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QC DLAB2, a Learning Tool for Students in Lattice QCD

ABSTRACT

Introducing Lattice QCD and its techniques to students is often quite challenging. In this paper we use a special package named QC DLAB2 as an educational tool for lattice QCD algorithms and hadrons spectroscopy. This package is a collection of MATLAB functions, characterized by short codes and fast run times. Being clear codes, written in MATLAB, you can make substantial changes in a few seconds. For these reasons, we have used this package to introduce LQCD to students and learn basic calculations. We have calculated the quark propagators and light hadrons spectrum, for different fermions actions and different gauge coupling constants, in order to understand simulation and inversion algorithms. The students can make their own changes and try different situations, in order to better understand what happens. We have seen how the understanding performance of the students increases when QC DLAB2 is added to the standard lessons. Using QC DLAB2, as a learning tool, Lattice QCD seems to be less difficult and challenging to understand.

Keywords: Lattice QCD, QC DLAB2, education, algorithms, coupling constant

Introduction

Lattice Quantum Chromodynamics (LQCD) is one of the most challenging subjects for undergraduate/graduate students and research fields for young scientists. It is a well - established non - perturbative approach for solving the quantum chromodynamics (QCD) theory of quarks and gluons, where the continuous space - time is replaced by a Euclidean lattice (Gattringer & Lang, 2010). Nowadays, Lattice QCD has become a standard tool in elementary particle physics and introducing it to master's students, as soon as possible, is a demand for the research in this or similar fields. The idea of this work was to test how effective could be the method "Learning by doing", in learning basic concepts, algorithms and simulations regarding Lattice QCD. After discussions with Prof. Artan Boriçi, creator and developer of the tool, it was proposed to use QCDCDLAB2, a package of MATLAB/GNU OCTAVE functions, based on short codes and run times (Boriçi, 2006, 2019). QCDCDLAB2 can be used as a tool for learn and practice lattice projects, and as a small laboratory to test and validate new research ideas in Lattice QCD. The focus of this work, was the use of it as a learning tool and the impact it could have to students fronting for the first time LQCD.

In the Department of Physics, Faculty of Natural Sciences, University of Tirana, lessons of Lattice QCD are presented partly in Elementary Particle Physics (Lecturer Prof. A. Boriçi) and Computational Physics (Lecturer R.Osmanaj), both semestral subjects. We made a test, in the last three years and measured the performance of the students in understanding LQCD and its techniques. The first year, we used the standard lessons, while the last two years, we used even more QCDCDLAB2 as a tool for lattice projects. We evaluate how much students understood the subject, not only by grades and project points, but even by the survey we made each year.

Literature Review

Lattice QCD

Quantum Chromodynamics is the theory of strong interactions, formulated in terms of quarks and gluons. It has some crucial properties such as: asymptotic freedom - discovered in 1973 by David Gross, Frank Wilczek (Gross & Wilczek, 1973) and David Politzer (Politzer 1973), who awarded the Nobel Prize in Physics 2004; color confinement and chiral symmetry breaking. Due to the nonlinear nature of the strong force and the large coupling constant at low energies, analytic solutions in low-energy QCD are hard or impossible to obtain. For this reason, lattice QCD was proposed by Wilson, in 1974, as a non - perturbative approach for solving quantum chromodynamics (QCD) (Wilson, 1974). It is a lattice gauge theory formulated on a lattice of points in space - time, representing quarks, and the links - representing gluons. The formulation of QCD in a discrete space - time introduces a momentum cut-off at the order $1/a$, where a is the lattice spacing, which regularizes the theory. This approximation approaches continuum QCD as

the spacing between lattice sites is reduced to zero. Because the computational cost of numerical simulations can increase dramatically as the lattice spacing decreases, results are often extrapolated to $a = 0$ by repeated calculations at different lattice spacings a . Wilson showed, that in the strong coupling regime, QCD is confining, meaning that the potential between two static charges grows linearly with the distance between charges (Wilson, 1974; Creutz 1979). Lattice simulations have confirmed chiral symmetry breaking too, and Yoichiro Nambu was awarded the 2008 Nobel Prize in Physics for explaining the phenomenon.

