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TWO-GRID OVERLAP SOLVER IN LATTICE QCD

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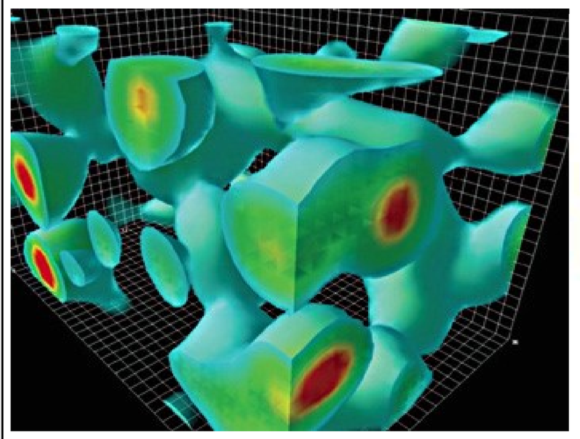
Abstract

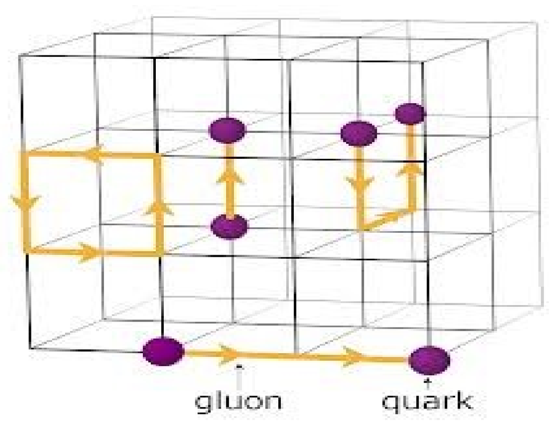
In lattice quantum chromodynamics with chiral fermions we want to solve linear systems which are chiral and dense discretizations of the Dirac operator, or the overlap operator. For this purpose, we use the equivalence of the overlap operator with the truncated overlap operator, which is a five dimensional 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.

Keywords: lattice QCD, multigrid algorithm, overlap solver, two-grid algorithm

Introduction

Lattice QCD is QCD formulated on a discrete Euclidean space time grid. In lattice QCD, fields representing quarks are defined at lattice sites, while the gluon fields are defined on the links connecting neighboring sites. Lattice regularization of chiral fermions is an important development of the theory of elementary particles. After many years of research in lattice QCD, it was possible to formulate QCD with chiral fermions on the lattice. There are two chiral formulations: a) domain wall fermions [2, 3] and b) overlap fermions [4, 5], which are closely related [6]. In particular, the truncated overlap variant of domain wall fermions [7] can b shown to be equivalent to overlap fermions in four dimensions at any lattice spacing [8].The physical information of these theories





is contained in quark propagators, which is the basic major computing problem in lattice QCD simulations. On the other hand it is important to build in lattice a chiral fermionic theory as chiral symmetry is characteristic of strong interactions. Therefore it should be made inversion of the chiral Dirac operator in the lattice which has high complexity (Narayanan & Neuberger 1995), (Neuberger, 1998), (Boriçi, 1999). For this purpose, simulations of lattice theory with U(1) group symmetry or the case of the Quantum Electrodynamics, in two dimensional space-times has always been a testing ground for algorithms. As the lattice volume is increased and simulations are repeated for a large number of statistically independent configurations, it significantly increases the need for computational power. An efficient direction to work with simulations of QCD theory in lattice, is development of fast inversion algorithms in order to gain time and computational cost.

Background

U(1) theory in two dimensional space-times dimensions has always been a testing ground for algorithms. This is even more desirable for chiral fermions in both variants, i.e. overlap and domain wall fermions.

The overlap operator:

$$D = c_1 I + c_2 A(A^* A)^{-\frac{1}{2}} ,$$

with A being the shifted Dirac operator $A = D_W - I$ such that D_W is singular. Here, $c_1 = (1+m)/2$, $c_2 = (1-m)/2$ are related to the bare quark mass m. D can be computed from the inverse square root of $A^* A$:

