A PERFORMANCE COMPARISON OF SIMULATeQCD AND FERMIQCD FRAMEWORKS FOR LATTICE QCD CALCULATIONS

RUDINA OSMANAJ[1], DAFINA XHAKO[2]

[1]Department of Physics, Faculty of Natural Sciences, University of Tirana

[2]Department of Physics Engineering, Faculty of Mathematical Engineering and Physical Engineering, Polytechnic University of Tirana

e-mail: rudina.zeqirllari@fshn.edu.al

Abstract

In this work we present a simple performance comparison of two main frameworks used by the Lattice QCD community for lattice calculations: FermiQCD and SIMULATeQCD, for the same algorithms, using Boriçi – Creutz fermions. Speaking for large scale simulations/calculations, the performance of the used package is the keyword to be focused. The idea of this work was to write and add to SIMULATeQCD the proper codes for Boriçi - Creutz action and test the performance of the inversion algorithms and the light hadrons propagators calculations with BC action, for both packages, so we can see which of them is the most appropriate package to be used for BC action for further studies. We have tested the performance of one of the most suitable inversion algorithms for BC fermions: Stabilized Biconjugate Gradient method, BiCGStab, implemented in SIMULATeQCD during this study. Also we present some simulations for the light hadrons spectrum with the BC action in quenched QCD, using SIMULATeQCD and have compared the results with our previous work, performed using FERMIQCD. The execution time and number of operations per second are evaluated in both cases. Simulations are made with gauge action on 48^4,64^4 lattices for a total number of 500 SU(3) gauge configurations and carried out on the Computational Physics Group's server in the Department of Physics, University of Tirana.

Key words**:** *Lattice QCD, SIMULATeQCD, FermiQCD, GPU, performance, Inversion algorithms.*

Përmbledhje

Në këtë punim paraqitet një krahasim i thjeshtë i performancës së dy paketave llogaritëse të përdorura në komunitetin e Kromodinamikës Kuantike Rrjetore për llogaritje e simulime: FermiQCD dhe SIMULATeQCD, për të njëjtat algoritme, duke përdorur fermionet Boriçi – Creutz. Duke qenë se flitet për simulime e llogaritje që kanë kosto të lartë llogaritëse, idea është të testojmë cila prej paketave ka performancë më të mirë për llogaritjet me anë të veprimit Boriçi - Creutz, në mënyrë që ajo të bëhet mjet për punimet e ardhshme me fermionet minimalisht të dubluara Boriçi - Creutz. Në paketën SIMULATeQCD janë implementuar dhe përshtatur të gjitha kodet e nevojshme për fermionet BC, si dhe është krahasuar performanca mes dy paketave në rastin e algoritmeve të invertimit dhe llogaritjeve të spektrit të hadroneve të lehtë. Janë testuar dhe krahasuar rezultatet dhe kohët e ekzekutimit për një prej algoritmeve të invertimit më të rëndësishëm për fermionet: Stabilized Biconjugate Gradient method, BiCGStab (i implemetuar prej nesh në këtë punim). Gjithashtu, janë kryer simulime të spektrit të hadroneve të lehtë në përafrimin me "fermione të ngrira" me anë të fermioneve BC, duke përdorur SIMULATeQCD dhe janë krahasuar me rezultatet e marra te realizuara duke përdorur FermiQCD në punimet tona më të hershme. Janë vlerësuar kohët e ekzekutimit dhe numri i veprimeve për sekondë në të dyja rastet. Simulimet janë kryer në rrjeta 48^4,64^4 dhe një total prej 500 konfiguracionesh SU(3), të realizuara në serverin e grupit të Fizikës Llogaritëse në Departamentin e Fizikës, Universiteti i Tiranës.

Fjalë kyçe: *Kromodinamikë Kuantike Rrjetore, SIMULATeQCD, FermiQCD, GPU, performancë, algoritme invertimi.*

Introduction

Quantum Chromodynamics (QCD) is the theory that describes the strong interaction, in terms of quarks and gluons and explains how quarks are binding together in hadrons. Let's remember that in the low energy regime, analytic or perturbative solutions are hard or almost impossible to obtain due to the nonlinear nature of the strong force and the large coupling constant. That's why a non - perturbative approach was proposed by Wilson in 1974: Lattice QCD. It is a lattice gauge theory formulated on a grid or lattice of points in space and time, where the links represent the gluon fields and the lattice sites the quarks. When the size of the lattice is taken infinitely large and its sites infinitesimally close to each other, the continuum QCD is

recovered (Wilson, 1974). The lattice formulation of QCD requires the discretization of the QCD action.

