MULTI-NODE PARALLELIZATION PERFORMANCE OF FIRST-PRINCIPLES CALCULATIONS

MOHAMMED BUBA

A dissertation submitted in partial fulfilment of the
requirements for the award of the degree of
Master of Science

Faculty of Science
Universiti Teknologi Malaysia

DECEMBER 2019

DEDICATION

This dissertation is dedicated to my father, who taught me that the best kind of knowledge to have is that which is learned for its own sake. It is also dedicated to my mother, who taught me that even the largest task can be accomplished if it is done one step at a time.

ACKNOWLEDGEMENT

This thesis effort would not have been possible without the tremendous support of my parents, brothers and sisters. I like to start by thanking my father for his courage and advice and my mother for her kind gesture, blessing and prayers toward the progress for my entire life and to my family members especially my wife Khadija for her encouragement, understanding and perseverance during my stay abroad.

I like to thank my dissertation supervisor, Dr. Razif Bin Razali, for his help and motivation throughout the time of this research and also for putting me through a right path to grasp the concept of parallel and distributed computing. I offer my regards to Prof. Dr. Amiruddin Bin Shaari for his valuable advice and guidance.

My fellow postgraduate student should also be recognised for their support and teamwork. My sincere appreciation also extends to all my research group members, especially Idris Chiromawa and Timothy Ahams for their proper suggestion and assistance at various occasions.

Finally, I thank TETFUND through the Federal Polytechnic Mubi, for proving complete funding for the entire studies and University Technology Malaysia for proving a conducive study environment which made it possible to accomplish my studies within the slotted period.

ABSTRACT

Quantum ESPRESSO (QE) is a computer simulation package based on Density Functional Theory (DFT) for calculating electronic and structural properties of a material at ground state, which gives an excellent balance of accuracy and computational cost. For a macromolecular system with a large number of atoms, it takes several hours to execute even a simple calculation. The integration of parallel library has made the package compatible to distributes work on many processors through the use of MPI. The computational cost is still challenging as single computer have a limited number of processors. A parallel computing environment of multi-nodes computing system called MPI Cluster is set up on a Linux Operating System to minimize the cost by providing more processors for parallelism. This dissertation investigation evaluates the performance of QE on the multi-node cluster system called MPI-Cluster. We distribute various k-points sampling workload over different MPI processors, to measure the speedup and scalability our multi-note cluster system. The result suggests that the improvement to scaling of speedup over many processors is limited only if the number of k-point to parallelize is greater than the number of processors. We also found the limit of speedup for parallelization of bands calculation is partially independent of the number of bands used and is linearly decreases as the number of MPI processors increased.

ABSTRAK

Quantum ESPRESSO (QE) adalah pakej simulasi komputer berdasarkan teori fungsian ketumpatan (DFT) untuk mengira sifat-sifat elektronik dan struktur sesuatu bahan pada keadaan dasar, yang memberikan keseimbangan ketepatan dan kos komputasi yang sangat baik. Untuk sistem makromolekul dengan sejumlah besar atom, diperlukan beberapa jam untuk melaksanakan pengiraan yang mudah. Penyepaduan perpustakaan selari telah menjadikan pakej itu serasi untuk mengedarkan kerja pada banyak pemproses melalui penggunaan MPI. Kos pengiraan masih mencabar kerana komputer tunggal mempunyai bilangan pemproses terhad. Persekitaran pengkomputeran selari sistem pengkomputeran pelbagai nod yang dipanggil MPI-Cluster ditubuhkan pada Sistem Operasi Linux untuk meminimumkan kos dengan menyediakan lebih banyak pemproses bagi parallelism. Siasatan disertasi ini menilai prestasi QE pada sistem kluster multi-node yang dipanggil MPI-Cluster. Kami juga telah mengagihkan pelbagai beban kerja pensampelan k-mata ke atas teras yang berbeza, untuk mengukur kelajuan dan skalabiliti sistem cluster multi-note kami. Hasilnya menunjukkan bahawa penambahbaikan untuk mempercepatkan kelajuan lebih banyak pemproses hanya terhad jika bilangan k-point untuk dipasangkan adalah lebih besar dari jumlah pemproses. Kami juga mendapati had laju kepantasan untuk pengkompilasi pengiraan band sebahagiannya tidak bergantung kepada bilangan band yang digunakan dan ia berkurangan kerana bilangan teras meningkat.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

