RAPID COMMUNICATIONS

PHYSICAL REVIEW D VOLUME 48, NUMBER 5 1 SEPTEMBER 1993

Idealized multigrid algorithm for staggered fermions

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(Received 7 April 1993)

An idealized multigrid algorithm for the computation of propagators of staggered fermions is investigated. Exemplified in four-dimensional SU(2) gauge fields, it is shown that the idealized algorithm preserves criticality under coarsening. The same is not true when the coarse grid operator is defined by the Galerkin prescription. Relaxation times in computations of propagators are small, and critical slowing is strongly reduced (or eliminated) in the idealized algorithm. Unfortunately, this algorithm is not practical for production runs, but the investigations presented here answer important questions of principle.

PACS number(s): 11.15.Ha, 02.60.Cb, 02.60.Dc

I. INTRODUCTION

In Monte Carlo simulations of lattice gauge theories with fermions the most time-consuming part is the computation of the gauge field dependent fermion propagators. Great hopes to compute propagators without any critical slowing down (CSD) are attached to multigrid (MG) methods [1–11]. However, up to now no practical MG algorithm has been found for fermions.

In this Rapid Communication an idealized MG algorithm is investigated for staggered fermions in four-dimensional SU(2) gauge fields. It will be shown that the idealized algorithm preserves criticality under coarsening, which is not true when the coarse grid operator is defined by the Galerkin prescription. This finding explains the failure of simple variational-like MG methods, at least for algorithms with nonoverlapping blocks or trivially overlapping blocks.

Relaxation times in computations of propagators with the idealized MG algorithm are small, and CSD is strongly reduced or eliminated. Unfortunately, this algorithm is not practical for production runs, but the investigations presented here answer important questions of principle.

II. MULTIGRID METHOD

For given f we wish to solve an equation

$$D_0 \chi = f \text{ with } D_0 = (-\not{D}^2 + m^2) \tag{1}$$

by MG methods, where $\not{D}$ is the gauge covariant staggered Dirac operator, and m is a small quark mass.

The following MG notation will be used. The fundamental lattice is denoted by Λ^0. The first block lattice Λ^1 is obtained by coarsening with a factor of L_b. Thus Λ^1 has L_b^d fewer sites than Λ^0 (in d space-time dimensions). Restriction and interpolation operators C and $\mathcal{A}$, respectively, are given by kernels $C(x,z)$ and $\mathcal{A}(z,x)$ with $z \in \Lambda^0$, $x \in \Lambda^1$. Note that $C(x,z)$ and $\mathcal{A}(z,x)$ are $N_c \times N_c$ matrices in a gauge theory with N_c colors. Also, C and $\mathcal{A}$ depend on the gauge field, although this is not indicated explicitly.

We use a blocking procedure for staggered fermions which is consistent with the lattice symmetries of free fermions [6]. This forces us to choose $L_b = 3$. Even L_b are not allowed. In four dimensions, coarsening by a factor of 3 reduces the number of points by 81. Therefore only a two-grid algorithm was implemented. The residual equation on the coarse grid was solved exactly by the conjugate gradient algorithm.

The averaging kernel C is chosen according to the ground-state projection definition [12,13,3,14]. In the present work C satisfies the gauge covariant eigenvalue equation(s)

$$(-\Delta_{N,x} C^*)(z,x) = \lambda_0(x)\, C^*(z,x) \tag{2}$$

together with a normalization condition $CC^* = \mathbb{1}$, and a covariance condition $C(x,\hat{x}) \propto \mathbb{1}$ where $\hat{x}$ denotes the center of block x. In Eq. (2), $\lambda_0(x)$ is the lowest eigenvalue of $-\Delta_{N,x}$, and $-\Delta_{N,x}$ is the gauge covariant fermionic "two-link lattice Laplacian," defined through $\not{D}^2 = \Delta + \sigma_{\mu\nu} F_{\mu\nu}$, with "Neumann boundary conditions (BC's)." A Neumann BC means that derivative terms in Δ are omitted where one site is in block x and the other one is in a neighboring block.