More often, the basic computational task in Lattice QCD, is the generation of ensembles of gauge fields configurations, according the probability density:

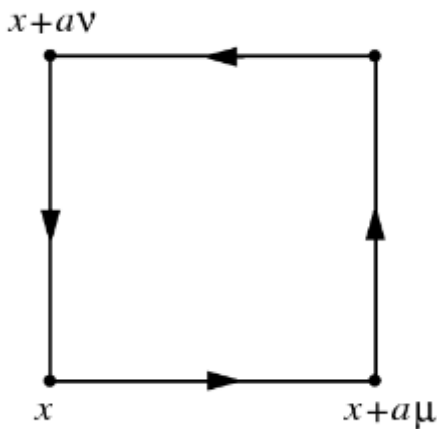
$$\rho_{QCD}(U) \sim \det(D^*D) e^{-S_g(U)}$$

where D is the lattice Dirac operator,

$$S_g = \beta \text{Re} \sum_{i, \mu < \nu} (1 - P_{\mu\nu, i})$$

is the gauge actions, $\beta = 6/g^2$ is the gauge - boson coupling constant, and $P_{\mu\nu}$ is the plaquette, a 4 - link product defined as in the figure:

Figure 1. *Lattice - Plaquette Representation*



These simulations typically utilize algorithms based upon molecular dynamics or micro canonical ensemble algorithms (Callaway & Rahman, 1982).

Numerical lattice QCD calculations using Monte Carlo methods combined with molecular dynamics or micro canonical ensemble can be computationally expensive, requiring the use of the largest available supercomputers. To reduce the computational cost, often is used the so-called quenched approximation, in which the quark fields are treated as non-dynamic "frozen" variables (Gattringer, Lang, 2010).

Lattice QCD has already successfully agreed with many experiments: the mass of the proton has been determined theoretically with an error of less than 2 percent, the transition from confined quarks to quark–gluon plasma.

QCDLAB2

QCDLAB is an educational and research tool for lattice QCD algorithms. It is a collection of MATLAB functions, based on a short code and run-time philosophy, written and developed by Artan Boriçi (Boriçi, 2006, 2007, 2019). The present version QCDLAB2, uses updated algorithms and simulations, developed and tested by Boriçi, Osmanaj & Xhako. QCDLAB2 is designed to be a high level language interface for lattice QCD techniques and simulations. It is based on the MATLAB/OCTAVE language, which offers some main features as:

- Vast build-in mathematical and linear algebra functions.
- Many functions form Blas, Lapack, Minpack, etc. libraries.
- Interpreted language.
- Dynamically loaded modules from other languages like C/C++, FORTRAN.
- Ability to compile OCTAVE codes using the Octave Compiler.

So, QCDLAB2 offers a two level language system: a higher level language, which is easier for numerical work and a lower level translation to C++ ((Boriçi, 2006) features that make the tool suitable for students who want to make explicit and visible changes, depending on the situations they want to simulate and study. It also maps linear operators of QCD to linear operators of the GNU Octave language (www.gnu.org). Although GNU Octave is an interpreted language, linear operators are precompiled. This property makes efficient coding and fast runtimes. However, GNU Octave is a one-threaded software and runs in one computing core only, that makes QCDLAB usage limited to moderate lattices. It is possible however to include multi-threaded C++ libraries such that the programs run in multiple cores. By the way, even in the actual form it is suitable for educational use.

In summary, QCDLAB serves three purposes: teaching, learning as well as algorithm prototyping. The latter helps developing a complex software by testing the basic idea of a new algorithm on GNU Octave using QCDLAB codes (Boriçi, 2019). The main codes of QCDLAB2 are divided in two groups: simulation and inversion algorithms. Further details can be found in <https://sites.google.com/site/artanborici/qcdlab>.

