THE CRITICAL SLOWING OF ALGORITHMS IN LQCD SIMULATIONS

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ABSTRACT

Chiral symmetry plays a critical role in lattice QCD simulations, particularly in modelling strong interactions. Simulations involving chiral fermions are computationally demanding due to the intricacies of the chiral Dirac operator. A primary challenge in lattice QCD calculations is dealing with simulations that involve light quarks. Traditional algorithms used in these simulations are susceptible to the problem of critical slowing down, causing the number of iterations required by the algorithm to scale inversely with the quark mass. To address this issue and explore the development of new algorithms, we conducted simulations using U (1) theory in two dimensions, which shares common features and algorithms with QCD. As a result, we introduced a novel algorithm called the preconditioned GMRESR, which had been previously reported and implemented using the QCDLAB software. In this paper, we calculate the inversion time for various quark masses and test them against three coupling constants. We also compare the results with another optimal algorithm typically used in such simulations. In our prior research, we conducted simulations on smaller lattice sizes. In this current work, we extend our investigations to a larger lattice volume of 256 x 256. Our results demonstrate that our algorithm significantly reduces simulation time when dealing with light quarks, outperforming the traditional

algorithms by approximately 12.5 times. In conclusion, increasing the lattice volume yields superior results, affirming the efficiency and effectiveness of our newly developed algorithm.
Keywords: inversion time, lattice QCD simulations, QCDLAB

1. INTRODUCTION

Quantum Chromodynamics (QCD) is the theory that describes the strong interactions between quarks and gluons, elucidating the physics of strong interactions across a range of energy regimes, from low to high energies. At high energies, we observe the phenomenon of asymptotic freedom in quarks, as highlighted in (Lüscher 2003), which allows us to employ perturbative calculations to understand the theory. In contrast, at low energies, quark confinement, first formulated by Wilson in 1974, becomes the dominant feature due to the strong coupling between quarks. In these low-energy regimes, non-perturbative methods, such as lattice QCD (LQCD) simulations (Wilson 1974), are necessary for analysis. Lattice QCD is a framework formulated on a lattice consisting of N points in both space and time. Quark fields are located on the lattice sites, while the gluon fields reside on the links connecting adjacent lattice sites. This lattice regularization of chiral fermions plays a pivotal role in the field of elementary particle physics. There are two principal methods for implementing QCD with chiral fermions on the lattice: domain wall fermions (Kaplan 1992; Furman and Shamir 1995) and overlap fermions (Narayanan and Neuberger 1993; Narayanan and Neuberger 1995), with the latter being closely related to the former (Boriçi 2005). Notably, the truncated overlap variant of domain wall fermions (Boriçi 2000), as demonstrated in (Boriçi 2006), is equivalent to overlap fermions in four dimensions. In these theories, the computation of quark propagators is fundamental. To construct propagators for other elementary particles, such as mesons and nucleons, one must combine quark propagators in a specific manner. As quarks are confined within hadrons and cannot be directly observed as physical particles, their masses must be indirectly determined. The primary computational challenge in lattice QCD lies in the calculation of the quark propagator.

2. MATERIALS AND METHOD

Simulations involving chiral fermions in lattice QCD are closely tied to the chiral Dirac operator, which is often represented by the Neuberger operator or the so-called overlap operator (Neuberger 1998). The computations of overlap quark propagators involve solving large linear systems of the form $D \cdot x = b$, where the operator D, a large and sparse matrix, represents the overlap Dirac operator on a four-dimensional space-time lattice. Here, $x \in CN$ denotes the quark propagator, and $b \in C^N$ represents the source.

Due to the inherent complexity of this operator, addressing this problem necessitates highly intensive computations.