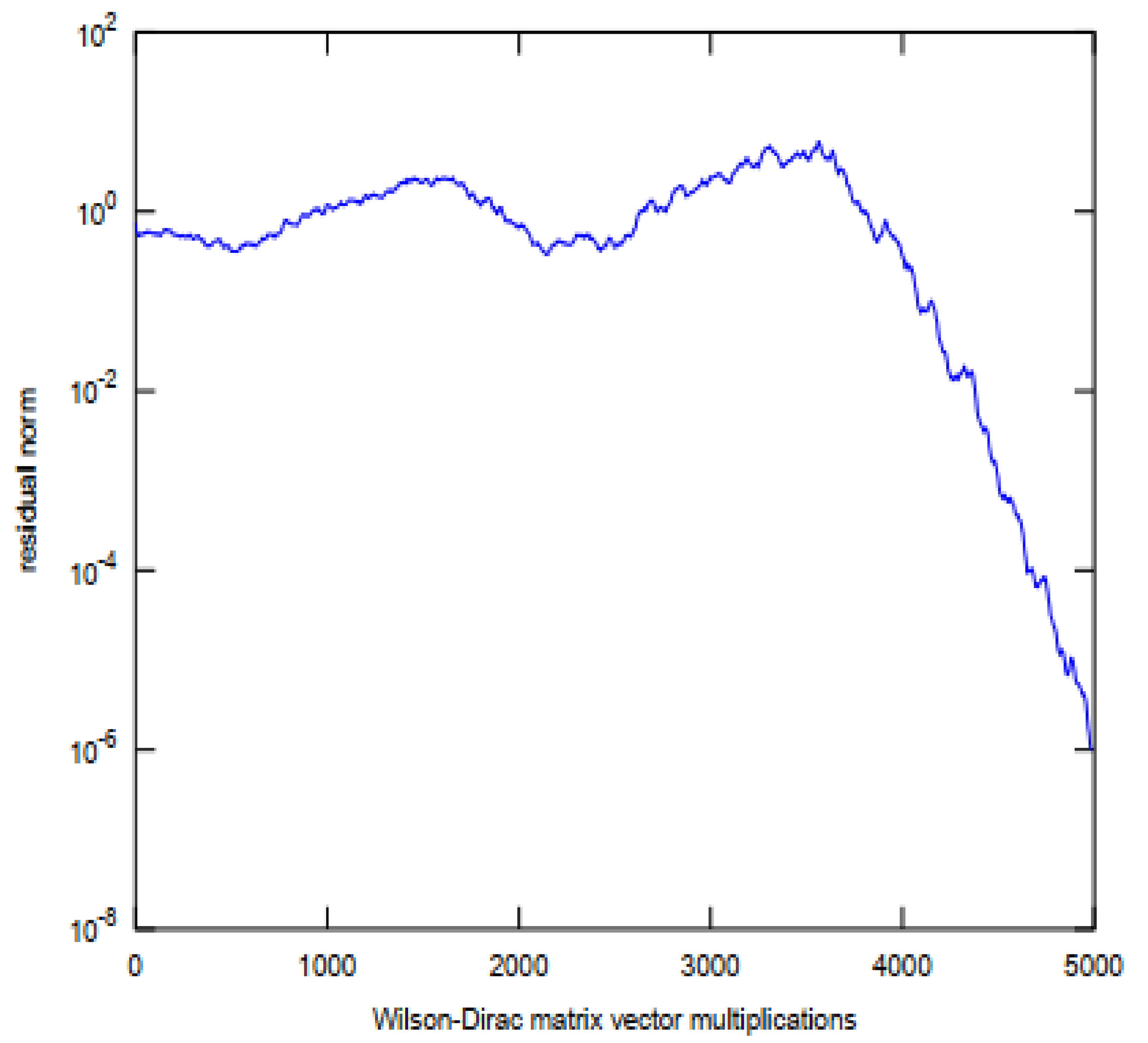
$$(A^* A)^{-\frac{1}{2}} = V\Sigma^{-1}V^* ,$$