The discretization of the fermions action part, according to the Nielsen - Ninomiya theorem, leads the appearance of additional, unphysical fermion states (Nielsen and Ninomiya, 1981). In order to solve this problem, several strategies are in use, such as Wilson fermions, minimally doubled fermions, overlap fermions, domain wall fermions etc. In all our previous works we have been focused on minimally doubled fermions, especially Boriçi - Creutz fermions (Creutz, 2008; Boriçi, 2008). This kind of fermions have been proposed as a type of lattice fermions, which preserve exactly the chiral symmetry and are strictly local, but breaks the hyper - cubic symmetry in a specific direction (Bedaque, 2008). The Dirac operator for these fermions in the momentum space:

$$D(p) = \sum_{\mu}[i\gamma_{\mu} \sin p_{\mu} + i(\Gamma - \gamma_{\mu})\cos p_{\mu}] \quad (1)$$

has two poles: $p_1 = (0,0,0,0)$ and $p_2 = (\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2})$, which correspond to the two physical flavours, having a preferred direction in the Euclidian space-time, defined by the line that connect them: the major hyper - cube diagonal. Let's remember that Γ is the sum of the gamma matrices (See for details (Boriçi, 2008). In our previous works, we have shown the effects of this broken symmetry in the light hadrons spectrum (Zeqirllari et al, 2011; Zeqirllari and Boriçi, 2014), have proposed a method of how to restore it partially using the chiral condensate (Osmanaj and Xhako, 2018) and have see also what happen when the hypercubic broken symmetry is restored (Osmanaj and Xhako, 2019; Osmanaj and Xhako, 2022). In most of the works done, we have used the FermiQCD package (Di Piero, 2002), where we have contributed continuously with codes regarding BC fermions. The codes written in FermiQCD are almost ideally suited to parallel computation and we have tested even the scalability of the codes in it (Osmanaj and Xhako, 2011, 2021).

Lattice QCD being very compute intensive and expensive requires often to find algorithms, programming methods and systems in order to decrease the computational time of the calculations performed in LQCD. Following the trends of High Performance Computing, GPUs have been ubiquitous in HPC and also in Lattice QCD applications.

Recently, SIMULATeQCD, a multi-GPU Lattice QCD framework, mainly developed and used by the HotQCD collaboration (Bazavov et al, 2009), has

been used widely in the Lattice QCD community, due to its high efficiency and performance in decreasing the computation time of the applications.

Materials and methods

The two main important tools for developing, applying and testing LQCD applications with Boriçi - Creutz fermions, as we mention above are FermiQCD and SIMULATeQCD, both packages used widely in Lattice Quantum Chromodynamics (LQCD). Let's first mention some of the important features of them and then describe where will consist our work.

FermiQCD

FermiQCD is a C++ library for fast development of parallel Quantum Field Theory (QFT) applications. Some detailed features of it are listed below:

• fully C++ (uses exceptions, streams, templates, inheritance, etc…)

• top-down design

• includes linear algebra and statistical package

• multiple lattices and fields

• automatic parallelization

• parallel random number generator

• parallel field::save and field::load methods (inherited)

• gauge_field for arbitrary SU(n)

• fermi_field for arbitrary SU(n)

• staggered_field for arbitrary SU(n) and even ndim

• Wilson, Clover, Asqtad actions (in SSE2 for SU(3)) (un-isotropic)

• Domain Wall action

• Fermilab action for heavy quarks (all dim=6 operators)

• minimum residue, stabilized bi-conjugate and uml inverters

• reads UKQCD, CANOPY, MILC and serial data formats

• easy

• safe: no need to use pointers

• flexible: can define your own fields and libraries by inheritance (Di Pierro, 2002; http://www.fermiqcd.net).

SIMULATeQCD

SIMULATeQCD is a multi-GPU, multi-node lattice code written using C++17, utilizing the OOP paradigm and modern C++ features. It is available on GitHub and licensed under the MIT license. Due to its design strategy, SIMULATeQCD makes it easy for developers to create new multi-GPU applications out of already existing modules. However, many well-tested applications for LQCD calculations already exist. These applications can serve as a starting point for new code, and they have already been used in a lot of physics projects. The most important difference between SIMULATeQCD and its predecessors' frameworks with GPUs lies in the clear distinction between organizational levels of the code, where much of the technical details are hidden from the highest level. This allows physicists without advanced C++ or hardware knowledge to write highly efficient code without having to understand low-level subtleties (Mazur et al, 2024). Some other important details of SIMULATeQCD are listed below:

- high-performing;
- works efficiently on multiple GPUs and nodes;
- Is flexible to changing architecture and hardware;
- Is easy to use for lattice practitioners with intermediate C++
- knowledge.

