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Inversion Algorithms for Boriçi – Creutz fermions

Rudina Osmanaj[1*], *Skënder* Minarolli[1], *Dafina* Xhako[2], *Klaudio* Peqini[1], *Dorian* Osmanaj[2] and *Enkelejd* Caca[2]

[1]Faculty of Natural Sciences, University of Tirana, Bvd "Zog I", Tiranë, Albania
[2]Polytechnic University of Tirana, Albania

Abstract. In this work we present some inversion algorithms used for minimally doubled fermions and a comparative study of them in the case of a specific class of MDF: Boriçi – Creutz fermions. We have studied three main algorithms: Biconjugate gradient stabilized method BICGStab, the Conjugate Gradient method applied to the Normal Equations CGNE and Generalized minimal residual method GMRES, used for the inversion of the Dirac operator (BC operator in this case) and have seen how suitable are for non - hermitian operators, how fast they converge, the memory use and the preconditioning options. The tests are performed in the cluster of the Faculty of Natural Sciences, in a 64^4 lattice for five different mass quarks. The results show that the BICGStab algorithm converges faster than the other algorithm tested for Boriçi Creutz fermions, has a low memory use and turns to be one of the more efficient for MDF uses. In the chiral limit each one of them, presents specific challenges, but in the overall BICGStab algorithm seems to be better than the others, making it the default solver for BC fermions.

1 Introduction

Quantum Chromodynamics (QCD) is the theory that describes strong interactions between quarks and gluons and is one of the most important part of the theoretical physics. Anyway, analytic solutions in low - energy QCD are hard or impossible due to the nonlinear nature of the strong force and the large coupling constant at low energies. One of the most powerful non - perturbative methods to study QCD is its discretization on a space - time lattice, known as Lattice QCD. In this approach, the continuous space - time is replaced by a four - dimensional grid, allowing for numerical evaluation of QCD path integrals through Monte Carlo methods. In this non perturbative approach proposed by Wilson in 1974, both gauge and fermions action are discretized [1].

There are several lattice fermions formulations, but we are focused on Boriçi - Creutz fermions [2, 3], part of minimally doubled fermions category, fermions that have been in center of many other previous studies of our group [4, 5, 6, 7, 8]. To address fermion doubling while preserving chiral symmetry more effectively than Wilson fermions, Boriçi–Creutz

* Corresponding author: rudina.zeqirllari@fshn.edu.al

fermions offer a promising discretization scheme. They achieve minimal doubling, leaving only two fermion species, while avoiding the full computational complexity of Ginsparg–Wilson fermions.[3, 12]

A very important computational challenge in Lattice QCD is the inversion of the Dirac operator, which arises when integrating out the fermionic degrees of freedom. Our focus will be on some main important inversion algorithms suitable for BC fermions. Among the most widely used Krylov subspace solvers in this context are:

- CGNE (Conjugate Gradient on Normal Equations) – applicable by converting a non-Hermitian problem into a Hermitian one;
- BiCGSTAB (BiConjugate Gradient Stabilized) – well suited for non-Hermitian systems with improved convergence over BiCG;
- GMRES (Generalized Minimal Residual) – a residual-minimizing algorithm ideal for challenging linear systems, though with higher memory costs.

Each of these algorithms represents a trade - off between speed, stability, and memory usage. The selection of the appropriate solver is crucial for efficient simulation of QCD with Boriçi – Creutz fermions [2,3].

Boriçi–Creutz Fermions

Motivated by the structure of electrons in two-dimensional graphene, Creutz introduced the idea of a lattice fermion operator which, in four dimensions, describes two flavors of Dirac fermions with exact chiral symmetry [3]. In order to obtain a lattice action with a zero at the origin, a new formulation of the lattice operator on orthogonal axes was proposed: the Boriçi–Creutz operator [2].