Methodology

The idea of this work was to test how effective could be the method "Learning by doing", in learning basic concepts, algorithms and simulations regarding Lattice QCD. After discussions with Prof. Boriçi, creator and developer of the tool, it was

proposed to use QCDCALAB2, a package of MATLAB/GNU OCTAVE functions, based on short codes and run times. (refernca) The focus of this work, was the use of it as a learning tool and the impact it could have to students fronting for the first time LQCD. We made a test, with the master's students, for three years/three semesters. The first year (2019) we used the standard methodology and lessons, and analyzed the student feedback and understanding performance of the main concepts, algorithms and simulations in Lattice QCD, part of two subjects: Elementary particle physics and Computational Physics. The last two years (2020, 2021), we added to the standard lessons, QCDCALAB2 as an educational tool for better understanding algorithms and lattice QCD concepts by doing themselves. After every lesson, the students had to be familiar with the package and realize several simulations/calculations in different conditions and see what happened, as homeworks or small lattice projects. In the end of each semester, we evaluate the performance during the final exam, regarding the Lattice QCD part, and the results of the survey done with the students of the specific year (each year the total number of master's students is around 40, and the mean grade of the students is 8). The main algorithms explained and learned using even QCDCALAB2 where divided in two parts:

- Simulation algorithms: Hybrid Monte Carlo Algorithm (Leap frog algorithm, Metropolis et al algorithm) (Duane, 1987).
- Inversion Algorithms: Krylov subspace methods (Conjugate Gradients, Conjugate Gradients on Normal Equations, Arnoldi Algorithm (Arnoldi, 1951), GMRES: Generalised Minimal Residual Method (Saad & Schultz 1986) Biconjugate Gradients (BiCG) algorithm, Biconjugate Grandients Stabilised algorithm (BiCGStab) (Van der Vorst, 1992; Gutknecht, 1993).

At the end of the semester, each year, we evaluate the results of the final test and perform a survey for understanding the impact that QCDCALAB2 had on students. The test and the survey questions where based in how much the students understood the algorithms used in Lattice QCD and if QCDCALAB2 was helpful or no.

Results

The results of the final test of our 40 master's students, regarding Lattice QCD (as part of the two subjects mentions above) and the results of the survey done, for every year are represented in Tables 1-8.

Table 1. Results of the Final Exams Dedicated to Lattice QCD (Points), Year 2019. Standard Methodology Lessons

Number of students	Points/Simulations algorithms	Points/Inversion algorithms
5	45-50/50	45-50/50
10	30-40/50	30-40/50
15	20-30/50	20-30/50
10	Below 20	Below 20

Table 2. Results of the Final Exams Dedicated to Lattice QCD (Points), Year 2020. QCMLAB2 Was Used as Educational Tool, for Homeworks and Lattice Projects

Number of students	Points/Simulations algorithms	Points/Inversion algorithms
13	45-50/50	45-50/50
20	30-40/50	30-40/50
5	20-30/50	20-30/50
2	Below 20	Below 20

Table 3. Results of the Final Exams Dedicated to Lattice QCD (Points), Year 2021. QCMLAB2 Was Used as Educational Tool, for Homeworks and Lattice Projects. All Lessons Were Online, due the COVID-19 Pandemic

Number of students	Points/Simulations algorithms	Points/Inversion algorithms
12	45-50/50	45-50/50
22	30-40/50	30-40/50
4	20-30/50	20-30/50
2	Below 20	Below 20

Table 4. Results of the Semestral Survey Regarding the Clarity and Comprehension of the Main Topics of Lattice QCD, (Percentage of Students), Year 2019. Standard Methodology Lessons

Clarity of the topic	Simulations algorithms	Inversion algorithms
Very clear	5%	8%
Clear	40%	43%
Enough clear	30%	25%
Not Enough clear	25%	24%

Table 5. Results of the Semestral Survey Regarding the Clarity and Comprehension of the Main Topics of Lattice QCD, (Percentage of Students) Year 2020. QCMLAB2 was Used as Educational Tool, for Homeworks and Lattice Projects

Clarity of the topic	Simulations algorithms	Inversion algorithms
Very clear	20%	20%
Clear	60%	58%
Enough clear	18%	19%
Not Enough clear	2%	3%

Table 6. *Results of the Semestral Survey Regarding the Clarity and Comprehension of the Main Topics of Lattice QCD, (Percentage of Students) Year 2021. QC DLAB2 Was Used as Educational Tool, for Homeworks and Lattice Projects. All Lessons Were Online, due the COVID-19 Pandemic*