When it comes to solving large linear systems in methods for chiral fermions, several optimal methods are derived from Krylov subspace methods (Boriçi 1996), including GMRES, CGNE, and SHUMR. However, these algorithms tend to experience significant slowdowns when dealing with light quarks and, in some cases, may even fail to converge. In Krylov inversion algorithms (Boriçi and Forcrand 1994; Brianzi *et al*., 2006; Favati *et al*., 2014), the time required for inversion escalates inversely with the quark mass. This phenomenon, known as the "critical slowdown of algorithms," has been well-documented in these simulations (Schaefer and Berlin 2011; Cossu *et al*., 2018; Schaefer 2011). Consequently, it is preferable to consider the case of lattice theory simulations for Quantum Electrodynamics, which possess U (1) group symmetry and are formulated in two space-time dimensions. Xhako and Boriçi (2014) introduced a faster inversion algorithm for chiral fermions, known as the preconditioned GMRESR algorithm. The key to the preconditioned part of this algorithm lies in the relationship between the overlap operator and the truncated overlap operator with a finite extra dimension.

To implement the preconditioned GMRESR algorithm, we utilized a specialized software package called QCDLAB (Boriçi 2006; 2007). QCDLAB is tailored for lattice QCD algorithms and simulations, and, in our case, we specifically employed QCDLAB 1.0. This version of the software includes the Schwinger model on the lattice, exemplifying U(1) group symmetry. While the Schwinger model differs from full lattice QCD, it shares many similarities with the algorithms used in lattice QCD simulations. With this algorithm, we calculated the domain wall fermion propagator and utilized the truncated overlap operator of domain wall fermions, albeit in the context of 2+1 dimensions, with N3 serving as the extra finite dimension. Our new algorithm is an additional code integrated into the QCDLAB 1.0 software, specifically designed for two-dimensional simulations.

In the context of inversion algorithms, one typical test involves examining the convergence history of the residual norm. This test graphically displays the results of the residual norm as the algorithm progresses, showcasing how the residual norm changes with the number of Dirac operator multiplications until convergence is achieved. Such an analysis for the preconditioned GMRESR algorithm was conducted in (Hyka (Xhako) and Osmanaj (Zeqirllari), 2018). The current paper also provides insights into the efficiency and speed of an algorithm used in numerical simulations of lattice QCD. One key aspect examined is how the algorithm's performance scales with the quark mass. In the case of optimal inversion algorithms based on Krylov methods, the time (t) required for inverting the chiral Dirac operator is scaled with the inverse of the quark mass (mq) measured in lattice units:

$$t \sim {m_q}^k \tag{1}$$

where k =-1 and this problem is called the critical slowing down. An inversion algorithm will be optimal one if the coefficient k ≈ 0, so totally independent from quark mass. Equation (1) in logarithmic scale will take the form $log t \sim k\, x\, log m_q$.

In our exploration of this phenomenon, we conducted computations for both the preconditioned GMRESR algorithm and the SHUMR algorithm, measuring the inversion time of the overlap operator (in seconds) for various quark masses. The methodology employed in this study remains consistent with our prior work, where we examined the critical slowing down of algorithms for light quark masses, as documented in (Xhako and Zeqirllari 2019). In the realm of lattice QCD algorithm development, for a more precise and dependable assessment of the efficiency of the algorithm in use, it becomes essential to test it on a larger lattice volume. This approach brings us closer to the conditions encountered in continuum QCD theory and allows for more accurate conclusions regarding algorithm efficiency.

3. RESULTS AND DISCUSSION

We conducted numerical simulations using 100 different statistically independent gauge field configurations randomly selected from a U(1) background. The coupling constant of the gauge field background was examined across three values: β = 1.0, β = 1.1, and β = 1.2, which were considered sufficient for deriving conclusive results. These simulations were performed on a lattice volume of 256 x 256. For each of the three coupling constants, the calculations were carried out across a range of quark masses, specifically mq = [0.5, 0.45, 0.4, 0.35, 0.3, 0.25, 0.2, 0.15, 0.1, 0.05, 0.01], all measured in lattice units. The same numerical simulations were performed for both the preconditioned GMRESR and the SHUMR algorithms. The numerical results from these simulations are presented in Tables 1 to 3, corresponding to the three tested values of the coupling constant: β = 1.0, β = 1.1, and β = 1.2. Additionally, the results are visually represented in Figures 1 to 3, as outlined in Equation (1).

