

My research uses analytical and numerical methods in the subjects of optics, electromagnetics, and acoustics. I am particularly interested in layered media problems which model the scattering of electromagnetic waves in a periodic structure. As a graduate student, I have focused on the numerical implementation of High-Order Perturbation of Surfaces (HOPS) methods including the Transformed Field Expansion (TFE) method developed by Nicholls [53, 54, 58] and Reitich [32, 34, 39, 49], the Field Expansion (FE) method developed by Bruno [25, 28, 29, 30] and Reitich, and the Operator Expansion (OE) method developed by Milder [24, 23, 26, 26, 35, 36], Craig [38], and Sulem [31]. HOPS methods are a High-Order Spectral (HOS) method [11, 91, 44, 48, 55, 72] which are particularly well-suited for PDEs posed on piecewise homogeneous domains. Of central interest to all of the HOPS methods are Dirichlet-to-Neumann Operators (DNOs) [19]. A major portion of my thesis work involves applying the TFE method to establish joint analyticity of DNOs with respect to both interfacial and frequency deformations. There are many interesting and open problems resulting from the interaction of electromagnetic waves and grating structures. In this document I discuss six different research goals that I plan to work on in the future. The second half of the document contains several problems that would make good projects for undergraduate or graduate students. In these, I focus on the numerical and theoretical aspects of the Riemann zeta function which is another source of outstanding problems in computational mathematics.

INTRODUCTION

The scattering of linear electromagnetic waves by a layered structure is a central model in many problems of scientific and engineering interest. Examples arise in areas such as geophysics [83, 79], imaging [52], materials science [22], nanoplasmonics [17, 73, 93], and oceanography [21]. In the case of nanoplasmonics, many topics such as extraordinary optical transmission [41], surface enhanced spectroscopy [14], and surface plasmon resonance (SPR) biosensing [75, 87] and [97, 99, 103, 106]. In all of the physical problems it is necessary to approximate scattering returns in a fast, robust, and highly accurate fashion. This proposal will expand upon a novel high-order perturbation of surfaces algorithm (HOPS) [109, 113, 114] designed for the numerical simulation of the layered periodic media (diffraction or scattering) problem.

While a variety of classical algorithms have been utilized for the simulation of this problem, it has recently been shown [104, 109, 113, 114] that such volumetric approaches (such as finite difference and finite/spectral element methods) are greatly disadvantaged due to the large number of unknowns for layered media problems. Another natural candidate is interfacial methods based upon integral equations (IEs) [40]. However, as discussed in [104, 109, 113, 114], these also face difficulties. Two major problems in our parametrized setting are:

1. For configurations parameterized by a real value ε (in our scheme the height/slope of the interface), an IE solver will return the scattering returns for only *one* particular value of ε . If this is changed, the solver must be run again.
2. IE solvers require inverting a dense, nonsymmetric positive definite system of linear equations at every stage of simulation.

In contrast, the high-order perturbation of surfaces (HOPS) approach [109, 113, 114] can effectively address these concerns. More specifically, in [113, 114] an alternative known as the method of field expansions (FE) is proposed which is based on the low-order calculations of Rayleigh [2] and Rice [4]. An expansion to high-order incarnation was first introduced by Bruno and Reitich [28, 29, 30] and then was later enhanced and stabilized by Nicholls and Reitich [63, 64, 78]. The later expansion is known as the transformed field expansion (TFE) method. The TFE method has two major advantages:

1. The method is built upon expanding the boundary parameter ε . Once the Taylor coefficients are known for the scattering quantities, the TFE method can recover all of the returns by summing the Taylor coefficients. It is unnecessary to begin a new summation for every value of ε .
2. The scheme is based on the perturbative nature of the interface which requires the inversion of a single, sparse operator corresponding to the flat-interface solution.