In the momentum space this operator has the following form:

$$D(p) = \sum_{\mu} i\gamma_{\mu} \sin p_{\mu} + \sum_{\mu} i\gamma'_{\mu} \cos p_{\mu} - 2i\Gamma$$

In this formulation, the gamma matrices appear in non - standard linear combinations that are aligned with the directions of the lattice. In particular, the combination

$$\Gamma = \frac{1}{2}\sum_{\mu=1}^{4} \gamma_{\mu}$$

selects a preferred direction in Euclidean spacetime, corresponding to the diagonal of the hypercube. The BC operator has two zeros:

$$p_1 = (0,0,0,0) \qquad\qquad p_2 = (\pi/2, \pi/2, \pi/2, \pi/2).$$

The zeros of this operator, which correspond to the two physical flavors, select a preferred direction in Euclidean spacetime, defined by the line connecting them. In the case of the Boriçi–Creutz operator, this direction is the diagonal of the hypercube. Consequently, hypercubic symmetry is broken [2, 14]. Several work for exploring and clarify BC fermions are done by the authors [4, 5, 6, 7, 8, 15, 16].

In this work we have tested these three algorithms in order to choose the most appropriate one for this class of fermions.

2 Materials and Methods

In lattice QCD, inversion algorithms are very import for solving linear equations in order to find the quark propagator, and include standard Krylov subspace methods or advanced techniques such as preconditioned algorithms and overlap solvers. These methods have evolved to address critical slowing down, which occurs when standard inversion algorithms become inefficient, especially at low quark masses, with improvements including preconditioning and multi - grid or multi - GPU approaches [6].

Below we make a review of some very known inversion algorithms used in Lattice QCD and then analyse them for minimally doubled Boriçi – Creutz fermions. We perform a comparative study of these algorithms in terms of convergence and memory usage in the case of BC fermions. We have studied three main algorithms: Biconjugate gradient stabilized method BICGStab, the Conjugate Gradient method applied to the Normal Equations CGNE and Generalized minimal residual method GMRES, used for the inversion of the Dirac operator (BC operator in this case) and have seen how suitable are for non - hermitian operators, how fast they converge, the memory use and the preconditioning options.

We focus on the numerical solution of the linear system

$$D\,x = b$$

where D is the discretized Dirac operator for Boriçi – Creutz fermions on a four-dimensional Euclidean lattice, b is a given source vector representing a point source on the lattice, and x corresponds to the quark propagator. All calculations were performed in double precision arithmetic to minimize numerical instabilities arising from the non-Hermitian nature of the Dirac matrix.

The gauge field configurations were generated independently and treated as fixed backgrounds during the inversion of D, using the Wilson gauge. For each configuration, the iterative solvers were applied to compute the propagator with a predefined stopping criterion

$$\frac{\| r_k \|_2}{\| b \|_2} \leq 10^{-8},$$

where $r_k = b - Dx_k$ is the residual vector at iteration k.

The following Krylov subspace algorithms were implemented and benchmarked:

- **CGNE**, to solve the equivalent Hermitian positive-definite system $D^{\dagger}Dx = D^{\dagger}b$;
- **BiCGSTAB**, applied directly to D, exploiting its ability to handle non-Hermitian systems efficiently;
- **GMRES**, an iterative solver for finding numerical solutions to non-symmetric, sparse, or dense systems of linear equations. [9]

The algorithms were implemented in C++ with performance - critical routines parallelized using MPI (FermiQCD). FermiQCD is a C++ library for fast development of parallel Lattice Quantum Field Theory computations that uses MPI for parallelization on distributed - memory architectures. [13] We have used this package in our previous works, for testing algorithms, programs scalability and lattice computations. [4,5,7].
The tests are performed in the cluster of the Faculty of Natural Sciences, in a 64^4 lattice for five different mass quarks, in the quenched approximation.
In order to ensure numerical stability, normalization of Krylov basis vectors and explicit reorthogonalization (in the case of GMRES) were employed. No preconditioning was applied in the baseline results presented here, in order to provide a fair algorithmic comparison. However, the solver framework allows for straightforward inclusion of preconditioners such as even–odd decomposition, which can further accelerate convergence.