The ground-state projection method is numerically implementable in four-dimensional non-Abelian gauge fields [14], and since the method is gauge covariant, no gauge fixing in computations of propagators is required. For staggered fermions in non-Abelian gauge fields two qualitatively different proposals were made for ground-state projection [6]. We call these proposals "the Laplace choice" and "the Dirac choice." The Laplace choice is the one described above. In the Dirac choice one substitutes a block-local approximation of $\not{D}^2$ for Δ in (2). This latter choice would be superior because it takes also the field strength term $F_{\mu\nu}$ into consideration. However, it was proved numerically [6,10] that the Laplace choice for C defines a good block spin in arbitrarily disordered

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gauge fields.[1] For this reason only the Laplace choice of C has been implemented yet.

III. SPECTRUM OF $-\not{D}^2$ AND CSD

The square of the staggered Dirac operator (plus mass term) couples only even lattice sites to even sites, and odd sites to odd sites. Therefore the matrix elements of $-\not{D}^2$ can be arranged in such a way that $-\not{D}^2$ can be written symbolically as

$$-\not{D}^2 = \begin{pmatrix} -\not{D}^2_{\text{even}} & 0 \\ 0 & -\not{D}^2_{\text{odd}} \end{pmatrix} , \tag{3}$$

where $-\not{D}^2_{\text{even/odd}}$ is $-\not{D}^2$ restricted to the even/odd sublattice.

Let us denote the spectrum of $-\not{D}^2$ by $\mathcal{S}(-\not{D}^2)$. It equals the union of the spectra of $-\not{D}^2_{\text{even}}$ and $-\not{D}^2_{\text{odd}}$: $\mathcal{S}(-\not{D}^2) = \mathcal{S}(-\not{D}^2_{\text{even}}) \bigcup \mathcal{S}(-\not{D}^2_{\text{odd}})$. The spectra are gauge invariant. Moreover, for any gauge field configuration one has the equality

$$\mathcal{S}(-\not{D}^2_{\text{even}}) = \mathcal{S}(-\not{D}^2_{\text{odd}}) \ . \tag{4}$$

A simple proof of (4) is as follows. Consider the lattice operator $-\not{D}^2_{\text{even/odd}}$ as a block matrix with $N_c \times N_c$ elements $-\not{D}^2_{\text{even/odd}}(z_1, z_2)$. The matrices $-\not{D}^2_{\text{even}}$ and $-\not{D}^2_{\text{odd}}$ are similar, and therefore they have the same spectrum. We recall that two matrices A and B are called similar if there exists an invertible matrix T such that $B = TAT^{-1}$. (We also recall that if v is an eigenvector of A with eigenvalue λ, then Tv is an eigenvector of B with eigenvalue λ.) In the case considered here, we look for a lattice operator T with the property

$$\sum_{z'} T(w,z')(-\not{D}^2_{\text{even}})(z',z) = \sum_{w'} (-\not{D}^2_{\text{odd}})(w,w')T(w',z) \tag{5}$$

where z, z' and w, w' denote even and odd lattice sites, respectively. Equation (5) is satisfied if we choose the matrix elements of T to be $T(w,z) = \not{D}(w,z)$. This choice of T is not invertible in pure gauges, but in that case the equality (4) of spectra is obvious anyhow.

In Ref. [15] a more complicated proof of (4) was given which uses an analyticity argument in connection with a hopping expansion of $(-\not{D}^2 + m^2)^{-1}$ for large mass.

In Refs. [9–11] the author pointed out that in conventional relaxation algorithms for propagators of staggered fermions there exists a scaling law for relaxation times τ which reads

$$\tau = \frac{\text{const}}{\triangle m^2} \quad \text{with} \quad \triangle m^2 = m^2 - m^2_{\text{cr}} \tag{6}$$

for small $\triangle m^2$, where $-m^2_{\text{cr}}$ is the lowest eigenvalue of $-\not{D}^2$, and const is *independent of the lattice size*. For bosonic propagators the validity of (6) is known analytically [11] and has also been confirmed to a high accuracy numerically [7,11].

A consequence of (4) is that in conventional relaxation algorithms for staggered fermions, CSD will be the same on the even and the odd sublattice.

