UNIVERSITI PUTRA MALAYSIA

PARALLEL COMPUTATION OF MAASS CUSP FORMS USING MATHEMATICA

CHAN KAR TIM

PARALLEL COMPUTATION OF MAASS CUSP FORMS USING MATHEMATICA

By

CHAN KAR TIM

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

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DEDICATIONS

To all the loved ones in my life . . .

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

PARALLEL COMPUTATION OF MAASS CUSP FORMS USING MATHEMATICA

By

CHAN KAR TIM

November 2013

Chair: Associate Professor Hishamuddin Zainuddin, PhD

Faculty: Science

Spectral studies on the eigenfunctions of Laplace-Beltrami operator on a cusp hyperbolic surface are known to contain both continuous and discrete eigenvalues. While the continuous eigenvalues are known analytically, whose eigenfunctions are usually spanned by the Eisenstein series, it is more subtle to solve for the discrete ones which can only be found numerically where the eigenfunctions are described by the Maass cusp forms. The main aim of this research is to compute the discrete eigenvalues and visualize the eigenfunctions for the modular group, commutator subgroup and principal congruence subgroup of level two in a parallel computing environment using GridMathematica software.

Our parallel programme comprises of two important parts namely the pullback algorithm and also the Maass cusp form algorithm. The latter is developed using an adapted algorithm of Hejhal and Then which is based on implicit automorphy and finite Fourier series. This algorithm applies to the computation of Maass cusp

forms on Fuchsian group whose fundamental domain has only one cusp namely the modular group and the commutator subgroup. Special attention is given to the computation of eigenvalues for the modular group because this part is intended to serve as the basis for further development of computation for the more complex surfaces. This parallel programme is further modified using a generalized Hejhal's algorithm to cater for fundamental domain that has several cusps namely the principal congruence subgroup of level two. To facilitate the complete pullback process of this group, a point locater algorithm is developed.

In this work, we present three different pullback algorithms for the surfaces we considered and carefully integrate them into our Maass cusp form algorithm. With it, we manage to compute 190 eigenvalues for the modular group where 111 belong to the odd class and 79 belong to the even class. The computational accuracy of the eigenvalues is expected to be accurate at least up to nine decimal places since the tolerance for the bisection module is set as 10^{-10}. For the commutator subgroup, we manage to compute 104 eigenvalues where 52 belong to the odd class and 52 belong to the even class. For the principal congruence subgroup of level two, 20 lower lying eigenvalues are computed. From these eigenvalues, 11 belong to the odd class and nine belong to the even class. The tolerance of the bisection module for these two subgroups are set as 10^{-9} and 10^{-6} respectively. As such, the computational accuracy of the eigenvalues are expected to be accurate at least up to eight for the former and five decimal places for the latter.

Eigenvalues from these surfaces are checked using selected procedures such as y independent solution, automorphy condition, Hecke relation and Ramanujan-Petersson conjecture for their authenticity. Later, we visualize the eigenstates of selected eigenvalues from each surface using GridMathematica. Some features that appear in the plots are explained. We have also compared the performance of parallel programming and normal programming here in order to justify the feasibility and advantages of using the parallel version of commercially available software for complex computations of Maass cusp forms. We find that the parallel programming is about 5.75 times faster than the normal programming while its efficiency is capped at 0.443.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

PENGKOMPUTERAN SELARI BAGI FUNGSI BENTUK JURING MAASS DENGAN MENGGUNAKAN MATHEMATICA

Oleh

CHAN KAR TIM

November 2013

Pengerusi: Profesor Madya Hishamuddin Zainuddin, PhD

Fakulti: Sains

Kajian spektrum pada fungsi eigen operator Laplace-Beltrami pada permukaan berjuring hiperbolik diketahui mempunyai nilai eigen yang selanjar dan diskrit. Sementara nilai eigen selanjar boleh dikira secara analitik dan fungsi eigennya dijana oleh siri Eisenstein, penyelesaian nilai eigen diskrit adalah lebih sukar dan hanya diketahui secara berangka dengan fungsi eigennya diberi oleh fungsi bentuk juring Maass. Tujuan utama kajian ini adalah untuk mengira nilai eigen diskrit dan memberi visualisasi fungsi eigen bagi kumpulan modular, subkumpulan komutator dan subkumpulan kongruen utama tahap dua dalam persekitaran pengkomputeran selari menggunakan perisian GridMathematica.