The performance of the algorithms was evaluated in terms of:

1. Number of iterations to convergence,
2. Wall-clock time,
3. Residual norm history

These evaluations provide a systematic comparison of the solvers' behavior in the case of Boriçi – Creutz fermions and offer practical guidance for selecting appropriate algorithms in large - scale Lattice QCD computations for this class of fermions, lattice fermions that the authors of the paper has worked for years, after the proposal of Boriçi in 2008 (co-author and collaborator in the mention papers. [2]
Let's make a short summary of the analysed inversion algorithms :

- The CGNE (Conjugate Gradient Normal Equation) algorithm is an iterative method used to solve linear systems, especially those arising from inverse problems that are large, non-symmetric, or ill-posed [11].

- In mathematics, the generalized minimal residual method (GMRES) is an iterative method for the numerical solution of an indefinite nonsymmetric system of linear equations. The method approximates the solution by the vector in a Krylov subspace with minimal residual. The Arnoldi iteration is used to find this vector. This method was developed by Yousef Saad and Martin H. Schultz in 1986 [11].

- In numerical linear algebra, the Biconjugate Gradient Stabilized method, often known as BiCGSTAB, is an iterative method developed by H. A. van der Vorst [10] for the numerical solution of nonsymmetric linear systems. It is a variant of the biconjugate gradient method (BiCG) and has faster and smoother convergence than the original BiCG as well as other variants such as the conjugate gradient squared method (CGS). It is a Krylov subspace method.

Shortly, these algorithms are written in pseudocodes as below:

CGNE (Conjugate Gradient on Normal Equations)

```
Inputs: A, b, x0, max_iter, tol
r = b - A * x0
y = A' * r  (Note: A' is transpose of A)
p = y
delta = y' * y
delta0 = delta

for k = 0 to max_iter - 1:
    Ap = A * p
    alpha = delta / (Ap' * Ap)
    x = x + alpha * p
    r = r - alpha * Ap

    y = A' * r
    delta_new = y' * y

    if sqrt(delta_new) < tol:
        break

    beta = delta_new / delta
    p = y + beta * p
    delta = delta_new
end
```

GMRES (Generalized Minimal Residual)

```
   Inputs: A, b, x0, m (restart parameter), max_iter, tol
   r0 = b - A * x0
   beta = norm(r0)
   v1 = r0 / beta
   H = zeros(m+1, m)

   for j = 1 to m:
       w = A * vj
       for i = 1 to j:
           H(i,j) = w' * vi
           w = w - H(i,j) * vi
       end
       H(j+1,j) = norm(w)
       v(j+1) = w / H(j+1,j)

       # Solve mini-least squares problem
       y = argmin ||beta*e1 - H*y||2
       x = x0 + V(:,1:j) * y

       if ||r|| < tol:
           break
#(If max_iter > m, restart with x0 = x)
```

BiCGSTAB (Biconjugate Gradient Stabilized)

```
   Inputs: A, b, x0, max_iter, tol
   r = b - A * x0
   r_hat = r (arbitrary vector, usually r0)
   rho = 1, alpha = 1, omega = 1
   v = 0, p = 0
   for i = 1 to max_iter:
       rho_new = r_hat' * r
       if rho_new == 0: break # Method fails

       if i > 1:
           beta = (rho_new / rho) * (alpha / omega)
           p = r + beta * (p - omega * v)
       else:
           p = r
       v = A * p
       alpha = rho_new / (r_hat' * v)
       s = r - alpha * v
       if norm(s) < tol:
           x = x + alpha * p
           break
       t = A * s
       omega = (t' * s) / (t' * t)
       x = x + alpha * p + omega * s
       r = s - omega * t
       if norm(r) < tol:
           break
       if omega == 0: break # Method fails
       rho = rho_new
end
```

The above algorithms are modified and implemented in FermiQCD and are available at: https://github.com/rosmanaj/LQCDsolvers_BC

3 Numerical results

In this section we present the numerical performance of the three iterative algorithms: CGNE, BiCGStab, and GMRES, applied to the inversion of the Boriçi – Creutz Dirac operator on a 64^4 lattice. The tests were performed for five different bare quark masses on the HPC cluster of the Faculty of Natural Sciences, in the quenched approximation.