Bi_2Te_3	-	Bismuth Telluride
BZ	-	Brillouin Zone
SCF	-	Self-Consistent Field
SOC	-	Spin-Orbit Coupling
DFT	-	Density Functional Theory
DOS	-	Density of State
GGA	-	Generalized Gradient Approximation
HF	-	Hartree Fock
KS	-	Kohn-Sham
LDA	-	Local Density Approximation
MPI	-	Message Passing Interface
PBE	-	Perdew-Berke-Erzndof
PAW	-	Plain-Augmented-wave
PDOS	-	Partial Density of State
QE	-	Quantum ESPRESSO
SE	-	Schrodinger Equation
TI	-	Topological Insulators
XC	-	Exchange and Correlation

LIST OF SYMBOLS

h	-	Plank's Constant
ψ	-	Wave function
ϕ	-	Single particle wave function
eV	-	Electron volt
Ry	-	Rydberg Constant
Γ	-	Gamma
E_g	-	Energy Band Gap

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Research Background

Nowadays computers have become an integral part of computational science to solve numerical problems. For problems which may not be easily solved analytically, computers and numerical method are of crucial importance. The field of computational chemistry deals mainly with calculation such as determination of energies, charge distribution, electronics and magnetic properties of compound or material. Its aim is to explain the molecular and electronics process observed in an experiment in order to predict them.

The emergence of Density functional theory (DFT) [1] in 1968 has been a great achievement that contributed significantly in theoretical studies of electronic and structural properties of a material. It is an approach to describe the quantum behaviour of the atom in setting up a practical value. It is a well-established quantum mechanical method for electronic calculations for molecules. Principally, in electronic structure calculations, a molecular system is described by a set of functions that depend on the set of coordinates of all the particles in the system. This set of function is known as a wave function in quantum mechanics. The energy of the system is calculated from the wave function through quantum mechanical operations and from the solution of these wave functions. The complex nature of the wave function makes the evaluation of the full system very complex and highly computationally expensive even for the simplest molecules. The Hohenberg-Kohn [2] formalism of DFT approximates this ab-initio approach and proposes electronics density instead of electronics coordinates wave function. Electronic structure calculations were one of the main areas of application in high-performance computing (HPC) for the last decades. Over the past years, this method has rapidly grown as the cutting edge of the quantum mechanical theory that has been used by a large number of researchers in material science and other

disciplines. While the methods used for these calculations have changed, the approach adopted by Car-Parrinello in 1985 [3] was one of the most common to be used. The Car-Parrinello method is a type of molecular dynamics, usually employing periodic boundary conditions, plane-wave basis sets, and density functional theory.

First-principles calculation within a framework of DFT is a renounced method for investigating material properties at the ground state. DFT in principle provides a true description of electronic behaviour and structural parameters at the atomic level of bulk material at ground states within some allowed approximation. The accuracy of calculation using the DFT approach is spanned within an error limit of 10^{-3} eV [4].

As a result of the extensive applications of DFT in studying electronic properties of a material, hundreds of computational software packages for material modelling and simulation arose among them is Quantum ESPRESSO (QE) [5]. It is a free, open-source software suite available under the GNU (General Public License). It is an embedded suite of computer code written primarily in Fortran for the calculation of electronics-structure and material modelling.

The suite is designed to operate on different kind of computer architectures and is equipped with various layers of mathematical libraries [6]. The code is able to run in series and in parallel, targeting multi-core operation systems through the multi-threaded parallel libraries such as BLAS or LAPACK [7] distributed using the Message Passing Interface (MPI) [8]

1.2 Message Passing Interface (MPI)

There is a computational demand from many sectors of research for greater computational speed from a computer system than is currently possible [9]. There are some specific applications like high energy simulation, engineering calculations, material science and simulations, which must be performed quickly. High-speed systems are greatly needed in these areas. One way to increase computational speed is to use multiple processors to solve a problem. The problem is split into parts, each of

which is performed by a separate processor in parallel. When the multiple processors work in parallel they need an interface by which they can communicate. The MPI is a library used by multiple processors to send messages back and forth using send and receive commands. This approach provides a significant increase in performance.