Table 1 Inversion time of chiral operator for coupling constant β = 1.0 in 256^2 lattice

No	Quark mass (in Lattice Unit)	Algorithms	Inversion time (in sec.)
1	0.5	SHUMR GMRESR	101.02 33.051
2	0.45	SHUMR GMRESR	103.52 38.155
3	0.35	SHUMR GMRESR	136.14 38.947
4	0.3	SHUMR GMRESR	189.94 40.870
5	0.25	SHUMR GMRESR	199.98 43.140
6	0.20	SHUMR GMRESR	295.76 47.231
7	0.15	SHUMR GMRESR	406.39 51.500
8	0.1	SHUMR GMRESR	1071.52 56.643
9	0.05	SHUMR GMRESR	3890.18 70.111
10	0.001	SHUMR GMRESR	15763.1 87.907

Table 2 Inversion time of chiral operator for coupling constant β = 1.1 in 256^2 lattice

No	Quark Mass (in Lattice Unit)	Algorithms	Inversion Time (in Seconds)
1	0.5	SHUMR GMRESR	101.95 35.671
2	0.45	SHUMR GMRESR	110.05 37.182
3	0.35	SHUMR GMRESR	129.86 39.201

4	0.3	SHUMR GMRESR	138.96 40.009
5	0.25	SHUMR GMRESR	179.82 40.951
6	0.20	SHUMR GMRESR	200.94 40.990
7	0.15	SHUMR GMRESR	278.04 41.250
8	0.1	SHUMR GMRESR	398.64 44.902
9	0.05	SHUMR GMRESR	809.34 52.671
10	0.001	SHUMR GMRESR	2110.13 64.096

Table 3. Inversion time of chiral operator for coupling constant $\beta = 1.2$ in 256^2 lattice

No	Quark mass (in Lattice unit)	Algorithms	Inversion time (in sec.)
1	0.5	SHUMR GMRESR	116.31 38.096
2	0.45	SHUMR GMRESR	121.01 38.871
3	0.35	SHUMR GMRESR	132.84 40.991
4	0.3	SHUMR GMRESR	155.58 41.071
5	0.25	SHUMR GMRESR	199.74 42.781
6	0.20	SHUMR GMRESR	225.82 43.940
7	0.15	SHUMR GMRESR	339.15 44.633
8	0.1	SHUMR GMRESR	589.95 46.180
9	0.05	SHUMR GMRESR	924.19 49.230
10	0.001	SHUMR GMRESR	1443.24 65.817

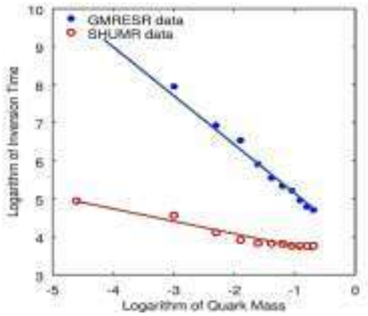

Fig. 1: The logarithmic scale of the inversion time using the preconditioned GMRESR and SHUMR algorithms, in 256 x 256 lattice and coupling constant 1.0. The linear fit gives k = - 0.093 for the preconditioned GMRESR and k = - 1.050 for SHUMR.

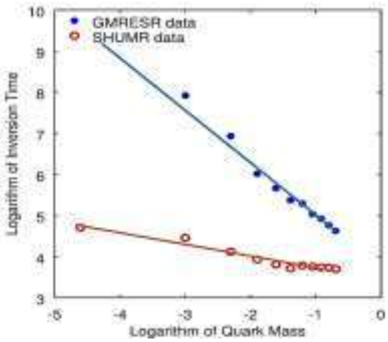

Fig. 2: The logarithmic scale of the inversion time using the preconditioned GMRESR and SHUMR algorithms, in 256 x 256 lattice and coupling constant 1.1. The linear fit gives k = - 0.084 for the preconditioned GMRESR and k = - 1.042 for SHUMR.