Clarity of the topic	Simulations algorithms	Inversion algorithms
Very clear	25%	27%
Clear	57%	58%
Enough clear	16%	12%
Not Enough clear	2%	3%

Table 7. *Results of the Survey (Percentage of Students), Year 2020*

Was QC DLAB helpful?	Simulations algorithms	Inversion algorithms
Yes	90%	93%
No	10%	7%

Table 8. *Results of the Survey (Percentage of Students), Year 2021*

Was QC DLAB helpful?	Simulations algorithms	Inversion algorithms
Yes	95%	90%
No	5%	10%

As it can be seen by the results in the table, we can note then the use of QC DLAB2 as a tool for understanding and learning Lattice QCD, has increased the performance of students in this field. The feedbacks of the students taken by the survey confirm what we expected. Even this year, when all the lessons were online, due the pandemic, the results taken are almost the same. QC DLAB2 has helped the students understand and "learn by doing".

Conclusions

Lattice QCD is a challenging field, sometimes difficult to be understood by students. The aim of this work was to find an interesting method to make it easier and attractive, and to learn the basic concepts and techniques that LQCD makes use. We were focused in the performance results of our master's students and the difference when standard methodology lesson is used, and when QC DLAB2 is introduced as an additive educational tool. "Learning by doing" method seems to be very effective and the student's performance has been increased significantly. We would recommend the use of QC DLAB2, as an educational tool, which can help students to better understand the techniques, algorithms and phenomenology of Lattice QCD.

Acknowledgments

This work makes use of the endless contribution of Artan Boriçi in Lattice QCD, the algorithms and the package he created and developed. Artan, passed

away on March 2021, after a long battle with COVID-19, and the authors of the paper dedicate this educational work to him.

References

- Arnoldi W. E, (1951) *Quart. Appl. Math.* 9 17.
- Boriçi, A. (2006). QCDLAB: designing lattice QCD algorithms with Matlab. *arXiv preprint hep-lat/0610054*.
- Boriçi, A. (2007). Speeding up domain wall fermion algorithms using QCDLAB. *arXiv preprint hep-lat/0703021*.
- Boriçi, A (2018) Lattice QCD with QCDLAB., *arXiv preprint arXiv:1802.09408*.
- Callaway D, Rahman A (1982). "Microcanonical Ensemble Formulation of Lattice Gauge Theory". *Physical Review Letters*. 49 (9): 613–616.
- Creutz M, (1979) Confinement and the Critical Dimensionality of Space-Time, *Phys. Rev. Lett.* 43, 553.
- Duane S et. al., (1987) Hybrid Monte Carlo, *Phys. Lett.* B195 216.
- Gattringer C, Lang C. B, (2010) Quantum Chromodynamics on the Lattice, *Springer*.
- Gross D.J, Wilczek F, (1973) Ultraviolet Behavior of Nonabelian Gauge Theories, *Phys. Rev.Lett.* 30 1343.
- Gutknecht M. H, (1993) Variants of BICGSTAB for Matrices with Complex Spectrum, *SIAM J. Sci.Comput.*14(5)1020.
- Kogut J.B, Susskind L, (1975) Hamiltonian Formulation of Wilson's Lattice Gauge Theories, *Phys.Rev. D11*, 395.
- Politzer H.D, (1973) Reliable Perturbative Results for Strong Interactions?, *Phys. Rev. Lett.* 30, 1346.
- Saad Y, Schultz M, (1986) *SIAM J. Sci. Stat. Comput.* 7 856.
- Sokal A. D, (1992) Bosonic Algorithms, in Quantum Fields on the Computer, *World Scientific* 211.
- Van der Vorst H.A, (1992), Bi-CGSTAB: A Fast and Smoothly Converging Variant of Bi-CG for the Solution of Nonsymmetric Linear Systems, *SIAM J. Sci. and Stat. Comput.* 13(2), 631.
- Wilson K. G, (1974) Confinement of Quarks, *Phys. Rev. D10* 2445.
- <https://www.gnu.org/software/octave>.
- <https://sites.google.com/site/artanborici/qcdlab>.