormous and the constraints of good acceptance severe. Nice solutions are not easy to find. Still between the cute but essentially trivial 1D examples we have presented here and the sophisticated example of Swendsen and Wang lies a vast unexplored region.

ACKNOWLEDGMENTS

We would like to acknowledge useful conversations with Achi Brandt, Eric Myers, Claudio Rebbi, and Alan Sokal. Also we would like to thank Lloyd M. Thorndyke, Carl S. Ledbetter, and Tom Jones of ETA Systems, Inc. and Robert M. Price and Tom Roberts of Control Data Corporation for their continued interest, support, and encouragement and access to the Scientific Information Services' CDC CYBER 205 at Kansas City, MO (Grant 13578 (TQ371HA)), where some of these calculations were performed, the National Allocation Committee for the John von Neumann National Supercomputer Center for access to the two CDC CYBER 205's at JVNC (Grants 110128, 551701, 551702, 551703, and 551704), the Control Data Corporation PACER Fellowship grants (Grants 85PCR06 and 86PCR01) for financial support, ETA Systems, Inc. for financial support (Grants 304658 and 1312963), the Natural Sciences and Engineering Research Council of Canada (Grants NSERC A8420 and NSERC A9030) for financial support and the Canada/Nova Scotia Technology Transfer and Industrial Innovation Agreement (Grants 87TTII01 and 88TTII01) for further financial support. R.C.B. thanks ETA Systems, Inc. for a grant which made his visit to Seillac, France possible.

REFERENCES

1. A. BRANDT, *Math. Comput.* **31**, 333 (1982); Multigrid methods, Lecture Notes in Mathematics Vol. 960 (Springer-Verlag, Berlin, 1982).
2. A. BRANDT, D. RON, AND D. J. AMIT, *in* Multigrid methods II, Lecture Notes in Mathematics Vol. 1228 (Springer-Verlag, Cologne, 1985).

3. P. C. HOHENBERG AND B. HALPERIN, *Rev. Mod. Phys.* **49**, 435 (1977).
4. K. E. SCHMIDT, *Phys. Rev. Lett.* 2175 (1983).
5. M. CREUTZ in *Lattice Gauge Theory Using Parallel Processors*, edited by Xiaoyuan Li, Zhaoming Qiu, and Hai-Cang Ren, (Gordon & Breach, New York, 1987), p. 105.
6. J. GOODMAN AND A. D. SOKAL, *Phys. Rev. Lett.* **56**, 1015 (1986).
7. L. P. KADANOFF, *Physics* **2**, 263 (1966).
8. K. WILSON, *Phys. Rev. D* **2**, 1438 (1970).
9. R. SWENDSEN AND J. S. WANG, *Phys. Rev. Lett.* **58**, 86 (1987).
10. C. M. FORTUIN AND P. W. KATELEYN, *Physica* **57**, 536 (1972).
11. R. C. BROWER, K. J. M. MORIARTY, E. MYERS, AND C. REBBI, in *Proceedings, Third Copper Mountain Conference on Multigrid Methods, Copper Mountain, Colorado, April 6-10, 1987*, edited by S. McCormick (Marcel–Dekker, New York, 1988), p. 85.

RECEIVED: May 1, 1987; REVISED: January 27, 1988

R. C. BROWER
Physics Department and Electrical, Computer and Systems Engineering Department
Boston University
Boston, Massachusetts 02215

R. GILES
Electrical, Computer and Systems Engineering Department
Boston University
Boston, Massachusetts 02215

K. J. M. MORIARTY
Institute for Advanced Study and
John von Neumann National Supercomputer Center
Princeton, New Jersey 08540

P. TAMAYO
Physics Department and Electrical, Computer and Systems Engineering Department
Boston University
Boston, Massachusetts 02215