IV. IDEALIZED MULTIGRID ALGORITHM

Up to now no practical MG method has been found for fermions. Mack pointed out that it is essential for fighting CSD in MG computations that interpolation kernels should be smooth [16]. This requirement is not satisfied in MG algorithms where one uses gauge covariant generalizations of piecewise constant interpolation with nonoverlapping blocks. Mack suggested an interpolation kernel $\mathcal{A}$ as a starting point for numerical work which was used successfully by Gawędzki and Kupiainen in constructive quantum field theory [17]. An idealized MG algorithm using the natural gauge covariant generalization of the Gawędzki-Kupiainen kernel had been investigated numerically in four-dimensional SU(2) gauge fields for bosonic propagators [7,11]. There CSD could be eliminated completely. Here we turn to an idealized MG algorithm for staggered fermions. This algorithm will not be practical for production runs, but it is important to answer questions of principle, and to recognize the features which a successful method must have.

Given the averaging kernel C, there exists an ideal choice of the interpolation kernel $\mathcal{A}$. It is determined as follows. For every function ("block spin") Φ on Λ^1, $\phi = \mathcal{A}\Phi$ minimizes the action $\langle \phi, D_0 \phi \rangle$ subject to the constraint $C\phi = \Phi$. For the purpose of numerical computations, it is convenient to determine the optimal $\mathcal{A}$ as the solution of the equation

$$\left([-\not{D}^2 + m^2 + \kappa C^* C]\mathcal{A}\right)(z,x) = \kappa C^*(z,x) \tag{7}$$

for large κ. C^* denotes the adjoint of C. The layers of an MG decouple completely when this $\mathcal{A}$ is used for interpolation, and when coarse grid operators D_1 are defined as $C(-\not{D}^2 + m^2)\mathcal{A}$. These coarse grid operators are automatically Hermitian and equal $\mathcal{A}^*(-\not{D}^2 + m^2)\mathcal{A}$.

The optimal $\mathcal{A}$ is favored by an argument of dynamics [8,11]. With the definition of smoothness that covariant derivatives are small, the above characterization of $\mathcal{A}$ as a solution of an extremization problem can be rephrased: that $\mathcal{A}$ is the smoothest interpolation kernel, subject to the constraint $C\mathcal{A} = \mathbb{1}$.

V. NUMERICAL RESULTS

Because of the considerations of Sec. III we decided to investigate the idealized two-grid algorithm only on the even sublattice. This restriction mitigates also the storage space requirements for the ideal $\mathcal{A}$ a little bit. Note that Eq. (7) can also be broken up into an equation for the interpolation kernel on the even sublattice and one on the odd one, if the averaging kernel C does not mix even and odd sites. This requirement is satisfied both for the Laplace and for the Dirac choices of Ref. [6]. In both proposals the coarse grid sites can be separated into

[1] For every averaging kernel C there exists an associated ideal interpolation kernel $\mathcal{A}$; see Sec. IV. C defines a good block spin if this $\mathcal{A}$ decays exponentially.

TABLE I. Lowest eigenvalues of the negative squared Dirac operator for staggered fermions on a fundamental lattice Λ^0, and the lowest eigenvalues of the ideal block operator $C(-\not{D}^2 + m_{\rm cr}^2)\mathcal{A}$ and of the Galerkin operator $C(-\not{D}^2 + m_{\rm cr}^2)C^*$.

