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Two-grid overlap solver in lattice QCD

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In lattice quantum chromodynamics with chiral fermions we want to solve linear systems which are chiral and dense discretizations of the Dirac operator, or the overlap operator. We propose that multigrid solver are the best choice to solve quickly this linear systems. In this paper we develop a two-grid algorithm. For this purpose, we use the equivalence of the overlap operator with the truncated overlap operator, which is a five dimensional formulation of the same theory. The coarsening is performed along the fifth dimension only. We have tested first this algorithm for small lattice volume 8^4 and we bring here our results for larger lattice size 16^4. We have done simulation in the range of coupling constants and quark masses for which the algorithm is fast and saves a factor of 6, even for dense lattice, compared to the standard Krylov subspace methods.

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1. Introduction

In the lattice QCD, quark fields or fermion fields are placed at the lattice nodes, and gluon fields, or calibration fields, are placed at the connections between nodes. To study the interactions between quarks one must calculate the quark propagator that is mathematically the inverse of the Dirac operator. It is important to formulate a lattice chiral fermion theory as chiral symmetry is characteristic of strong interactions. Thus, in this article we will calculate the propagators of lattice chiral quarks by means of a Dirac chiral operator, such as the Neuberger overlap operator. Since this operator connects two subspaces by means of transcendental operational functions, as will be discussed below, the computational methods are also highly complex.

In this article we bring a faster calculation method than the standard ones, the so called the two-grid algorithm method, which speeds up the solution thanks to the more efficient approximation of the Dirac operator's low eigenvalues [11]. This algorithm was proposed a decade ago but has only been tested for a single pairing constant [1]. In this paper he will study a set of values of pairing constants of the calibration field and for larger lattice volume. The aim is to build and test the algorithm with two networks for different values of the pairing constant of the calibration fields and for quark masses even lighter than in the reference [1]. The algorithm will be compared to a standard algorithm, often used in network QCD as one of the fastest methods to calculate network quark spreaders, the Conjugate Gradients algorithm for normal equations or CGNE (Conjugate Gradients on Normal) Equation) [7].

1.1 Chiral fermions using the Neuberger operator

In 1982, Ginsparg and Wilson concluded that a Dirac chiral operator could be found in the lattice who meets the condition called the Ginsparg-Wilson relationship [6].

$$\{D,\gamma_5\} = aD\gamma_5 D \qquad (1)$$

We note that in the continuous boundary the relation to chirality is recovered. One candidate operator that completes this relationship is the Neuberger overlap operator [10]:

$$D = c_1 I - c_2 V, \qquad (2)$$

where is a unitary matrix, I is the identity matrix and $A = M - aD_W$. The overlap operator D is non-Hermitian operator. This operator can also be expressed equivalently using the sign function,

$$D = c_1 I - c_2\gamma_5 sign(H_W) \qquad (3)$$

where $H_W = \gamma_5(M - aD_W)$, M is a shift parameter in the interval (0,2), which we have fixed $M = 1.8$ in the case of our study, $c_1$dhe c_2 are two constants that are determined by equations, $c_1 = \frac{1+m_q}{2}$, and $c_2 = \frac{1-m_q}{2}$. Where $m_q$is the quark mass and D_W is the Wilson-Dirac operator,

$$D_W = \frac{1}{2}\sum_\mu[\gamma_\mu(\partial_\mu^* + \partial_\mu) - a\partial_\mu^*\partial_\mu] \qquad (4)$$

and ∂_μ, ∂_μ^* are the forward and backward differences operators, closest neighbors:

$$\partial_\mu f(x) = \frac{1}{a}(f(x+ae_\mu) - f(x)), \qquad \partial_\mu^* f(x) = \frac{1}{a}(f(x) - f(x-ae_\mu)), \qquad (5)$$

where e_μ are orientation orts by direction $\mu.\gamma_\mu$ are matrices 4 x 4 who obey Clifford-Dirac algebra. Thus, if the lattice has N nodes, since the calibration fields take values in the SU(3) group, then the Dirac matrix in the lattice is of the order 12N. The advantages of Neuberger chiral fermions are: a) the chiral symmetry of the lattice QCD is exact since the action of the fermions is invariant to chiral transformations [8], we notice that the anticommutation relation (1), when we switch to