MPI's goals are performance, scalability and portability. These features make MPI the most dominant model used in high-performance computing today. It has become the de facto standard for communication between different processors both for shared memory and distributed memory.

1.3 Problem Statement

One of the major challenges of theoretical studies for materials using material simulation software packages is computational time consumption. The complex nature of simulating some material has led to computational time to remain very high which pose a great challenge in computational condensed matter. Therefore, there is a growing demand for much more efficient implementations of DFT. Parallel computing involves the use of multiple processors (cores) of central processing units (CPU) of a computer to minimize these challenges. Researchers have been using parallel computing for several years when working on a computationally difficult task such as simulation in high energy physics and bulk materials. The challenges still continue as every computer have a limited number of processors that will available to contribute to parallel computing. A large complex problem requires hundreds or even thousands of processing hour to solve one problem and which is not feasible to achieve in an ordinary computer. As such, the use of an interconnected set of computers called Cluster emerges which allows simultaneous use of many computer processors to solve one computational problem. Clustered computers are specifically designed to take a large set of data and divide them into component parts and distribute them across the system entire processors thereby allowing the Cluster's individual node to process their unique task and finally collect them in their entirety.

QE suite is fitted with parallelism libraries code that enables it to split work into chunks of data or workload and distribute it across multiple processors of the system thereby minimizing the computational cost. In this work, we established a computational environment on a Linux operating system called MPI Cluster, where QE is being configured to use any number of processing resources available. The main aim of this dissertation will not improve a scientific code, but to investigate the distribution of parallelism over a locally connected cluster. We will investigate the parallel scalability of QE over MPI-Cluster for performing ground state total energy calculation; which is particularly important as often the total energy calculation needs to be performed many times during the geometry optimization of the atomic and electronic structure.

1.4 Research Objectives

(a) To evaluate the parallel computational performance of Linux multi-node cluster system for simulation of a material based base on DFT approach.

(b) To evaluate the effect of parallelism on DFT ground state energy calculations for computing Self-Consistency Field (SCF) and bands.

(c) To analyze parallel performance (speed-up) and scalability of the application of Quantum ESPRESSO simulation package on a Linux multi-node cluster system.

1.5 Scope of the Research

In this research, a high-performance computing multi-node cluster system is established on the Linux Operation system using LAN wireless communication. QE being the simulation package used for this work, is configure to share common computer processors of the cluster system. The following approach is adopted to achieve our objective.

(i) An MPI cluster of 5 computers with a total of 44 cores (mpi processors) is set up on a Linux operating system.

(ii) QE is installed to use the available computer processors of the cluster.

1.6 Thesis outline

Chapter 1, discussed the background of research, problem statement and scope of the study. Chapter 2 provide the basic theory and mathematical background of quantum mechanics that explained concepts of DFT and some overview of previous work done on topological insulators. The current parallelisation level of QE is briefly described and the basic concept of cluster computing is also introduced in Chapter 2. Chapter 3 present the basic steps for establishing MPI Cluster, computational details and method adopted. Performance of QE in MPI Cluster has been evaluated and presented in Chapter 4. The result for parallelization strategy over k-points and bands is presented in Chapter 4 and finally, the performance tests Result for scalability and speedup of QE over MPI-Cluster is also presented in Chapter 4. Chapter 5 summarizes the work and provides outlook for future work. List of references and appendices are presented at the end of this thesis.

REFERENCES

[1] D. S. Sholl, "Density functional theory," *Electrocatal. Comput. Exp. Ind. Asp.*, pp. 117–138, 2010.

[2] S. T. Epstein and C. M. Rosenthal, "The Hohenberg-Kohn theorem," *J. Chem. Phys.*, vol. 64, no. 1, pp. 247–249, Jan. 1976.

[3] M. C. Payne, J. D. Joannopoulos, D. C. Allan, M. P. Teter, and D. H. Vanderbilt, "Molecular dynamics and ab initio total energy calculations," *Physical Review Letters*, vol. 56, no. 24. p. 2656, 1986.