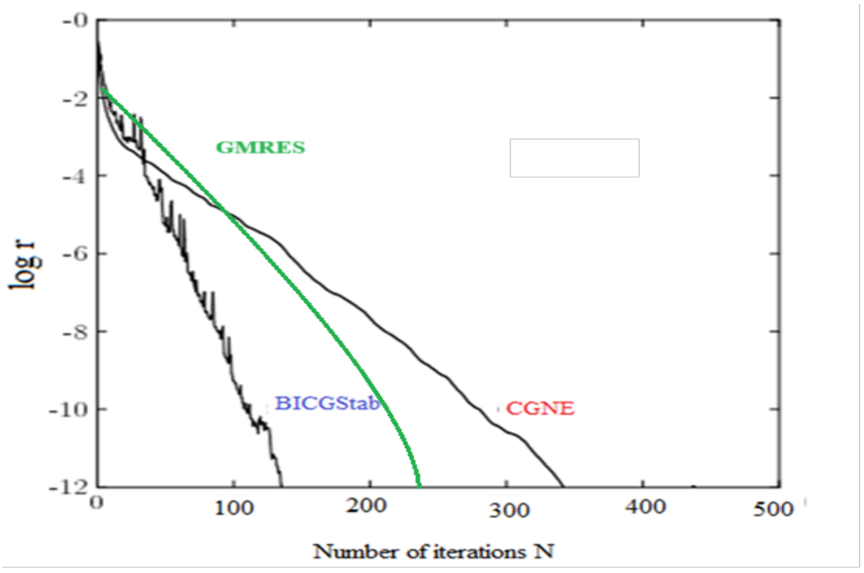

Fig. 1. The logarithm of the residual norm as a function of the number of iterations for the three cases.

As can be seen from the graphic in figure 1, where is presented the logarithm of the residual norm as a function of the number of iterations:

- **BiCGStab** reaches the required tolerance in the fewest iterations, showing a steep decrease in residuals.
- **GMRES** also converges steadily, but requires more iterations compared to BiCGStab.
- **CGNE** converges much more slowly, exhibiting a gradual decrease in residuals over a longer iteration span.

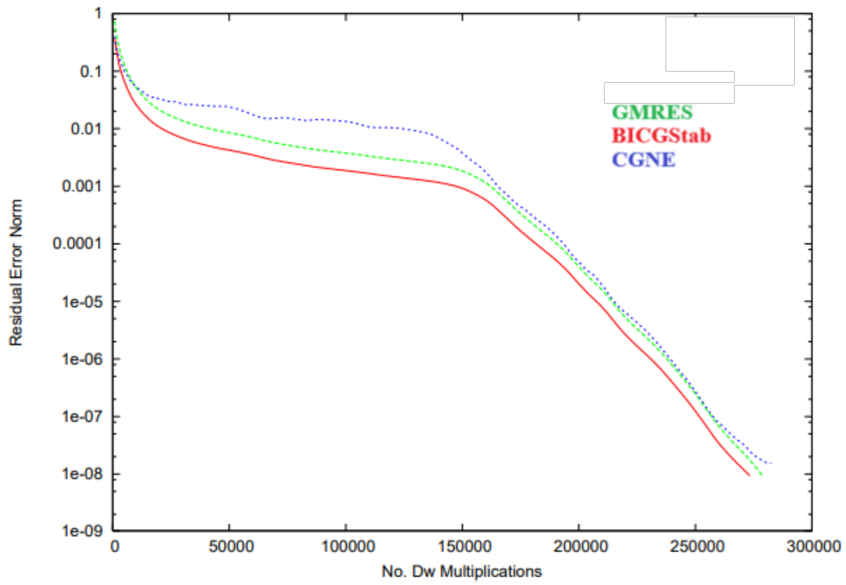

Fig. 2. The residual error norm as a function of the number of Dirac matrix multiplications