Further technical details can be founded in:

https://github.com/LatticeQCD/SIMULATeQCD.

So, in order to make faster and more efficient the Lattice QCD applications with BC fermions, we decided to implement this new action to the SIMULATeQCD framework and test the performance of some inversion algorithms and calculation using BC. We can compare the taken results using FermiQCD with the ones from SIMULATeQCD and choose the best tool for further projects with minimally doubled fermions Boriçi - Creutz.

The first step of this work was to implement to SIMULATeQCD the Boriçi - Creutz action and one of the inversion algorithms most suitable for this type of fermions: Stabilized Biconjugate Gradient method, BiCGStab (Van der Vorst, 1992), written in a short pseudo - code as is shown in the figure below.

BiCGSTAB

Given an initial solution x(0) compute $r = b - Ax(0)$

$\rho_0 = 1$, $\rho_1 = r(0)'r(0)$, $\alpha = 1$, $\acute{\omega} = 1$, $p = 0$, $v = 0$

for $k = 1,2, \ldots$ until convergence

$\beta = (\rho_k / \rho_{k-1})(\alpha/\acute{\omega})$

$p = r + \beta(p - \acute{\omega}v)$

$v = Ap$

$\alpha = \rho_k/(r(0)'v)$

$s = r - \alpha v$

$t = As$

$\acute{\omega} = (t's)(t't)$

$x(k) = x(k-1) + \alpha p + \acute{\omega}s$

$r = s - \acute{\omega}t$

$\rho_{k+1} = -\acute{\omega}r(0)'t$

end

Figure 1. The pseudo - code for the Stabilized Biconjugate Gradient method for solving the linear matrix equation $Ax = b$

Let's remember why the inversion algorithms are important in Lattice QCD. Since we have to simulate the lattice QCD theory with chiral fermions we will use the chiral Dirac operator: Boriçi - Creutz. The calculation of the quark propagator means that we have to solve large linear systems of the type:

$$Ax = b \;\leftrightarrow Dx = b \tag{2}$$

where the operator *D* is a large matrix operator representing the corrected BC - Dirac operator on a four-dimensional space-time lattice:

$$D_{BC}(p) = \sum_{\mu}[i\gamma_{\mu}\sin p_{\mu} + i\left(\Gamma - \gamma_{\mu}\right)\cos p_{\mu}] + i(c_3 - 2)\Gamma \tag{3}$$

x is the quark propagator and *b* the source of quark. This problem requires very intensive computations and high computing power, that's why choosing the proper algorithm, programming using CPUs or GPUs is very important in order to decrease this costs and is the motivation of our work.

After we have implemented Boriçi - Creutz fermions in the framework of multi - GPUs SIMULATeQCD, we have followed the below described

procedure.
The calculations are performed on the Computational Physics Group's server in the Department of Physics, University of Tirana, using FermiQCD and SIMULATeQCD, with Boriçi - Creutz operator. Quenched gauge configurations are generated with the Wilson gauge action at $\beta = 5.8$, 6 on lattices of size 48^4 and 64^4. For 500 configurations at each of the two lattice sizes, BC quark propagators are calculated for a single point source and all color - spin combinations.
Propagators are calculated for five values of the hopping parameter κ: 0.138, 0.140, 0.142, 0.144, 0.147, corresponding to five lattice mass quarks. To compute the quark propagators we have used static point sources located at $t_0 = (0, 0, 0, 1)$ on 500 configurations. As a solver, we have used the Stabilized Biconjugate Gradient method, BiCGStab (Osmanaj et al, 2014; Osmanaj and Xhako, 2021, 2022).

The existing codes of SIMULATeQCD are improved and new codes need for these calculations are written.
The back end of SIMULATeQCD operates close to the hardware level to achieve high performance, for example through dedicated classes for memory management and communication between host and devices, as lattice applications are usually bound by bandwidth. The four-dimensional lattice also needs to be translated to one-dimensional memory, which is handled by an indexing class.