[4] P. Suryanarayana, K. Bhattacharya, and M. Ortiz, "Coarse-graining kohn-sham density functional theory," *J. Mech. Phys. Solids*, vol. 61, no. 1, pp. 38–60, 2013.

[5] P. Giannozzi *et al.*, "QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials," *J. Phys. Condens. Matter*, vol. 21, no. 39, pp. 9–11, 2009.

[6] J. Romero, E. Phillips, G. Ruetsch, M. Fatica, F. Spiga, and P. Giannozzi, "A performance study of quantum ESPRESSO's PWscf Code on multi-core and GPU Systems," *Lect. Notes Comput. Sci. (including Subser. Lect. Notes Artif. Intell. Lect. Notes Bioinformatics)*, vol. 10724 LNCS, pp. 67–87, 2018.

[7] E. Anderson *et al.*, *LAPACK Users' Guide*. Society for Industrial and Applied Mathematics, 1999.

[8] MPI, "MPI : A Message-Passing Interface Standard Version 2.2," *Forum Am. Bar Assoc.*, vol. 8, no. UT-CS-94-230, p. 647, 2009.

[9] B. Wilkinson and M. Allen, "PARALLEL PROGRAMMING TECHNIQUES AND APPLICATIONS USING NETWORKED WORKSTATIONS AND PARALLEL COMPUTERS 2nd Edition," 2005.

[10] J. C. Slater, "Band theory," *J. Phys. Chem. Solids*, vol. 8, pp. 21–25, Jan. 1959.

[11] Y. Ping, D. Rocca, and G. Galli, "Electronic excitations in light absorbers for photoelectrochemical energy conversion: first principles calculations based on many body perturbation theory," *Chem. Soc. Rev.*, vol. 42, no. 6, p. 2437, Feb. 2013.

[12] G. Onida, L. Reining, and A. Rubio, “Electronic excitations: density-functional versus many-body Green’s-function approaches,” *Rev. Mod. Phys.*, vol. 74, no. 2, pp. 601–659, Jun. 2002.

[13] K. S. Thygesen and A. Rubio, “Conserving G W scheme for nonequilibrium quantum transport in molecular contacts,” *Phys. Rev. B*, vol. 77, no. 11, p. 115333, Mar. 2008.

[14] R. G. Parr, “Density Functional Theory in Chemistry,” in *Density Functional Methods In Physics*, Boston, MA: Springer US, 1985, pp. 141–158.

[15] R. American Physical Society., G. Rignanese, X. Gonze, F. Giustino, and A. Pasquarello, *Physical review letters.*, vol. 100, no. 18. American Physical Society, 2008.

[16] M. Jain, J. R. Chelikowsky, and S. G. Louie, “Reliability of Hybrid Functionals in Predicting Band Gaps,” *Phys. Rev. Lett.*, vol. 107, no. 21, p. 216806, Nov. 2011.

[17] D. Hirose, Y. Noguchi, and O. Sugino, “Quantitative characterization of exciton from *GW* +Bethe-Salpeter calculation,” *J. Chem. Phys.*, vol. 146, no. 4, p. 044303, Jan. 2017.

[18] H. Koc, H. Ozisik, E. Deligöz, A. M. Mamedov, and E. Ozbay, “Mechanical, electronic, and optical properties of Bi 2 S 3 and Bi 2 Se 3 compounds: first principle investigations,” *J Mol Model*, vol. 20, no. 4, pp. 1–12, 2014.

[19] Y. Sharma, P. Srivastava, A. Pratap, and N. S. Saxena, “First-principles Study of Electronic and Optical Properties of Bi[sub 2]Se[sub 3] in its Trigonal and Orthorhombic Phases,” in *AIP Conference Proceedings*, 2010, vol. 1249, no. 1, pp. 183–187.

[20] Y. Noguchi, O. Sugino, M. Nagaoka, S. Ishii, and K. Ohno, “A *GW* +Bethe-Salpeter calculation on photoabsorption spectra of $(CdSe)_3$ and $(CdSe)_6$ clusters,” *J. Chem. Phys.*, vol. 137, no. 2, p. 024306, Jul. 2012.

[21] S. Cottenier and S. Cottenier, *Density Functional Theory and the Family of (L)APW-methods: a step-by-step introduction*, no. L. 2004.