β	$\lvert\Lambda^0\rvert$	$-m_{\rm cr}^2$ = lowest eigenvalue of $-\not{D}^2$	Lowest eigenvalue of $C(-\not{D}^2 + m_{\rm cr}^2)\mathcal{A}$	Lowest eigenvalue of $C(-\not{D}^2 + m_{\rm cr}^2)C^*$
∞	6^4	7.98×10^{-29}	3.09×10^{-21}	9.04×10^{-13}
5.0	6^4	0.0013413	-1.40×10^{-11}	1.0341375
3.0	6^4	0.3497739	6.68×10^{-12}	2.8529730
2.8	6^4	0.2441995	7.27×10^{-11}	2.8412484
2.8	6^4	0.2748178	4.33×10^{-12}	3.2338422
2.7	6^4	0.2004647	-6.42×10^{-11}	3.4374150
2.6	6^4	0.1740946	-2.78×10^{-11}	3.1884409
2.5	6^4	0.0698942	-5.96×10^{-13}	3.0198011
2.4	6^4	0.0010729	-1.82×10^{-11}	3.1265394
2.2	6^4	0.0007099	9.50×10^{-11}	3.4488349
2.0	6^4	0.0000732	6.08×10^{-10}	3.5620285
0.0	6^4	0.0000287	-1.21×10^{-10}	3.7354123
∞	12^4	8.15×10^{-29}	-2.33×10^{-14}	9.13×10^{-13}
3.0	12^4	0.0779810	-7.96×10^{-12}	2.3190549
2.7	12^4	0.0368447	-1.15×10^{-11}	2.3967694
2.5	12^4	0.0005742	-1.03×10^{-10}	2.6881098
2.4	12^4	0.0001865	-1.10×10^{-8}	2.8248637

even and odd sites, and the ideal effective Dirac operator $-C\not{D}^2\mathcal{A}$ (as well as the Galerkin operator $-C\not{D}^2C^*$) can be decomposed analogously to (3).

Here we made the Laplace choice and computed C by the efficient algorithm of Ref. [14]. Numerical work was done in SU(2) lattice gauge fields on 6^4 and 12^4 lattices, covering all possible values of $\beta = 4/g^2$ between ∞ and zero. The system (7) was solved by means of the conjugate gradient algorithm where iterating was stopped when the rms residual was less than 10^{-10}. The statement that $-C\not{D}^2\mathcal{A}$ is automatically Hermitian was confirmed up to round-off errors of order 10^{-9} or less.

A. Lowest eigenvalues

Let us first look at the lowest eigenvalues of $-\not{D}^2$ on the fundamental lattice Λ^0, and see how they are transferred to the block lattice Λ^1. The role of this transfer for the performance of the parallel-transported MG method of Ben-Av, Brandt, and Solomon was pointed out in Ref. [2].

First the lowest eigenvalues $-m_{\rm cr}^2$ of $-\not{D}^2$ were determined by inverse iteration. This method allows us to determine $-m_{\rm cr}^2$ to an accuracy of 10^{-7} or better [7]. Then optimal interpolation kernels $\mathcal{A}$ were computed as solutions of Eq. (7) with $m^2 = m_{\rm cr}^2$, and for $\kappa = 10^5$. Results for $-m_{\rm cr}^2$ and for the lowest eigenvalues of the ideal coarse grid operator $C(-\not{D}^2 + m_{\rm cr}^2)\mathcal{A}$ are given in Table I. The last column of Table I contains results for the Galerkin definition of the coarse grid operator. This operator is used in variational MG methods where interpolation is done by C^*. (The Galerkin operator retains the locality properties of $-\not{D}^2$ in arbitrary gauge fields.)

One sees that for any value of the gauge coupling the idealized algorithm maps a critical system on Λ^0 onto a critical system on the block lattice. In contrast, the variational MG algorithm does not have this property. The Galerkin operator $C(-\not{D}^2+m_{\rm cr}^2)C^*$ is far from being critical in nontrivial gauge fields.

The results of Table I supply another explanation for the failure of the variational MG algorithm which was ascertained in Refs. [9–11]. One cannot expect that a (nearly) critical problem on Λ^0 can be solved by means of an auxiliary problem with fewer degrees of freedom on Λ^1, if the auxiliary problem is not critical as well. The Galerkin operator is only critical in trivial gauge fields,[2]

TABLE II. Accuracy of $C\mathcal{A} = \mathbb{1}$ for staggered fermions. $\|C\mathcal{A} - \mathbb{1}\|_\infty$ denotes the maximal trace norm of $C\mathcal{A}(x,y) - \delta(x-y)$ over all pairs (x,y) of block lattice sites, and $\|C\mathcal{A} - \mathbb{1}\|_2$ is the rms of these norms.