For a single incident wavelength, the TFE method is among the most efficient available in our layered media setting. In more recent work, I have investigated configurations parameterized by *two* real parameters - ε (the height/slope of the interface) and δ (the frequency). In upcoming work, I will publish two papers involving a rigorous proof of joint analyticity in expanding both ε and δ with detailed numerical simulations. The first paper shows that the TFE method can be extended from a single parameter ε to multiple parameters of interest to the geometry of the problem. The second paper confirms the theorem by rigorously testing numerical simulations of large boundary and frequency parameters ε and δ . Further analysis will zone in on adding new parameters of interest to layered media problems, investigating points (known as Rayleigh singularities) where the Taylor series fails to converge, analyzing analyticity results in multilayered configurations, implementing parallel programming techniques, investigating alternative techniques for boundary/surface data, and improvements to the computational cost of the HOPS algorithm.

RESEARCH GOALS

Research Objectives: My primary objectives are to expand the TFE method through a new proof of convergence, investigate expanding around singularities, evaluating analyticity theorems in multilayered configurations, adding new parallel programming functionality, exploring alternative methods to recover surface data without Dirichlet-to-Neumann Operators, and to reduce the execution time of the HOPS algorithm. I will investigate both analytical and numerical techniques. My research is concerned with the following questions:

Goal 1- Choice of Parameters: Does the geometry of the perturbation impact how large the size of the perturbation can be?

Goal 2- Rayleigh Singularities: Can we build a full HOPS algorithm based on points where the Taylor expansion is invalid?

Goal 3- Multiple Layers: Can we prove analyticity results when the number of layers is greater than three? Do the same theorems hold for ten or one hundred layers?

Goal 4- Parallel Programming: Can we implement parallel programming techniques so that our HOPS code runs on N processors?

Goal 5- Alternatives to DNOs: Do we need to use DNOs to recover surface data from information stored in the transformed field? Is there an alternative method which preserves the inversion of a single, sparse operator at the interface?

Goal 6- Computational Costs: Can we reduce the execution time per time step in our HOPS algorithm?

Research Methods: My existing HOPS code is written in Matlab. Following Fang [108], I will investigate a parallel implementation in C++ or Fortran. By using classical Sobolev space theory [43], regular perturbation theory [46], and previous results [123, 119, 88, 82, 118], I will investigate theoretical enhancements to the TFE method and improve existing functionality of the HOPS algorithm. In [118], Nicholls describes how to prove analyticity results in three or more

layers using a τ -allowable layer configuration. I intend to generalize these results to ten or more layer configurations. I will review the electromagnetics and inverse scattering literature to find alternatives to DNOs.

Goal 1. Choice of Parameters: Does the geometry of the perturbation impact how large the size of the perturbation can be?

Our HOPS method is based on two smallness assumptions:

1. Boundary perturbation: $g(x) = \varepsilon f(x)$, $\varepsilon \in \mathbb{R}$, $\varepsilon \ll 1$,
2. Frequency perturbation: $\omega = (1 + \delta)\underline{\omega} = \underline{\omega} + \delta\underline{\omega}$, $\omega \in \mathbb{R}$, $\delta \ll 1$,

with the additional assumption that f is sufficiently smooth ($f \in C^2$ [53, 62] or even Lipschitz [68]). Numerical simulations show that our HOPS algorithm can handle larger perturbations of ε (the height/slope) in comparison to δ (the frequency). With modest test parameters and a period of $d = 2\pi$, we are able to perturb the value of ε (to $\varepsilon = 0.1$ or even $\varepsilon = 0.2$) and still get reasonable convergence results. At a value around $\varepsilon = 10^{-4}$, our HOPS algorithm converges to machine precision provided that we sum to high enough Taylor orders.