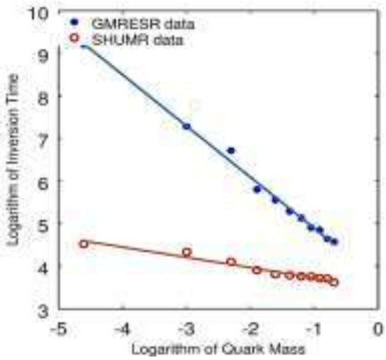

Fig. 3: The logarithmic scale of the inversion time using the preconditioned GMRESR and SHUMR algorithms, in *256 x 256* lattice and coupling constant 1.2. The linear fit gives k = - 0.073 for the preconditioned GMRESR and k = -1.011 for SHUMR.

Figures 1 to 3 illustrate the relationship between the inversion time (measured in seconds) of the overlap chiral operator and the quark mass for both the preconditioned GMRESR and SHUMR algorithms. These graphs are presented on a logarithmic scale to determine the coefficient k. As previously explained, we utilized the preconditioned GMRESR and SHUMR algorithms on a 256 x 256 lattice with a U (1) gauge field. Across three different background fields, it's evident that the preconditioned GMRESR algorithm exhibits a significantly smaller coefficient k compared to the SHUMR algorithm. Table 1 demonstrates that the preconditioned GMRESR algorithm scales with the quark mass as ${m_q}^{-0.093}$), while the SHUMR algorithm scales as ${m_q}^{-1.050}$. Consequently, the coefficient k for the SHUMR algorithm is 11.3 times greater than for the preconditioned GMRESR algorithm at a constant β = 1.0. In Table 2, the preconditioned GMRESR algorithm escalates with the quark mass as ${m_q}^{-0.084}$, and the SHUMR algorithm follows a scaling law of ${m_q}^{-1.042}$. This leads to the SHUMR algorithm having a coefficient k 12.4 times greater than that of the preconditioned GMRESR algorithm when β = 1.1. Table 3 reveals that the preconditioned GMRESR algorithm's scaling with quark mass is ${m_q}^{-0.073}$, whereas the SHUMR algorithm scales as ${m_q}^{-1.011}$. Consequently, the coefficient k for the SHUMR algorithm is 13.8 times greater than that for the preconditioned GMRESR algorithm when the coupling constant is β = 1.2.

4. CONCLUSIONS

When testing our new algorithm (as introduced in Xhako and Boriçi 2014) on a lattice volume of 256 x 256, we observed that the coefficient k for the SHUMR algorithm was 12.5 times greater than that for the preconditioned GMRESR algorithm, across different coupling constants. In our earlier work, detailed in (Xhako and Zeqirllari 2019), where we used a smaller lattice volume, we found that the coefficient k for the SHUMR algorithm was approximately 4.5 times greater than that for the preconditioned GMRESR algorithm, also across different coupling constants. In conclusion, the inversion time of the chiral operator in lattice QCD simulations, when utilizing the preconditioned GMRESR algorithm, does not exhibit the same dependence on the inverse of the quark mass as observed in the SHUMR algorithm. Based on these results, we can confidently affirm the efficiency of our algorithms, even when applied to denser lattices, bringing us closer to the realm of continuum QCD. This suggests that the lattice QCD community can readily employ our algorithm in their calculations.

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REFERENCES

Boriçi A. 1996. Krylov subspace methods in Lattice QCD, PhD thesis, CSCS TR-96-27, ETH Zurich.

Boriçi A. 2000. Truncated overlap fermions. *Nuclear Physics B - Proceeding Supplements*. **83-84**, 771-773.