β	$\lvert\Lambda^0\rvert$	$\|C\mathcal{A} - \mathbb{1}\|_2$	$\|C\mathcal{A} - \mathbb{1}\|_\infty$
∞[a]	6^4	3.98×10^{-15}	2.13×10^{-14}
5.0	6^4	6.62×10^{-7}	1.87×10^{-6}
3.0	6^4	2.77×10^{-6}	9.43×10^{-6}
2.8	6^4	2.59×10^{-6}	8.66×10^{-6}
2.8	6^4	3.69×10^{-6}	1.07×10^{-5}
2.7	6^4	3.76×10^{-6}	1.18×10^{-5}
2.6	6^4	3.18×10^{-6}	1.02×10^{-5}
2.5	6^4	2.43×10^{-6}	8.15×10^{-6}
2.4	6^4	2.39×10^{-6}	6.76×10^{-6}
2.2	6^4	1.51×10^{-6}	4.48×10^{-6}
2.0	6^4	9.40×10^{-7}	2.95×10^{-6}
0.0	6^4	2.84×10^{-7}	9.23×10^{-7}
∞	12^4	2.32×10^{-6}	2.32×10^{-5}
3.0	12^4	1.02×10^{-6}	1.12×10^{-5}
2.7	12^4	1.00×10^{-6}	1.11×10^{-5}
2.5	12^4	9.08×10^{-7}	1.05×10^{-5}
2.4	12^4	7.92×10^{-7}	9.12×10^{-5}

[a]In case of the pure gauge on the 6^4 lattice (and only in this case), the ideal MG scheme is identical to the Galerkin definition with $\mathcal{A} = C^*$ ("covariant piecewise constant" interpolation); since C is normalized as $CC^* = \mathbb{1}$, the finite norms of $C\mathcal{A} - \mathbb{1}$ in this case are due to round-off errors.

[2]In exact arithmetics the entries for $\beta = \infty$ (realized as random pure gauge fields) in Table I would be zero for any lattice size.

TABLE III. Dependence of relaxation times τ on $\triangle m^2$ in the ideal MG algorithm with lexicographic SOR for computing propagators of staggered fermions on 6^4 lattices. (The two configurations at $\beta = 2.8$ are different.)

		τ for $\triangle m^2 =$						
β	ω	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
∞	1.17	0.8	0.8	0.7	0.7	0.7	0.7	0.7
5.0	1.35	1.2	1.3	1.4	1.4	1.4	1.4	1.4
3.0	1.70	4.0	4.5	4.8	4.9	4.9	4.9	4.9
2.8	1.70	3.6	4.4	5.4	5.8	5.9	5.9	5.9
2.8	1.75	5.2	6.6	7.1	7.7	7.8	7.8	7.8
2.7	1.65	3.5	4.5	5.0	6.1	6.2	6.2	6.2
2.6	1.65	3.2	4.5	5.2	6.0	6.1	6.1	6.0
2.5	1.65	3.2	4.4	6.8	7.5	7.6	7.6	7.6
2.4	1.72	4.5	7.2	12	16	17	17	17
2.2	1.70	6.2	15	20	43	53	54	80
2.0	1.60	5.0	13	54	139	199	211	213
0.0	1.45	28	36	119	524	1156	1505	1570

and only there is CSD eliminated by the variational MG method in computations of propagators.

The effect of adding a mass term $\triangle m^2$ to $(-\not{D}^2 + m_{\rm cr}^2)$ is as follows. The values given in the last two columns of Table I are shifted by the amount determined by $\triangle m^2$. This is obvious in case of the Galerkin operator because the averaging kernel is normalized such that $CC^* = \mathbb{1}$. In the case of the idealized algorithm, $C\mathcal{A}$ tends to $\mathbb{1}$ for $\kappa \to \infty$. For finite κ one finds deviations from $\mathbb{1}$. Examples are given in Table II. These deviations are small enough to have no effect in practice. When one computes the lowest eigenvalues of $-C\not{D}^2\mathcal{A}$, one recovers the negative critical masses of the gauge fields to the same accuracy as they are given in Table I. Hence, the small negative values partly found for the lowest eigenvalues of $C(-\not{D}^2 + m_{\rm cr}^2)\mathcal{A}$ are really due to numerical inaccuracies.