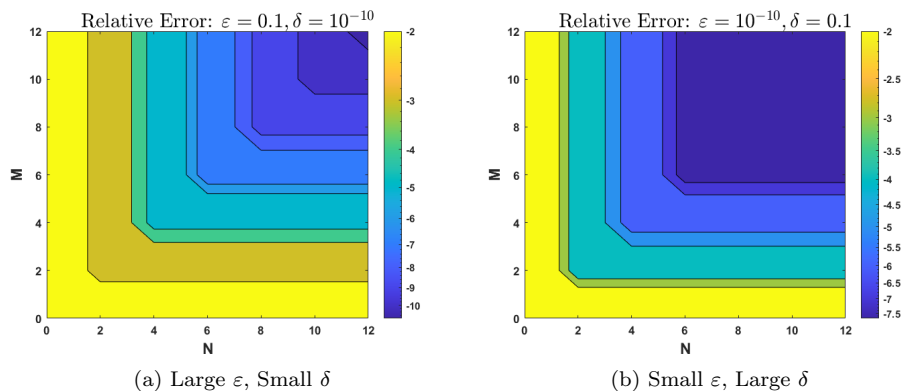


Figure 1: A contour plot of the relative error computed with our HOPS algorithm by holding ε and δ fixed. In Figure 1(a) we set $\varepsilon = 0.1, \delta = 10^{-10}$ and compute up to $N = M = 12$ Taylor orders. In Figure 1(b) we set $\varepsilon = 10^{-10}, \delta = 0.1$ and compute up to $N = M = 12$ Taylor orders. Supplementary testing confirms that our HOPS algorithm is better suited towards larger ε .

Predictions: The HOPS method relies on creating an artificial boundary condition through what is known as a Dirichlet-to-Neumann operator. The DNO is responsible for recovering transformed field solutions by data stored at the interface. I strongly suspect that the DNO mitigates moderate to large perturbations of the height/slope. By following techniques developed in [118, 58, 82], I intend to rigorously prove that the TFE method is analytic and convergent when ε is large. This is an extension of my previous work where I showed that the TFE method is jointly analytic in a small perturbation of both ε and δ . In order to test new physical parameters, I will study the engineering literature [121, 120] and analyze which parameters are best suited towards the domain flattening change of variables [6, 12] central to the TFE method.

Goal 2. Rayleigh Singularities: Can we build a full HOPS algorithm based on points where the Taylor expansion is invalid?

A fundamental equation in the HOPS algorithm is

$$\alpha_p^2 + \gamma_p^2(\delta) = k^2$$

where k represents the wavenumber, and $\alpha = k \sin(\theta)$, $\gamma = k \cos(\theta)$, are parameters corresponding to refraction/reflection of the incidence angle θ . It is well known that a Rayleigh singularity [3, 93] (also known as a Wood's anomaly) occurs when $\alpha_p^2 = k^2$ for any integer $p \neq 0$. That is, if $\gamma_p(\delta) = 0$ for $p \neq 0$ then the Taylor series expansion of $\gamma_p(\delta)$ is invalid. In [117], Nicholls investigated changing the Taylor expansion to a Puiseux expansion [71]:

$$\gamma_p(\delta) = \sum_{m=0}^{\infty} \gamma_{p,m} \delta^{m+1/2} = \delta^{1/2} \sum_{m=0}^{\infty} \gamma_{p,m} \delta^m.$$

However, he found that this approach ran into external difficulties (§6 of [117]) simplifying explicit forms of the Dirichlet and Neumann trace operators.

Predictions: Rayleigh singularities are a central obstruction to the convergence of our HOPS algorithm. In all of our numerical tests, we select custom frequency ranges which maximize the radius of convergence of our algorithm by expanding away from the singularities. Alternative methods such as Padé summation also fail to be analytic in a neighborhood of a Rayleigh singularity. By investigating known techniques [69, 115, 122, 5, 13] of perturbation series, I will perform a series expansion of $\gamma_p(\delta)$ that doesn't diverge when $\gamma_p(\delta) = 0$.

Goal 3. Multiple Layers: Can we prove analyticity results when the number of layers is greater than three? Do the same theorems hold for ten or one hundred layers?