Aturcara selari kami terdiri daripada dua bahagian penting iaitu algoritma pengunduran dan juga algoritma fungsi bentuk juring Maass. Algoritma kedua ini telah dibangunkan dengan menggunakan algoritma terubahsuai Hejhal dan Then yang berdasarkan automorf tersirat dan siri Fourier terhingga. Algoritma ini boleh digunapakai untuk mengira fungsi bentuk juring Maass bagi kumpulan Fuchsian

yang domain asasnya hanya berjuring tunggal contohnya kumpulan modular dan subkumpulan komutator. Perhatian khas diberikan kepada pengiraan nilai eigen bagi kumpulan modular kerana bahagian ini bertujuan untuk dijadikan sebagai asas pembangunan pengiraan selanjutnya untuk permukaan yang lebih kompleks. Aturcara selari ini seterusnya diubahsuai menggunakan algoritma Hejhal teritlak untuk menampung domain asas yang mempunyai beberapa juring contohnya subkumpulan kongruen utama tahap dua. Untuk memudahkan proses pengunduran lengkap kumpulan ini, satu algoritma penentu lokasi dibangunkan.

Dalam kajian ini, kami bentangkan tiga algoritma pengunduran yang berbeza untuk permukaan-permukaan kajian kami dan dengan cermat mengintegrasikan mereka ke dalam algoritma fungsi bentuk juring Maass. Dengan algoritma ini, kami berjaya mengira 190 nilai eigen bagi kumpulan modular di mana 111 dimiliki oleh kelas ganjil manakala 79 lagi dimiliki oleh kelas genap. Ketepatan pengiraan nilai eigen dijangka tepat sekurang-kurangnya sehingga sembilan tempat perpuluhan sejak toleransi bagi modul pembahagian dua bahagian ditetapkan sebagai 10^{-10}. Untuk subkumpulan komutator, kami dapat mengira 104 nilai eigen yang mana 52 adalah milik kelas ganjil dan 52 lagi milik kelas genap. Bagi subkumpulan kongruen utama tahap dua pula, 20 nilai eigen paras rendah berjaya dikira. Daripada nilai eigen ini, 11 dimiliki oleh kelas ganjil manakala sembilan lagi dimiliki oleh kelas genap. Toleransi modul pembahagian dua bahagian bagi kedua-dua subkumpulan ini masing-masing ditetapkan sebagai 10^{-9} dan 10^{-6}. Dengan ini, ketepatan pengiraan nilai eigen dijangka adalah tepat sekurang-kurangnya sehingga lapan untuk subkumpulan pertama dan lima tempat perpuluhan untuk subkumpulan yang kedua.

Nilai eigen yang diperoleh dari permukaan-permukaan ini kemudian disahkan melalui prosedur-prosedur yang dipilih seperti penyelesaian y bebas, syarat automorf, hubungan Hecke dan andaian Ramanujan-Petersson. Seterusnya, kami menggambarkan tahap eigen bagi nilai-nilai eigen terpilih dari setiap permukaan menggunakan GridMathematica. Ciri-ciri yang muncul dalam gambar ini kemudian diperjelaskan. Kami juga telah membandingkan prestasi pengaturcaraan selari dengan pengaturcaraan biasa di sini untuk membuktikan kebolehlaksanaan dan kelebihan menggunakan perisian selari yang boleh didapati secara komersial untuk pengiraan fungsi bentuk juring Maass yang kompleks. Kami dapati pengaturcaraan selari adalah kira-kira 5.75 kali lebih cepat daripada pengaturcaraan biasa manakala kecekapannya dihadkan pada 0.443.

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I certify that a Thesis Examination Committee has met on **12 November 2013** to conduct the final examination of **Chan Kar Tim** on his thesis entitled "**Parallel Computation of Maass Cusp Forms Using Mathematica**" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the **Doctor of Philosophy**.

Members of the Thesis Examination Committee were as follows:

Zainal Abidin bin Talib, Ph.D.
Professor
Faculty of Science
Universiti Putra Malaysia
(Chairperson)

Kamel Ariffin bin Mohd Atan, Ph.D.
Professor Dato'
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Zulkifly bin Abbas, Ph.D.
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

S. Twareque Ali, Ph.D.
Professor
Department of Mathematics and Statistics
Concordia University
Canada
(External Examiner)

NORITAH OMAR, Ph.D.
Associate Professor and Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 19 December 2013

This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy.

The members of the Supervisory Committee were as follows:

Hishamuddin Zainuddin, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Chairperson)

Halimah Mohamed Kamari, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

Isamiddin S. Rakhimov, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

BUJANG BIN KIM HUAT, PhD
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

DECLARATION

I declare that the thesis is my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously, and is not concurrently, submitted for any other degree at Universiti Putra Malaysia or at any other institution.