Boriçi A. 2005. Computational methods for the fermion determinant and the link between overlap and domain wall fermions, in QCD and Numerical Analysis III, ed. Boriçi et al, Springer.

Boriçi A. 2006. QCDLAB: designing lattice QCD Algorithms with MATLAB, High Energy Physics - Lattice (hep-lat), arXiv:hep-lat/0610054.

Boriçi A. 2006. Truncated Overlap Fermions: the link between overlap and domain wall fermions, in V. Mitrjushkin and G. Schierholz (edts.), Lattice Fermions and Structure of the Vacuum, Kluwer Academic Publishers.

Boriçi A. 2007. Speeding up Domain Wall Fermion Algorithms using QCDLAB, Invited talk given at the 'Domain Wall Fermions at Ten Years', Brookhaven National Laboratory, arXiv:hep-lat/0703021.

Boriçi A, Forcrand P. 1994. Fast Krylov space methods for calculation of quark propagator. In: Physics computing '94. (1994). Proceedings, 6th Joint EPS-APS International Conference, PC'94, Lugano, Switzerland, pp. 711–714. arXiv: hep-lat/9405001.

Brianzi P, Favati P, Menchi O, Romani F. **2006**, A framework for studying the regularizing properties of Krylov subspace methods. *Inverse Problems*, 22: 1007–1021.

Cossu G, Boyle P, Christ N, Jung Ch, Jüttner A, Sanfilippo F. 2018. Testing algorithms for critical slowing down. EPJ Web of Conferences 175, 02008, https://doi.org/10.1051/epjconf/201817502008.

Favati P, Lotti G, Menchi O, Romani F. 2014. Generalized Cross-Validation applied to Conjugate Gradient for discrete ill-posed problems. *Applied Mathematics and Computation*, **243:** 258–268.

Furman V, Shamir Y. 1995. Axial symmetries in lattice QCD with Kaplan fermions. *Nuclear Physics B*, **439(1-2),** 54-78.

Hyka (Xhako) D, Osmanaj (Zeqirllari) R. 2018. Fast algorithms for chiral fermions in 2 dimensions, EPJ Web of Conferences 175, 14005 https://doi.org/10.1051/epjconf/201817514005.

Kaplan DB. 1992. A Method for Simulating Chiral Fermions on the Lattice. *Physics Letters B*, **228 (3-4):** 342-347.

Lüscher M. 2003. Lattice QCD — from quark confinement to asymptotic freedom. *Annales Henri Poincaré* **4** (Suppl 1), 197–210. https://doi.org/10.1007/s00023-003-0916-z.

Narayanan R, Neuberger H. 1993. Infinitely many regulator fields for chiral fermions. Phys. Lett. B 302, 62.

Narayanan R, Neuberger H. 1995. A construction of lattice chiral gauge theories. *Nuclear Physics B,* **443 (1-2):** 305.

Neuberger H. 1998. Exactly massless quarks on the lattice. *Physics Letters B,* **417(1-2):** 141-144.

Schaefer S. 2011, Algorithms for lattice QCD: progress and challenges, AIP Conference Proceedings 1343, 93 https://doi.org/10.1063/1.3574948.

Schaefer S, Berlin HU. 2011. Critical slowing down and error analysis in lattice QCD simulations, ALPHA Collaboration Nuclear Physics B, 845 93-119 DOI: 10.1016/j.nuclphysb.2010.11.020.

Wilson KG. 1974. Confinement of Quarks. *Physical Reviewed D*, 10: 2445.

Xhako D, Boriçi A. 2014, Fast Algorithms for Simulating Chiral Fermions in U(1) Lattice Gauge Theory. *American Journal of Physics and Applications,* **2(2):** 67-72.

Xhako D, Zeqirllari R. 2019, Chiral Fermions Algorithms in Lattice QCD. *East European Journal of Physics*, 1: 34-39. https://doi.org/10.26565/2312-4334-2019-1-02.