In [118], Nicholls discusses how to apply the HOPS methodology in multilayered configurations. He considers a multilayered material with M interfaces at

$$z = a^{(m)} + g^{(m)}(x, y), \quad 1 \leq m \leq M,$$

which are $d_x \times d_y$ periodic

$$g^{(m)}(x + d_x, y + d_y) = g^{(m)}(x, y), \quad 1 \leq m \leq M,$$

separating $(M + 1)$ -many layers.

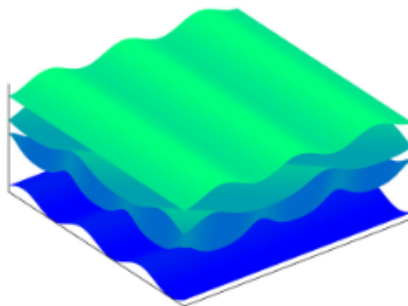


Figure 2: A five-layer problem configuration with layer interfaces $z = a^{(m)} + g^{(m)}(x)$.

One of the main results proven in this paper is the analyticity of the DNOs with respect to the interfacial parameter ε . I would like to extend this result to the joint analyticity of both the interfacial parameter ε and frequency parameter δ . I also want to prove more exotic analyticity results when the number of layer configurations increases to ten or one hundred.

Predictions: My existing HOPS code can handle ten or more layer configurations. The majority of the numerical work was completed in the analysis done in my thesis where I wrote separate subroutines to calculate DNOs in the upper and lower transformed fields. In order to implement multilayered configurations, I would need to write no more than five new subroutines. However, I am concerned about the execution time of the HOPS algorithm with a large number of layer configurations (to be addressed in the next research goal). I will run into difficulty with analyticity theorems in more than three dimensions (the majority of our work has been in two and three dimensions). I intend to build upon the τ -allowable layer configuration techniques developed by Nicholls and invent new techniques in higher dimensions.

Goal 4. Parallel Programming: Can we implement parallel programming techniques so that our HOPS code runs on N processors?

A former student of my advisor, Zheng Fang, implemented C++ code [108] to parallelize the computation of the Operator Expansion (OE) method with Navier’s equations [47, 90]. The analysis done in my dissertation is based on an application of the Transformed Field Expansion (TFE) method to the Helmholtz equation [10]. However, given the similarities between the numerical implementation of the OE and TFE methods, I should be able to reuse some of the C++ code written by Fang.

If I cannot reuse the work done by Fang, then it would be worthwhile to write my own parallel implementation of the TFE method. While Matlab does have some parallel programming functionality, I would prefer to use a language such as C++ or Fortran. My previous experience in the software industry and in national labs tells me that it is beneficial to invest in parallel programming techniques. I will investigate the feasibility of a parallel implementation of our three HOPS methods - the Operator Expansion (OE) method, the Field Expansion (FE) method, and the Transformed Field Expansion (TFE) method.

Predictions: In two or three dimensions, most of our HOPS code is efficient and has a runtime less than an hour. On a local library machine (with Matlab installed), I can run almost all of my numerical simulations in less than thirty minutes. However, with one hundred or more layer configurations, I suspect that many simulations will take longer than a week to run on one processor. As a result, I will investigate a parallel implementation of the TFE method and the Helmholtz equation. I currently have access to supercomputing resources (through workstations at UIC and Argonne National Laboratory) and would need equivalent resources as a postdoc. After I complete the parallel implementation of the TFE method, I will work on the OE and FE methods.

Goal 5. Alternatives to DNOs: Do we need to use DNOs to recover surface data from information stored in the transformed field? Is there an alternative method which preserves the inversion of a single, sparse operator at the interface?