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continuous QCD, thus for a → 0, gives the condition of chiral symmetry as it should be in continuous space-time; b) we have fermion theory without doubling, fermions are defined in a single way. The problems encountered in this study method are related to the high computational complexity, due to the complicated form, as a matrix function, of the Neuberger operator.

1.2 Truncated overlap fermions

The Neuberger overlap fermions are equivalent to the truncated overlap fermions, in a 5-dimensional formulation, with the fifth Euclidean dimension N5 [3]. Through this equivalence it becomes possible to adapt and use multigrid according to the fifth dimension. The basic idea is the division into space according to an additional dimension of the left and right chirality defined on the two opposite sides of the border or domain wall. Along the fifth dimension we have no calibration fields. The Dirac operator is now given as a matrix with N5 x N5 4-dimensional operating blocks.

$$M_{TOV}(m_q) = \begin{pmatrix} a_5 D_W - I & (a_5 D_W + I)P_+ & & -m_q(a_5 D_W + I)P_- \\ (a_5 D_W + I)P_- & a_5 D_W - I & \ddots & \\ & \ddots & \ddots & (a_5 D_W + I)P_+ \\ -m_q(a_5 D_W + I)P_+ & & (a_5 D_W + I)P_- & a_5 D_W - I \end{pmatrix} \tag{6}$$

where a_5 is the lattice parameter according to the 5th dimension and $P_\pm$ are the chirality projection operators given by: $P_\pm = \frac{I_4 \pm \gamma_5}{2}$. Such fermions are called domain wall fermions (DWF)[12].

The question that arise naturally is: "*Are domain wall fermions somehow related to the overlap fermions?*" To answer this question, effective theory must be constructed in four dimensions. For this we find the form of Dirac's effective operator, $D^{(N5)}$, in four dimensions [3], from which we have:

$$D^{(N_5)} = \frac{1+m_q}{2} I - \frac{1-m_q}{2} \gamma_5 \tanh\left(\frac{N_5}{2} \log\left(\frac{1-a_5 H_W}{1+a_5 H_W}\right)\right), \tag{7}$$

where $H_W = \gamma_5(M - aD_W)$. In continuum limit $N_5 \to \infty$ we have operator:

$$D^{(\infty)} = \frac{1+m_q}{2} I - \frac{1-m_q}{2} \gamma_5 sign(H_W). \tag{8}$$

2. The TWO-GRID algorithm

An efficient way for solving linear systems arising from differential equations in the lattice is the use of Multigrid Algorithms [11]. In this paper we will apply the two-grid algorithm according to the fifth dimension in the case of the truncated overlap fermions. So, we want to solve the linear system:

$$Dx = b, \tag{9}$$

where D is the overlap operator or Neuberger operator, the right-hand side or quark source, and x are the quark propagators. In order to use the two-grid algorithm we use the equivalence of the overlap operator with truncated overlap operator. Thus, the coarse lattice system:

$$D^{(N_5)} y = r, \tag{10}$$

can be obtained from the 5-dimensional system solution:

$$M_{TOV}(m_q)P\chi = M_{TOV}(1)P\eta, \tag{11}$$

with P we denote the permutation matrix:

$$P = \begin{pmatrix} P_+ & P_- & & \\ & P_+ & \ddots & \\ & & \ddots & P_- \\ P_- & & & P_+ \end{pmatrix}$$

where from the vectors χ and η, $\chi = (y, \chi^{(2)}, \dots, \chi^{(N_5)})^T$ and $\eta = (r, o, \dots, o)^T$, the y and r vectors of the coarse lattice system are determined. Below we present the TWO-GRID algorithm that we have developed to solve this problem:

The TWO-GRID algorithm

Let them be $x_1 \in C^N$ and $r_1 = b - Dx_1$.
We assign two tolerances: tol for the system in the dense lattice and $tol0$ for the system in the coarse lattice.
for *i=1,2, ...* ***do***
Form the sparse lattice vector $\eta_i = (r_i, o, \dots, o)^T$, where the number of zero vectors 4-dimensions it is $N_5 - 1$.
Solve the linear system $M_{TOV}(m_q)P\chi_{i+1} = M_{TOV}(1)P\eta_i$ until the residual is less than $tol0\|M_{TOV}(1)P\eta_i\|_2$.
We derive the correction of the approximate 4-dimensional solution y_{i+1} from that 5-dimensional $\chi_{i+1} = (y_{i+1}, \chi_{i+1}^{(2)}, \dots, \chi_{i+1}^{(N_5)})^T$.
Update the solution on the 4-dimensional lattice $x_{i+1} = x_i + y_{i+1}$
We calculate the residual lattice $r_{i+1} = b - Dx_{i+1}$.
Stop if $\|r_{i+1}\|_2 < tol\|b\|_2$.
end for

We coded the above algorithm in MATLAB/Octave. As expected, due to the complex shape of the Neuberger operator, computer calculations require a lot of physical time. Thus, an inversion with the CGNE algorithm takes about 60 minutes on the Intel (R) Core (TM) 2 Duo CPU T5470@1.60GHz. That's why we turned to FORTRAN codes which takes about 20 minutes on the same processor.

3. Results and Discussions

In addition to the above algorithm coded in MATLAB/Octave, several ready-made QCDLAB package functions have been used [4], one of which is the CGNE (Conjugate Gradients on Normal Equation) algorithm. The purpose of its use is to compare with the two-grid algorithm. Both algorithms are calculated in fixed calibration field, in lattice volume 16^4, with calibration field coupling constants $\beta = 6/g^2$ from $\beta = 5.8$ to $\beta = 5.5$, with step 0.1. For a fixed value of this parameter, we tested the two grid algorithm for different quark masses, starting from heavy mass quarks 0.13 to lighter quarks with mass 0.03 with step 0.01. It was observed that for each fixed value of the pairing constant, the masses of the quarks for which the two-grid algorithm works varies from one configuration to another. We summarize the results in the following tables for each configuration, which give a clear picture of the different quark masses, the number of multiplications by the Wilson matrix, and the residual rate in each step. In our calculations we have determined the accuracy of the order 10^{-8}. The residual rate values with the smallest sign (<) means that for the corresponding quark mass the two-grid algorithm increases the accuracy required by us. Whereas the quark masses without the < sign, have a stagnation of residual values quoted in the table. We will consider that the two-grid algorithm does not converge for these quark masses. Specifically, for the first configuration obtained for β = 5.8, referring to the data in Table 1, it is seen that our algorithm converges for quark masses m = 0.09, m = 0.07, m = 0.06, m = 0.03, for others quark masses have stagnation. In the second configuration obtained for β = 5.7, referring to the data in Table 2, the two-lattice algorithm converges for quark masses m = 0.12, m = 0.09, for others quark masses have stagnation. In the third configuration obtained for β = 5.6, referring to the data in Table 3, the two-lattice algorithm converges for quark masses m = 0.12, m = 0.11, m = 0.07, m = 0.06, for other masses we have stagnation. In the fourth configuration obtained for β = 5.5, referring to the data in Table 3, the two-lattice algorithm converges for quark masses m = 0.13, m = 0.11, m = 0.1, m = 0.09, m = 0.08, m = 0.05, for other measures we have stagnation. In parallel, the same procedure was performed with the CGNE algorithm. The obtained results are presented in the following graphs, where the convergence history of the two-grid algorithm (TWO-GRID) and that of CGNE is given as a function of the number of multiplications performed with the Wilson matrix. Figure 1 is taken for the first configuration generated with coupling constant β = 5.8 and different quark masses as shown in the figure. Similarly Figure 2 gives the convergence history of the two algorithms for coupling constant β = 5.7, Figure 3 for β = 5.6 and Figure 4 for β = 5.5.