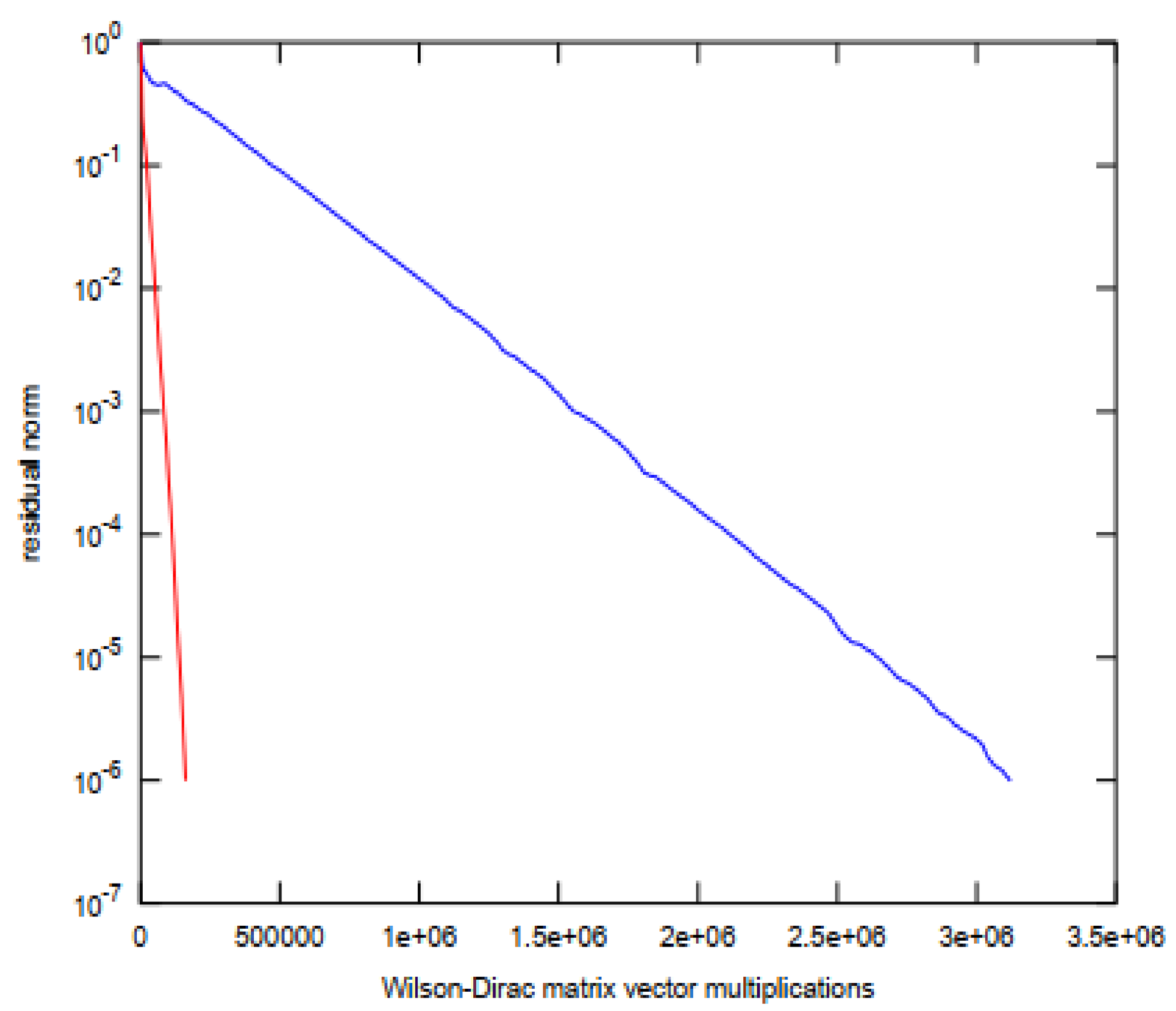
where Σ are the singular values of $A = U\Sigma V^*$.

Since the full matrix D is not required, the multiplication of D with a vector can be computed using Krylov subspace algorithms such as the double pass Lanczos algorithm and Zolotarev approximation for the inverse square root of the Lanczos matrix T. The algorithm requires a lower bound ε of the smallest eigenvalue of $A^* A$.

In the following example we take $\varepsilon = 10^{-7}$, which requires the Zolotarev rational polynomial to be of the order $n = 60$, i.e. the number of T inversions is thus $n/2 = 30$. One iteration of the above algorithm using the Lanczos algorithm running the Octave script on an Intel Celeron 430 processor at 1.73 GHz spent about 7 seconds.

Results





Conclusions

In the following we give an example of the overlap inversion using the SHUMR (blue) and preconditioned GMRESR (red) algorithms, without projection of small eigenvalues of $A^* A$ on a 32 x 32 lattice background U(1) field at $\beta = 1$ and $m = 0.01$. The convergence history of the SHUMR residual norm is given below.

The SHUMR algorithm is decribed in [1], whereas GMRESR in [2]. The multigrid preconditioner is described in [3], whereas the details of truncated overlap fermions in [4]. The Lanczos method for the inverse square root can be found in [5], whereas the Zolotarev approximation in [6].

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