Suppose we are given a linear system of the form $AV = R$. Expanding in both interfacial and frequency perturbations gives

$$A(\varepsilon, \delta) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A_{n,m} \varepsilon^n \delta^m, \quad R(\varepsilon, \delta) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} R_{n,m} \varepsilon^n \delta^m,$$

where the solution takes the form

$$V(\varepsilon, \delta) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} V_{n,m} \varepsilon^n \delta^m.$$

A straightforward calculation gives at order $\mathcal{O}(\varepsilon^n, \delta^m)$

$$A_{0,0}V_{n,m} = R_{n,m} - \sum_{\ell=0}^{n-1} A_{n-\ell,0}V_{\ell,m} - \sum_{r=0}^{m-1} A_{0,m-r}V_{n,r} - \sum_{\ell=0}^{n-1} \sum_{r=0}^{m-1} A_{n-\ell,m-r}V_{\ell,r},$$

or

$$V_{n,m} = A_{0,0}^{-1} \left(R_{n,m} - \sum_{\ell=0}^{n-1} A_{n-\ell,0}V_{\ell,m} - \sum_{r=0}^{m-1} A_{0,m-r}V_{n,r} - \sum_{\ell=0}^{n-1} \sum_{r=0}^{m-1} A_{n-\ell,m-r}V_{\ell,r} \right).$$

From which at order $\mathcal{O}(\varepsilon^0, \delta^0)$ we obtain the flat-interface solution $V_{0,0} = (A_{0,0})^{-1} R_{0,0}$. A central feature in all of our HOPS schemes is that we can invert $A_{0,0}$ (a sparse operator) through the use of Dirichlet-to-Neumann operators. However, it would be interesting to find an alternative technique which preserves the inversion of our sparse operator.

Predictions: Our HOPS methodology (and all of our numerical algorithms) depend on the inversion of a single, sparse operator (which will always be A_0 for the linear system $AV = R$). Trace theory tells us that we can define a Dirichlet operator \mathcal{D} in order to map the “zero-trace” value of our Dirichlet data to the “boundary-trace” value. In this manner, the DNO is responsible for recovering the flat-interface solution from transformed field data. I intend to search the PDE literature for alternative techniques. I strongly suspect that there are other techniques (used in inverse scattering problems) which will provide competitive numerical results.

Goal 6. Computational Costs: Can we reduce the execution time per time step in our HOPS algorithm?

We are interested in computing the reflectivity map [114, 124], R , for N_ε many values of ε and N_δ many values of δ . By definition, any surface method requires the use of a number of discretization points which we will denote by N_x . The TFE approach retains N perturbation orders in ε , while our HOPS algorithm demands the additional consideration of M Taylor orders in δ . In recent work, I show that the total cost of computing the reflectivity map by our HOPS algorithm is

$$\mathcal{O}(N^2 M^2 N_x \log(N_x) + N_\varepsilon N_\delta),$$

while the cost of more traditional methods such as integral solvers takes

$$\mathcal{O}(N_\varepsilon N_\delta (N_x)^3).$$

Therefore, the HOPS approach is more competitive when N_ε and N_δ are large.

Predictions: By definition, our algorithm requires $\mathcal{O}(N_\varepsilon N_\delta)$ steps to sum over every value of ε and δ in Matlab. Our focus will be on reducing the cost of $\mathcal{O}(N^2 M^2 N_x \log(N_x))$ from the HOPS/TFE methodology. In particular, I will investigate reducing the total cost of our algorithm to

$$\mathcal{O}(NMN_x \log(NM) \log(N_x) + N_\varepsilon N_\delta)$$

by reducing the problem space at every step [59, 84, 116, 107, 66]. In the numerical paper, I show that the total cost of the computing the TFE recursions at order (N, M) is $\mathcal{O}(NMN_x \log(N_x))$. By careful consideration of a joint Taylor expansion in (ε, δ) , I will study how to recover the flat-interface solution with cost

$$\mathcal{O}(\log(NM)N_x \log(N_x)).$$

Remark: All of the research goals described above are focused on the numerical and theoretical applications of High-Order Perturbation of Surfaces (HOPS) methods. I am also interested in problems in fluid mechanics [20, 33, 110, 102], finite element theory [100, 74, 70], numerical analysis [95, 96, 37, 76, 92, 65], and water waves [89, 77, 112, 47]. An interesting problem I was introduced to as a graduate student was that of undular bores [8] which is connected to the existence and uniqueness [9, 80, 105] of the Benjamin–Bona–Mahony (BBM) equation. As a postdoc, I would be happy to study a problem in a related field. I think that a lot of work is being developed in the applications of finite element theory.