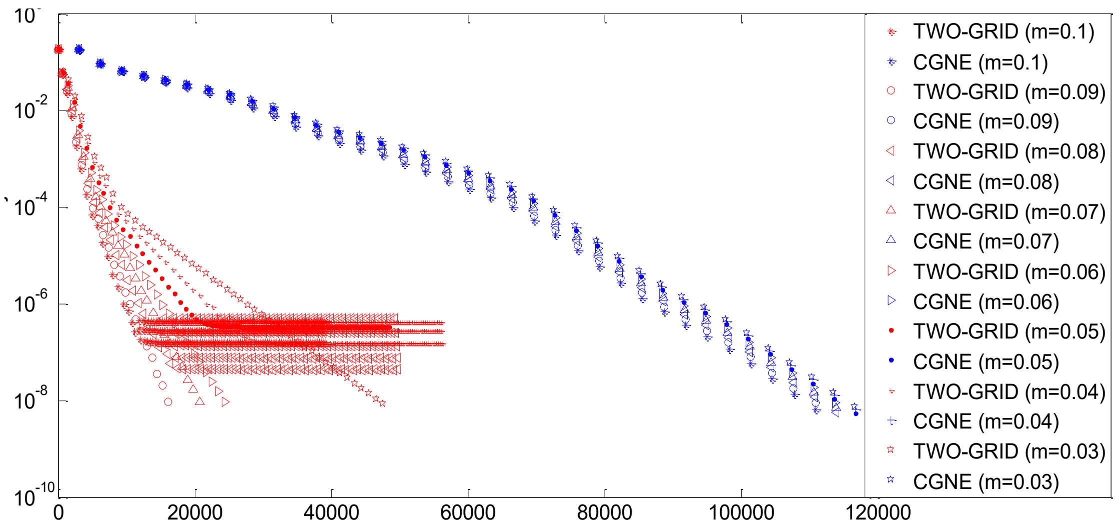

Figure 1. The convergence history of the residual norm as the function of the number of Dirac-Wilson multiplications for TWO-GRID and CGNE algorithms on 16^4 lattice background SU(3) field at coupling constant β=5.8 .