Furthermore, there is a class that maps sets of lattice sites to GPU threads, such that operations on multiple sites are run in parallel. The big advantage of this class is that the operations on each site can be written as high-level functors that do not require any knowledge about the specifics of GPU programming. The back end of the code is finally completed with classes that manage file input/output and logging (Mazur et al, 2024).

Results and discussion

After implementing the BICGStab algorithm for inverting the BC - Dirac operator and the action itself, in SIMULATeQCD, we have measured the execution time of solving the linear equation $Dx=b$, with the both frameworks, in the same server. The results are presented in the graphic of the figure 1, where we can see clearly that the same algorithm converge

faster and the time needed for the execution is smaller, when SIMULATeQCD, the multi- GPUs framework is used.

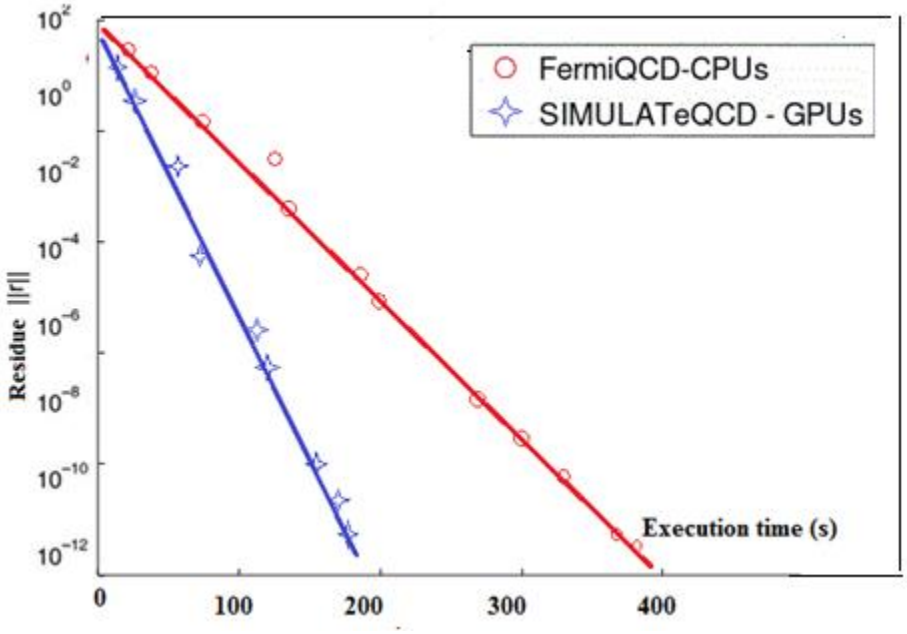

Figure 2. Time needed for solving the BC - Dirac equation $Dx=b$ (Inverting the matrix), using BICGStab algorithm, implemented in FermiQCD (CPUs) and SIMULATeQCD (GPUs)

As we explained above, we have performed some other calculations regarding the light hadrons spectrum, already tested in previous works with FermiQCD (Osmanaj and Xhako, 2022), compared these results with the both packages and also evaluate the performance of them, using the number of operations per second needed.

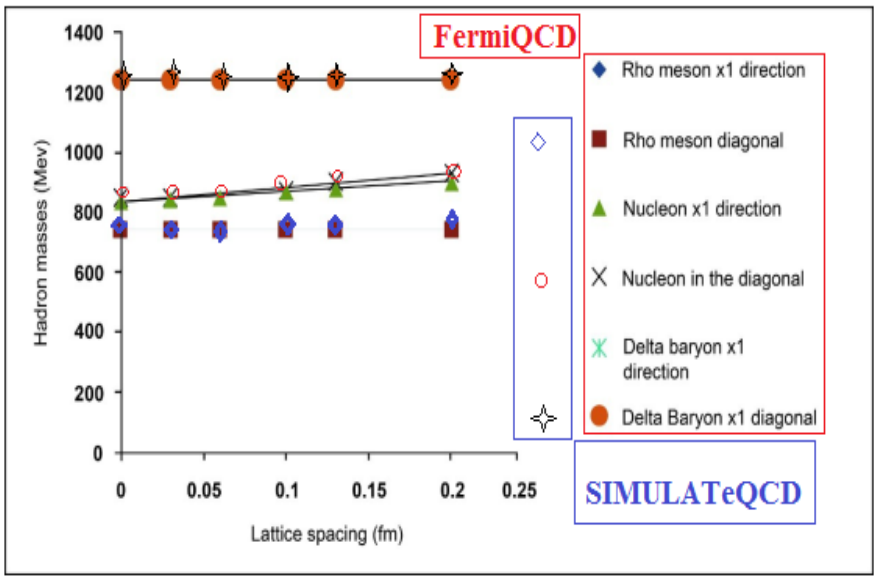

Figure 3. Light hadrons spectrum using FermiQCD (in red) and SIMULATeQCD (in blue). The calculations of the masses using SIMULATeQCD performed only in the hypercubic diagonal, where there is no need for the corrected BC actions

As we can see the calculated masses (see details in (Osmanaj and Xhako, 2022)) in the diagonal direction give almost (errors included) the some values with the both packages, a result that make us confident that SIMULATeQCD can be a potential tool to be used even for BC fermions.