Student Projects

One of my favorite functions in all of mathematics is the Riemann zeta function. Let $s = \sigma + it$. Then the Riemann zeta function is defined by [15, 98]

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}, \quad \text{for } \sigma > 1.$$

By analytic continuation we can extend the Riemann zeta function to the whole complex plane with a simple pole at $s = 1$. The zeta function satisfies the functional equation

$$\zeta(s)\pi^{s/2}\Gamma(s/2) = \zeta(1-s)\pi^{(1-s)/2}\Gamma\left(\frac{1-s}{2}\right).$$

From the definition and functional equation, it is easy to compute $\zeta(s)$ for $\sigma > 1$ or $\sigma < 0$. Suppose $s = -2k$ where k is a positive integer. Then we can use the functional equation to write the zeta function as

$$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s) \zeta(1-s),$$

and observe that

$$\begin{aligned} \zeta(-2k) &= 2^{-2k} \pi^{-2k-1} \sin(-\pi k) 2k! \zeta(1+2k) \\ &= -2^{-2k} \pi^{-2k-1} \sin(\pi k) 2k! \zeta(1+2k) \\ &= 0. \end{aligned}$$

Therefore $\zeta(-2k) = 0$ when k is a positive integer. These are known as “trivial zeros” and are uninteresting. We are interested in locating the non-trivial zeros in the critical strip where $0 < \sigma < 1$. One of the most famous conjectures in mathematics is known as the Riemann hypothesis. It was proposed by Bernhard Riemann [1] in 1859 and states that $Re(s) = 1/2$ ($s = \sigma + it$) for every nontrivial zero of the Riemann zeta function. If the conjecture is true then every nontrivial zero in the critical strip $0 < \sigma < 1$ lies on the critical line consisting of the complex numbers $s^{cl} = 1/2 + it$. Starting from around the early 1930s [57, 60], a lot of researchers started writing computer programs to verify that the Riemann hypothesis is true. The majority of these computer programs are based on variations of the following three methods:

1. The Euler-Maclaurin Summation Formula [61, 42, 56]
2. The Riemann–Siegel Formula [51, 45, 126, 18]
3. The Odlyzko–Schönhage algorithm [27, 85, 111, 86]

Due to the ease of implementation and the flexibility of modern programming languages, there are a lot of possibilities for student projects. These are accessible to both undergraduate and graduate students and could be worked on in teams (where a computer science student could write code and a pure math student would work on theoretical and analytical derivations).

Numerical Projects

A (highly motivated) undergraduate or graduate student could work on a variety of different projects involving calculations of the Riemann zeta function. These projects would involve implementing (preferably C/C++ or Fortran) code to calculate zeros of the Riemann zeta function. They could also focus on the distribution of spacing between zeros or parallel programming techniques. Some project ideas are:

Project 1- Calculating nontrivial zeros through the Euler-Maclaurin Summation formula.

Project 2- Calculating nontrivial zeros through the Riemann–Siegel formula.

Project 3- Calculating nontrivial zeros through the Odlyzko–Schönhage algorithm.

Project 4- Parallelizing the code for projects (1)-(2).

Project 5- Investigating what is known as Montgomery’s pair correlation conjecture and the distribution of spaces between zeros.

A student who is interested in pure mathematics could provide several key derivations to assist with programming.