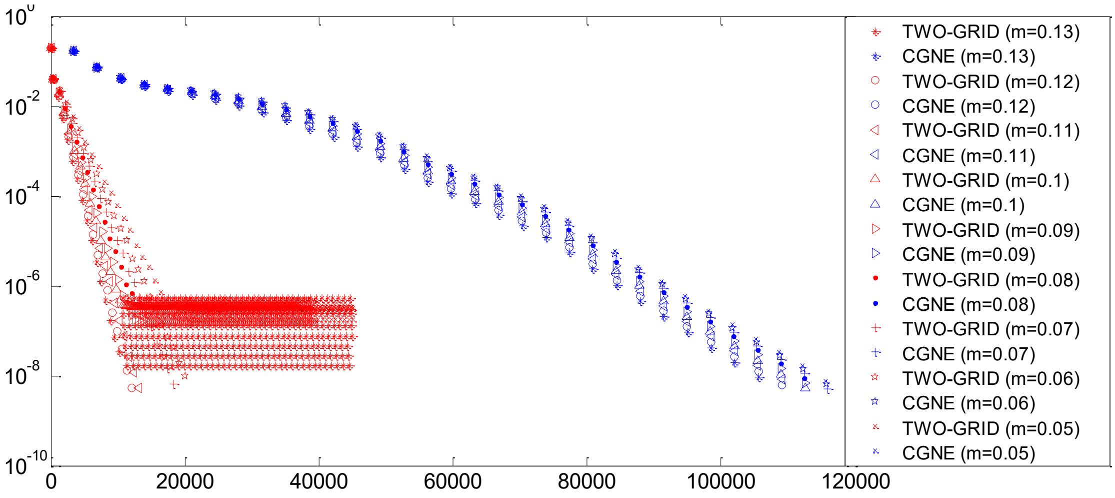

Figura 2. The convergence history of the residual norm as the function of the number of Dirac-Wilson multiplications for TWO-GRID and CGNE algorithms on 16^4 lattice background SU(3) field at coupling constant β=5.7.

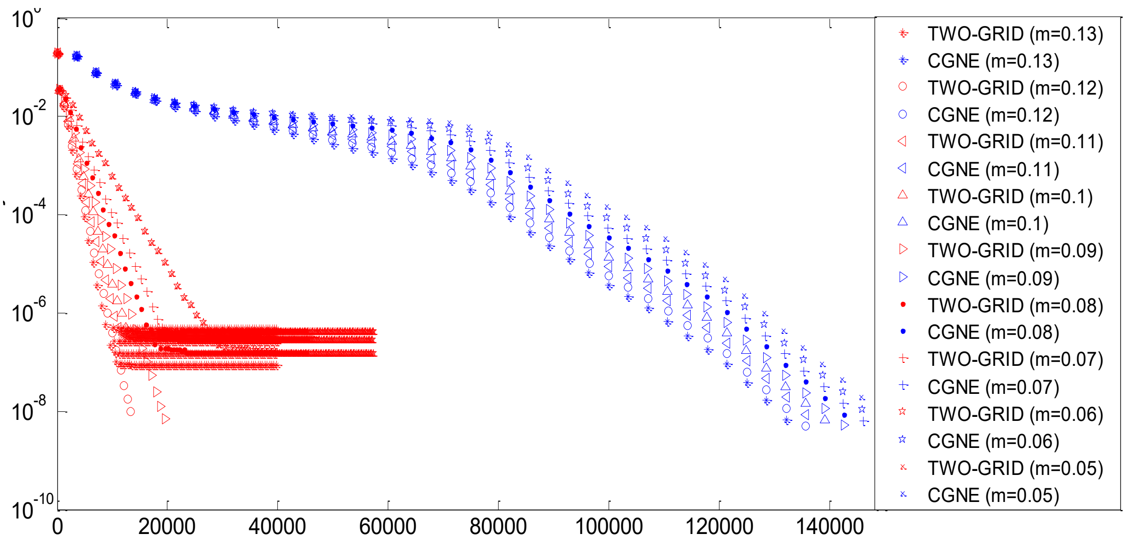

Figure 3. The convergence history of the residual norm as the function of the number of Dirac-Wilson multiplications for TWO-GRID and CGNE algorithms on 16^4 lattice background SU(3) field at coupling constant β=5.6.