[22] ’ % E Schrodinger and ; § F Klein, “The Wave Mechanics of an Atom with a Non-Coulomb Central Field. Part I. Theory and Methods,” 1926.

[23] W. Pauli and W., “Über den Zusammenhang des Abschlusses der Elektronengruppen im Atom mit der Komplexstruktur der Spektren,” *Zeitschrift für Phys.*, vol. 31, no. 1, pp. 765–783, Feb. 1925.

[24] J. C. Slater, “Note on Hartree’s Method,” *Phys. Rev.*, vol. 35, no. 2, pp. 210–211, Jan. 1930.

[25] P.-O. Löwdin and B. O. Roos, “Molecular Quantum Mechanics.”

[26] F. Jensen, “Introduction to Computational Chemistry.”

[27] J. P. Perdew, “Density-functional approximation for the correlation energy of the inhomogeneous electron gas,” *Phys. Rev. B*, vol. 33, no. 12, pp. 8822–8824, Jun. 1986.

[28] J. P. Perdew and Y. Wang, “Accurate and simple analytic representation of the electron-gas correlation energy,” *Phys. Rev. B*, vol. 45, no. 23, pp. 13244–13249, Jun. 1992.

[29] P. A. M. Dirac and P. A. M., “Note on Exchange Phenomena in the Thomas Atom,” *Math. Proc. Cambridge Philos. Soc.*, vol. 26, no. 3, pp. 376–385, Jul. 1930.

[30] J. P. Perdew, K. Burke, and M. Ernzerhof, “Generalized Gradient Approximation Made Simple,” *Phys. Rev. Lett.*, vol. 77, no. 18, pp. 3865–3868, Oct. 1996.

[31] J. P. Perdew, K. Burke, and M. Ernzerhof, “Generalized Gradient Approximation Made Simple,” *Phys. Rev. Lett.*, vol. 77, no. 18, pp. 3865–3868, Oct. 1996.

[32] M. M. Ugeda *et al.*, “Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor,” *Nat. Mater.*, vol. 13, no. 12, pp. 1091–1095, Dec. 2014.

[33] S. Huang and Shouting, “Electronic, Optical, and Thermal Properties of Reduced-Dimensional Semiconductors,” *ProQuest Diss. Theses; Thesis (ph.d.)--washingt. Univ. St. Louis, 2013.; Publ. Number AAT 3563486; ISBN 9781303118173; Source Diss. Abstr. Int. Vol. 74-09(E), Sect. B.; 187 p.*, 2013.

[34] J. M. Crowley, J. Tahir-Kheli, and W. A. Goddard, “Accurate Ab Initio Quantum Mechanics Simulations of Bi_2Se_3 and Bi_2Te_3 Topological Insulator Surfaces,” *J. Phys. Chem. Lett.*, vol. 6, no. 19, pp. 3792–3796, Oct. 2015.

[35] O. V. Yazyev, E. Kioupakis, J. E. Moore, and S. G. Louie, “Quasiparticle effects in the bulk and surface-state bands of Bi 2 Se 3 and Bi 2 Te 3 topological insulators,” *Phys. Rev. B*, vol. 85, no. 16, p. 161101, Apr. 2012.

[36] W. Kohn and L. J. Sham, “Self-Consistent Equations Including Exchange and

Correlation Effects," *Phys. Rev.*, vol. 140, no. 4A, pp. A1133–A1138, Nov. 1965.

[37] Y. Sharma *et al.*, "Electronic structure, optical properties and Compton profiles of Bi2S3 and Bi2Se3," *Solid State Sci.*, vol. 14, no. 2, pp. 241–249, Feb. 2012.

[38] A. Lawal and A. Shaari, "Density functional theory study of electronic properties of Bi2Se3 and Bi2Te3," *Malaysian J. Fundam. Appl. Sci.*, vol. 12, no. 3, Jan. 2017.

[39] A. Wacker, "An Introduction to the Concept of Band Structure," no. 3, pp. 1–34, 2018.

[40] H. Yserentant, "A short theory of the Rayleigh-Ritz method," *Comput. Methods Appl. Math.*, vol. 13, no. 4, pp. 495–502, Oct. 2013.