CHAN KAR TIM

Date: 12 November 2013

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LIST OF SYMBOLS AND ABBREVIATIONS

r	Computed eigenvalue
λ	True eigenvalue
Ψ	Time dependent wavefunction
ψ	Time independent wavefunction
Δ	Laplace-Beltrami operator
$\mathbb{Z}$	Integers
$\mathbb{R}$	Real number
$\mathbb{C}$	Complex number
$\mathbb{R} \cup \infty$	Euclidean boundary of the upper half plane
$\hat{\mathbb{C}}$	Riemann sphere
$\Gamma \backslash \mathcal{H}$	Hyperbolic Riemann surface
$\mathcal{X}$	Compact Riemann surface
$\mathcal{H}$	Upper half plane
$PSL(2, \mathbb{R})$	Projective special linear group with 2×2 real matrices
$PSL(2, \mathbb{Z})$	Projective special linear group with 2×2 integer matrices
Γ	Discrete group
$\Gamma(1)$	Modular group
Γ'	Commutator subgroup
$\Gamma(2)$	Principal congruence subgroup of level two
$\mathcal{S}$	Surface of constant negative curvature
$\mathcal{F}$	Fundamental domain for the modular group
$\mathcal{D}$	Fundamental domain for the commutator subgroup
$\mathcal{D}'$	New fundamental domain for the commutator subgroup
$\mathcal{F}_2$	Fundamental domain for the principal congruence subgroup

$\mathcal{M}(\Gamma, \lambda)$	The space of Maass waveform for Γ and eigenvalue λ
$\mathcal{M}(\Gamma(M), \lambda)$	The space of Maass oldform
$\mathcal{M}(\Gamma(N), \lambda)$	The space of Maass newform
ϵ	Tolerance of wave function
c_j	A cusp depending on index j
L	Width of a cusp
K_{ir}	K-Bessel function
κ	Number of inequivalent cusps
$\mathcal{F}_{2a}$	Fundamental domain with respect to inequivalent cusp c_1
$\mathcal{F}_{2b}$	Fundamental domain with respect to inequivalent cusp c_2
$\mathcal{F}_{2c}$	Fundamental domain with respect to inequivalent cusp c_3
GCD	Greatest common divisor
MCF	Maass cusp form
FFT	Finite Fourier transform

CHAPTER 1

INTRODUCTION

1.1 Brief Introduction to Chaotic Systems

The first dynamical system to be proven chaotic was given by Jacques Hadamard in 1898 (Gutzwiller, 1990). This system is usually referred to as the Hadamard dynamical system or Hadamard's billiards where he considered free motion of a mass point constrained to move on a compact Riemann surface of constant negative curvature (Avelin, 2007; Gutzwiller, 1990). The motion at each point is very unstable due to the saddle points of the surface. As such these kind of systems usually exhibit strong chaotic behaviour which means that the chaotic systems were mixing throughout the phase space. Later in 1924, Emil Artin discovered the Artin billiard which described the geodesic motion of free particle on a non-compact Riemann surface, $\Gamma\backslash\mathcal{H}$ where $\mathcal{H}$ is the upper half plane and Γ is the modular group (Bolte et al., 1992). Non-compact Riemann surfaces of finite area usually have vertices that are located infinitely far away (i.e. cusps) and they can be used as mathematical models for many physical situations such as in the scattering problem where a particle or a wave enters a container from the outside (i.e. infinitely far away) (Gutzwiller, 1990). These kind of dynamical billiards have attracted wide attention of the mathematician as these systems are connected to problems in number theory, differential geometry and group theory (Bogomolny et al., 1995). While in physics, there is interest to establish direct links between the trajectories (i.e. orbits) of classically chaotic system and the properties of the system in quantum domain. The quantum versions of the dynamical billiards are then called the quantum billiards and they obey the law of quantum mechanics. This kind of relation between quantum mechanics and classical chaos has become the subject of study in quantum chaos which has found applications in cosmology

(Then, 2007) and condensed matter (Hurt, 2000; Gubin and Santos, 2012).

1.2 Problem Statement

Different types of configuration spaces have been studied in the context of quantum chaos (Bogomolny et al., 1995; Then, 2007), and these include the punctured surface (with one or more cusps) which is of our interest here. The corresponding quantum system is governed by the stationary state Schrödinger equation, $H\psi = E\psi$ with the Hamiltonian $H = -\Delta$, where $\Delta = y^2(\partial_x^2 + \partial_y^2)$ is the Laplace-Beltrami operator ($\hbar = 2m = 1$). When we consider spectral resolution of the Laplacian, its spectrum contains both continuous (i.e. scattering state) and discrete (i.e. bound state) parts (Then, 2007). The continuous part of the spectrum is spanned by the Eisenstein series which is known analytically (Then, 2005). The discrete part is usually spanned by a discrete eigenfunction called Maass waveform which is a non-holomorphic modular form introduced by Hans Maass in 1949 (Terras, 1985). Maass waveforms are simply smooth and square integrable eigenfunctions of the Laplacian on the punctured surface. It is well known that Maass waveform with eigenvalues $\lambda \geq 1/4$ has no constant term in their Fourier expansion and they are called the Maass cusp form (MCF). This waveform vanishes exponentially fast in each cusp. Since the discrete part is non analytical, one has to compute them numerically.