For these calculations and the inversion process we have measured the TFLOPs and compare the results so we can see which of the frameworks have a better performance, for the same algorithms, in the same server. The collected data are presented in Table 1, and then in the graphic in figure 4.

Table 1. Data for Figure 3, Scaling the BC - Dirac fermions with a single right hand side (rhs) b, on a 48^4 lattice

CPUs	TFLOP/s	GPUs	TFLOP/s
1	1	1	1.5
4	3.1	4	5.2
8	5.2	8	7.1
16	8.1	16	10.2
32	13.4	32	18.35

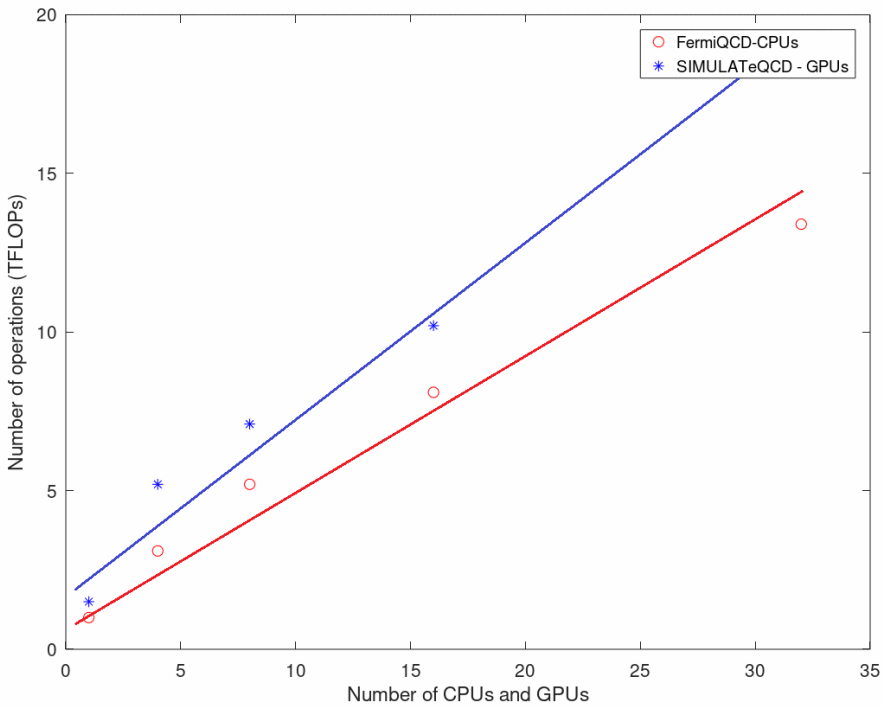

Figure 4. The evaluated performance of FermiQCD (CPUs) and SIMULATeQCD (GPUs) using the number of iterations per second.

Scaling the BC - Dirac fermions with a single right hand side (rhs) b, on a 48^4 lattice.

As can be seen from the graphic, the performance is much better with SIMULATeQCD rather than FermiQCD, a fact that make us consider this multi - GPUs framework, as a tool for further projects with Boriçi - Creutz fermions.

Conclusions

In this work we tested the performance for Lattice QCD calculations with minimally doubled fermions Boriçi - Creutz, for the same used algorithms implemented in two important frameworks used in the LQCD community: FermiQCD and SIMULATeQCD, in order to choose the proper tool for further research projects in this area. We clearly saw from the results that SIMULATeQCD has a better performance in time in the calculations we have done. Furthermore, SIMULATeQCD being highly modularized, gives the possibility that anyone with modest knowledge of C++ can get started writing production code right away. One of the most important characteristics of SIMULATeQCD is that it is relatively straightforward to implement new algorithms, as we did with the BICGStab algorithms. Testing the results and performance, and considering the advantages we mention above, we would recommend this tool for further research with BC fermions.

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