From the above figure, which shows the residual error norm as a function of the number of Dirac matrix multiplications or a more direct measure of computational cost is shown that:

- **BiCGStab** consistently requires fewer matrix multiplications to reach convergence,
- **GMRES** performs slightly better than CGNE but still demands more resources than BiCGStab,
- **CGNE** remains the least efficient in this setting.

This confirms that BiCGStab is not only faster in terms of iterations but also computationally less expensive.

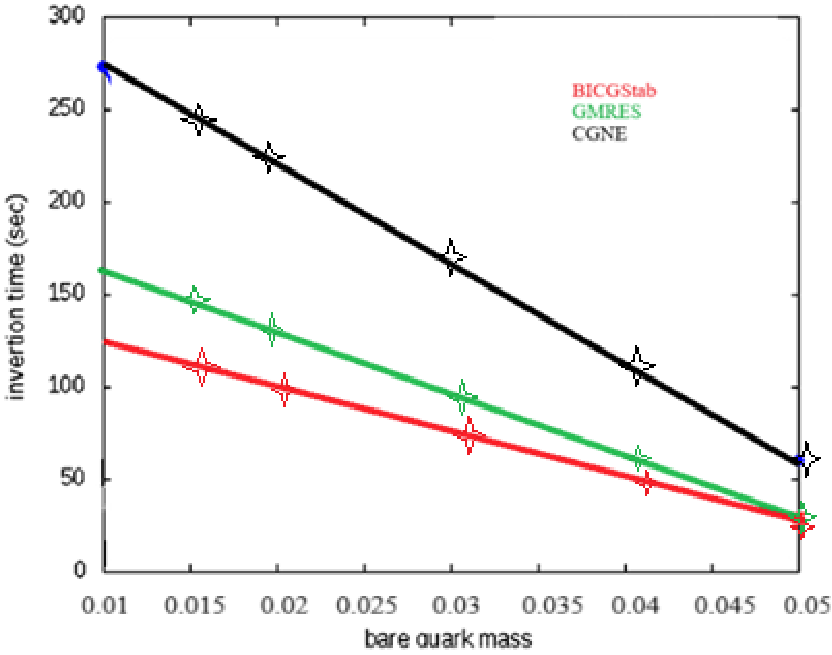

Fig. 3. The inversion time as a function of the bare quark mass

The last figure, figure 3, summarizes the inversion time as a function of the bare quark mass. As expected:

- The inversion time decreases with increasing quark mass for all algorithms
- BiCGStab consistently yields the lowest inversion times, followed by GMRES and then CGNE.
- The performance gap becomes more pronounced in the chiral limit (lower masses), where numerical difficulties are largest.

In the case of BC fermions, it can be seen that BICGStab seems to be the most appropriate solver.

4 Conclusions and future work

Boriçi – Creutz fermions present an alternative for simulations in Lattice QCD, due to the properties they have as lattice fermions. An important part of LQCD calculations has to do with the inversion of the Dirac operator and in this work several inversion algorithms were numerically analysed in the case of BC fermions. The shown results confirm that BiCGStab offers the best balance between speed, convergence stability, and memory footprint for the inversion of the BC Dirac operator. BiCGStab is the most efficient among the tested algorithms, achieving convergence with the least number of iterations and lowest computational cost. It converges faster than CGNE and GMRES. The performance difference between the algorithms becomes more significant as the system approaches the chiral limit.

All the taken results, makes BiCGStab the natural choice as a default solver for minimally doubled fermions, particularly the Boriçi – Creutz formulation. Anyway further details have to be considered in our future works. We will explore preconditioning techniques for improved convergence, extend tests to other classes of MDF and investigate performance in dynamical simulations.

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