In our research, we are interested in the eigenvalues of the bound states for the surfaces arising from the modular group $\Gamma(1)$, commutator subgroup Γ' and the principal congruence subgroup of level two $\Gamma(2)$. We use an algorithm developed by Hejhal (Hejhal, 1999) for computation of Maass cusp forms on cofinite Fuchsian groups that usually have cusp. Hejhal's algorithm is heuristic and represents a major step forward with regards to both numerical stability and range of applicability (Booker et al., 2006).

Computational work of MCF on modular surface is not new and has been done by researchers such as Hejhal and Rackner (1992), Then (2005), Strömberg (2005) and the references listed therein. Nevertheless, their work remain known only to specialists in the area because of the complexity of the algorithm involved. To make this work more accessible to non-specialists, Siddig and Zainuddin (2009) used a popular commercial software Mathematica for the computation of Maass waveforms since Mathematica has a wider user base and are easily accessible to beginners. Besides, there are many built-in functions including the K-Bessel function and this greatly simplify the programme. However, using Mathematica for the computation is time consuming. Due to this reason, this motivates us to use GridMathematica, a parallel version of Mathematica which is realizable on a cluster of workstations for computation. At present, to the best of our knowledge, there is only one Mathematica package that handles specifically the MCF computations and particularly there is none using GridMathematica. With the implementation of parallel computing on computation of MCF, the time for computing higher ranges of eigenvalues for the modular surfaces and eigenfunctions for more complex surfaces such as the singly punctured two torus and the triply punctured two sphere will be greatly reduced.

1.3 Objectives of Research

The main purpose of this research is to develop a programme that is workable in parallel computing environment (GridMathematica) to compute the eigenvalues on modular group, commutator subgroup and also the principal congruence subgroup of level two. Overall, the objectives of this research are as follows:

1) To set up a cluster of workstation using Rock Cluster and GridMathematica.
2) To optimize the previously developed Mathematica programme for modular group and implement it in GridMathematica (parallel computing).
3) To compare the performance of parallel programming and normal programming in modular group.
4) To develop a pullback algorithm for commutator subgroup and principal congruence subgroup of level two.
5) To compute eigenvalues and visualization of Maass cusp forms for modular group, commutator subgroup and principal congruence subgroup of level two using GridMathematica.

1.4 Outline of Thesis

This thesis is divided into eight chapters. In Chapter One, we give a brief introduction and the objectives of current research. Chapter Two presents the reviews on the computations of Maass waveforms and also works that have been linked with Hejhal's algorithm. In addition, it also reviews various directions of computational works on Maass forms. Some applications based on computing eigenvalues and research related to punctured surface are also discussed in this chapter.

Chapter Three explains the mathematical preliminaries for the hyperbolic geometries and also the discrete subgroup. Special attention is given to the surfaces of interest where their definitions, fundamental domains and generators are explained. The theoretical background on the Maass waveforms which includes modified K-Bessel function, Hecke operators and oldforms and newforms are also discussed.

Some theories of the root finding method are also presented here.

Chapter Four describes the implementation of parallel computation on a cluster of workstation. Physical assembly of the hardware as well as the installation of software are explained here. This is followed by parameters setting, algorithm implementation and how to optimize the programme. Last section of this chapter explains on the parallelization of the programme.

Chapter Five is devoted to the computation of Maass cusp form for the modular group using GridMathematica. In this chapter, two of the most important algorithms, namely Maass cusp form algorithm and pullback algorithm are explained. Numerical results as well as comparison of performance between normal and parallel programming of the computation of modular group are presented here. Finally, some pictures of the waveform based on selected eigenvalues are produced.

Chapter Six contains the computational work for Maass cusp form for the commutator subgroup using GridMathematica. A modified MCF algorithm based on the previous chapter is deployed here. A new pullback algorithm based on generators of Γ' is constructed. With some modifications to our programme, we presented here the numerical results as well as the topography of the waveforms.

Chapter Seven presents the computational work for the principal congruence subgroup of level two using GridMathematica. We begin with the construction of the fundamental domain and its subdomain for this subgroup. Pullback algorithm is then developed after the consideration of the cusp representative, point's location, complete pullback and automorphic relation as well as the minimal height of the fundamental domain. A point locater algorithm is provided here to look for location of each point. A modified MCF algorithm which is meant for computing eigenvalues for a surface with three cusps is presented here. This is followed by its numerical results and pictures of the waveforms.

The final chapter provides the conclusion of this work. We also make a few suggestions here for future works and improvements.

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