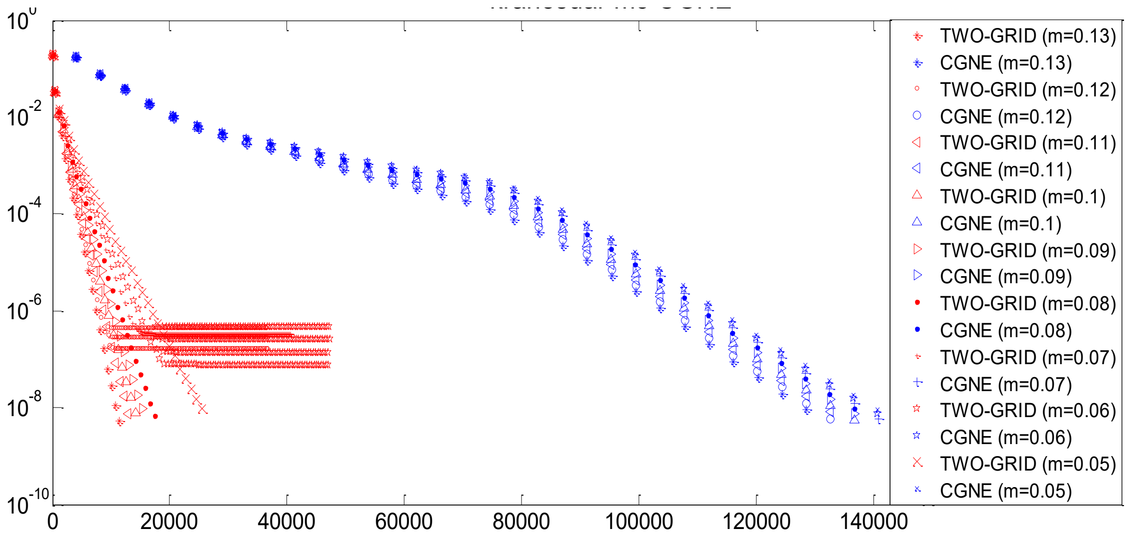

Figure 4. The convergence history of the residual norm as the function of the number of Dirac-Wilson multiplications for TWO-GRID and CGNE algorithms on 16^4 lattice background SU(3) field at coupling constant β=5.5.

Table 1. Data obtained from the convergence history of the TWO - GRID algorithm for the configuration with coupling constant 5.8.

Quark mass	The number of Dirac-Wilson multiplications	Residual norm
0.1	9552	10^{-5}
0.09	16152	$<10^{-8}$
0.08	12450	10^{-6}
0.07	20700	$<10^{-8}$
0.06	24366	$<10^{-8}$
0.05	17898	10^{-5}
0.04	26148	10^{-6}
0.03	47580	$<10^{-8}$

Table 2. Data obtained from the convergence history of the TWO - GRID algorithm for the configuration with coupling constant 5.7.

Quark mass	The number of Dirac-Wilson multiplications	Residual norm
0.13	8052	10^{-5}
0.12	13362	$<10^{-8}$
0.11	9606	10^{-5}
0.1	10956	10^{-5}
0.09	19566	$<10^{-8}$
0.08	15306	10^{-5}
0.07	17292	10^{-5}

0.06	24240	10^{-5}
0.05	24240	10^{-5}

Table 3. Data obtained from the convergence history of the TWO - GRID algorithm for the configuration with coupling constant 5.6.

Quark mass	The number of Dirac-Wilson multiplications	Residual norm
0.13	7512	10^{-5}
0.12	12108	$<10^{-8}$
0.11	13098	$<10^{-8}$
0.1	8958	10^{-5}
0.09	10080	10^{-5}
0.08	11286	10^{-5}
0.07	18282	$<10^{-8}$
0.06	20076	$<10^{-8}$
0.05	15612	10^{-5}

Table 4. Data obtained from the convergence history of the TWO - GRID algorithm for the configuration with coupling constant 5.5.

Quark mass	The number of Dirac-Wilson multiplications	Residual norm
0.13	11430	$<10^{-8}$
0.12	7674	10^{-5}
0.11	12948	$<10^{-8}$
0.1	14118	$<10^{-8}$
0.09	15312	$<10^{-8}$
0.08	17400	$<10^{-8}$
0.07	12378	10^{-5}
0.06	14670	10^{-5}
0.05	25452	$<10^{-8}$

It is clear that ***the two-grid algorithm for each configuration is about 6 times faster*** than the CGNE for those quark masses to which it converges. These preliminary results show that the two-grid algorithm is very promising. Before giving final conclusions, we will first have to find the origin of the non-convergence for certain measures. Our calculations do not show any regularity which leads us to believe that we are dealing with a lack of algorithm instability, an instability that we need to study in the future before advancing the study in even larger lattice volumes.

4. Acknowledgments

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