[41] M. J. Flynn, "Some computer organizations and their effectiveness," *IEEE Trans. Comput.*, vol. C–21, no. 9, pp. 948–960, 1972.

[42] M. Frigo and S. G. Johnson, "The Design and Implementation of FFTW3," *Proc. IEEE*, vol. 93, no. 2, pp. 216–231, Feb. 2005.

[43] R. J. Block, S. Sarukkai, and P. Mehra, "Automated performance prediction of message-passing parallel programs," in *Proceedings of the ACM/IEEE Supercomputing Conference*, 1995, vol. 1, pp. 709–738.

[44] X. Cai *et al.*, "Performance Modeling of PDE Solvers," 2003, pp. 361–399.

[45] G. R. Luecke, B. Raffin, and J. J. Coyle, "Comparing the communication performance and scalability of a Linux and a NT cluster of PCs, a Cray origin 2000, an IBM SP and a Cray T3E-600," in *Proceedings - 1st IEEE Computer Society International Workshop on Cluster Computing, IWCC 1999*, 1999, pp. 26–35.

[46] C. J. Woods, P. Brown, and F. R. Manby, "Multicore parallelization of Kohn-Sham theory," *J. Chem. Theory Comput.*, vol. 5, no. 7, pp. 1776–1784, 2009.

[47] E. E.S.C, "EIM E.S.C - Embedded Super Computing."

[48] "What is Linux? | Linux.com | The source for Linux information." [Online]. Available: https://www.linux.com/what-is-linux. [Accessed: 09-Jul-2019].

[49] C.-T. Yang, K.-W. Cheng, and K.-C. Li, "An Efficient Parallel Loop Self-scheduling on Grid Environments," 2004, pp. 92–100.

[50] R. Evard, N. Desai, J.-P. Navarro, and D. Nurmi, "Clusters as Large-Scale Development Facilities 1."

[51] I. M. (Isaak M. TSîdil′kovskiĭ, *Band structure of semiconductors*. .

[52] D. Campi, L. Paulatto, G. Fugallo, F. Mauri, and M. Bernasconi, "First-principles calculation of lattice thermal conductivity in crystalline phase change materials: GeTe, Sb2Te3, and Ge2Sb2Te5 First-principles calculation of lattice thermal conductivity in crystalline phase change materials: GeTe, Sb 2 Te 3 , and Ge 2 Sb 2 Te 5," *Phys. Rev. B*, vol. 95, p. 24311, 2017.

[53] I. Aguilera, C. Friedrich, and S. Blügel, "Spin-orbit coupling in quasiparticle studies of topological insulators," *Phys. Rev. B*, vol. 88, p. 165136, 2013.

[54] A. Lawal and A. Shaari, "Density functional theory study of electronic properties of Bi2Se3 and Bi2Te3," *Malaysian J. Fundam. Appl. Sci.*, vol. 12, no. 3, Jan. 2017.

[55] K. S. Novoselov *et al.*, "Two-dimensional atomic crystals.," *Proc. Natl. Acad. Sci. U. S. A.*, vol. 102, no. 30, pp. 10451–3, Jul. 2005.

[56] K. S. Novoselov *et al.*, "Two-Dimensional Gas of Massless Dirac Fermions in Graphene," Sep. 2005.

[57] G. Spektor, A. David, G. Bartal, M. Orenstein, and A. Hayat, "Spin-patterned plasmonics: towards optical access to topological-insulator surface states," *Opt. Express*, vol. 23, no. 25, p. 32759, Dec. 2015.

[58] H. J. Monkhorst and J. D. Pack, "Special points for Brillouin-zone integrations," *Phys. Rev. B*, vol. 13, no. 12, pp. 5188–5192, Jun. 1976.

[59] P. E. Blöchl, "Projector augmented-wave method," *Phys. Rev. B*, vol. 50, no. 24, pp. 17953–17979, Dec. 1994.

[60] W. Setyawan and S. Curtarolo, "High-throughput electronic band structure calculations: Challenges and tools," *Comput. Mater. Sci.*, vol. 49, no. 2, pp. 299–312, 2010.

[61] H. P. Flatt and K. Kennedy, "Performance of parallel processors," *Parallel Comput.*, vol. 12, no. 1, pp. 1–20, 1989.