B. Performance of the idealized algorithm

Finally, we report results of computations of propagators by means of an idealized algorithm. We used coarse grid operators $C(-\not{D}^2 + m^2)\mathcal{A}$ with masses $m^2 = m_{\rm cr}^2 + \triangle m^2$, $\triangle m^2 > 0$ and small. For all values of $\triangle m^2$ only one interpolation kernel $\mathcal{A}$ was used, namely, the "critical" one which solves (7) with $m^2 = m_{\rm cr}^2$. Actually, one should use an m^2-dependent $\mathcal{A}$ kernel, viz. the solution of (7) with m^2 being the mass under consideration. However, in case of bosonic propagators the procedure described here was successful [7,11], and therefore we used it also as a first attempt in case of staggered fermions.

Tables III and IV comprise results for relaxation times as a function of $\triangle m^2$ on 6^4 and 12^4 lattices, respectively. The values given for the relaxation parameter ω are optimal within ± 0.05. (For the configuration on the 12^4 lattice at $\beta = 2.5$, $\omega = 1.72$ is close to optimum, while the results for $\omega = 1.65$ are given as additional information.)

We rediscover here an observation which was made earlier [7,11]: The use of a relaxation parameter ω different from one in MG computations contradicts the conventional wisdom. According to this wisdom the only job of the relaxation procedure on Λ^0 is to smoothen the error, and this job is well done by Gauss-Seidel iteration. The conventional wisdom was confirmed by numerical results in trivial gauge fields [11]. However, the picture changes for propagators in nontrivial gauge fields.

In order to be sure about the correct determination of the value of $m_{\rm cr}^2$, it was checked that conventional successive over-relaxation (SOR) and the variational MG algorithm (with the Laplace choice of C) both exhibited CSD, i.e., relaxation times τ follow perfectly the scaling law (6). The constant in (6) is of order one.

The results of Tables III and IV show that the $1/\triangle m^2$ divergence of τ's on lattices of a fixed size is eliminated in the idealized MG algorithm. Relaxation times are

TABLE IV. Dependence of relaxation times τ on $\triangle m^2$ in the ideal MG algorithm with lexicographic SOR for computing propagators of staggered fermions on 12^4 lattices. (The values given for $\beta = 2.5$ were obtained in the same gauge field configuration.)

		τ for $\triangle m^2 =$						
β	ω	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
∞	1.32	1.5	1.7	1.7	1.7	1.7	1.7	1.7
3.0	1.65	2.9	3.2	3.3	3.5	3.5	3.5	3.5
2.7	1.65	2.9	3.4	4.0	4.5	4.5	4.5	4.5
2.5	1.72	4.2	4.9	6.9	8.4	8.7	8.8	8.8
2.5	1.65	3.2	3.8	6.9	8.8	9.3	9.4	9.4
2.4	1.65	3.3	5.0	15.4	23.6	27.7	28.0	28.0

bounded and small. (Only for very disordered gauge fields at physically uninteresting values of the gauge coupling, τ's are not so small, but nevertheless bounded.) We conclude from Tables III and IV that CSD in computation of propagators is strongly reduced. It is hard to judge a possibly remaining volume effect, but one might be tempted to say that CSD can be eliminated for practical purposes, in principle. At this point one should also recall that in the investigations reported here, only one $\mathcal{A}$ kernel was used for all values of m^2. If one used an m^2-dependent kernel, the results would probably improve further; at least they cannot become worse.

Note added in proof: The terminology of "Galerkin operator" used in this article follows the one introduced in Refs. [3] and [4]. In terms used in the mathematical literature, also the idealized coarse grid operator $C(-\not{D}^2 + m^2)\mathcal{A}$ is a Galerkin operator. I am indebted to Alan D. Sokal for this remark.

ACKNOWLEDGMENTS

I wish to thank Gerhard Mack for many stimulating discussions. Financial support by Deutsche Forschungsgemeinschaft is gratefully acknowledged. The computations reported here were performed on the Cray Y-MP of HLRZ Jülich.

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