Project 1. Calculating nontrivial zeros through the Euler-Maclaurin Summation formula.

The Euler–Maclaurin Summation formula gives a very effective tool for evaluating a sum of values of a function at integers.

Theorem (Euler-Maclaurin Summation). *Let a and b be integers satisfying $a \leq b$, and let M be a natural number. Suppose $f(x)$ is an M times continuously differentiable function over $[a, b]$. Then, we have*

$$\sum_{n=a}^b f(n) = \int_a^b f(x) dx + \frac{1}{2} (f(a) + f(b)) + \sum_{k=1}^{M-1} \frac{B_{k+1}}{(k+1)!} \left(f^{(k)}(b) - f^{(k)}(a) \right) - \frac{(-1)^M}{M!} \int_a^b B_M(x - [x]) f^{(M)}(x) dx.$$

Here, B_{k+1} is the Bernoulli number and $B_M(x)$ is the Bernoulli polynomial, $[x]$ is the greatest integer less than or equal to x , and the sum on the right-hand side is understood to be 0 if $M = 1$.

If m is a positive integer then the value of $\zeta(s)$ at $s = 1 - m$ is given by

$$\zeta(1 - m) = -\frac{B_m}{m}.$$

Following [51], it can be shown that the Euler-Maclaurin Summation formula provides a method for calculating zeros of the Riemann zeta function. However, as discussed by Bober and Hiary in [111], it is more practical to choose a number N and write

$$\zeta(s) = \sum_1^N \frac{1}{n^s} + \int_N^\infty \frac{1}{y^s} [dy] = \sum_1^N \frac{1}{n^s} + s \int_N^\infty \frac{\{y\}}{y^{s+1}} + c(N) \frac{s}{1-s},$$

which converges for $\sigma > 0$ by analytical continuation. If we choose N properly then $\zeta(s) - \sum_1^N 1/n^s$ won’t be too large and we can compute the difference by the Euler-Maclaurin summation formula. It requires $\mathcal{O}(t)$. Thankfully, the other methods are faster.

Project 2. Calculating nontrivial zeros through the Riemann–Siegel formula.

As a starting point, both Pugh [45] and Takusagawa [126] wrote excellent introductions to a computer implementation of the Riemann-Siegel formula. The classical textbook [50] by Edwards also contains a very readable exposition. The main difficulty lies within computing the coefficients that arise from the Riemann-Siegel Z function. A paper from Haselgrove [7] in the 1960s provides a table which can be used to simplify and speedup computer programming.

A mathematician named Carl Siegel went through Riemann’s work and defined the Riemann-Siegel Z function as

$$Z(t) := e^{i\theta(t)}\zeta(1/2 + it),$$

where

$$\theta(t) := \arg\left(\Gamma\left(\frac{1}{4} + \frac{it}{2}\right)\right) - \frac{\log \pi}{2}t,$$

is known as the Riemann–Siegel theta function. The Riemann-Siegel formula is an approximation formula for $Z(t)$. Once $Z(t)$ is known, a straightforward approximation of $\theta(t)$ can be used to compute $\zeta(s)$. The Z function is important because $Z(t)$ is real when t is real and it has the same absolute value as $\zeta(1/2 + it)$, i.e. $|Z(t)| = |\zeta(1/2 + it)|$. $Z(t)$ has sign changes at zeros on the critical line where $s = 1/2 + it$, so it can be used to locate zeros.

I wrote [my own](#) implementation of the Riemann-Siegel formula and am familiar with implementations in different programming languages. The [Riemann Zeta Search Project](#) was created to locate large values of the Riemann zeta function on the critical line. As of October 2021, they have obtained the following records ($Z(t)$ is the Riemann-Siegel Z function):

- More than 5.5 million candidates where $Z(t) > 1,000$.
- More than 100 candidates where $Z(t) > 10,000$.
- The largest value of $Z(t)$ calculated where $t = 310678833629083965667540576593682.05$.

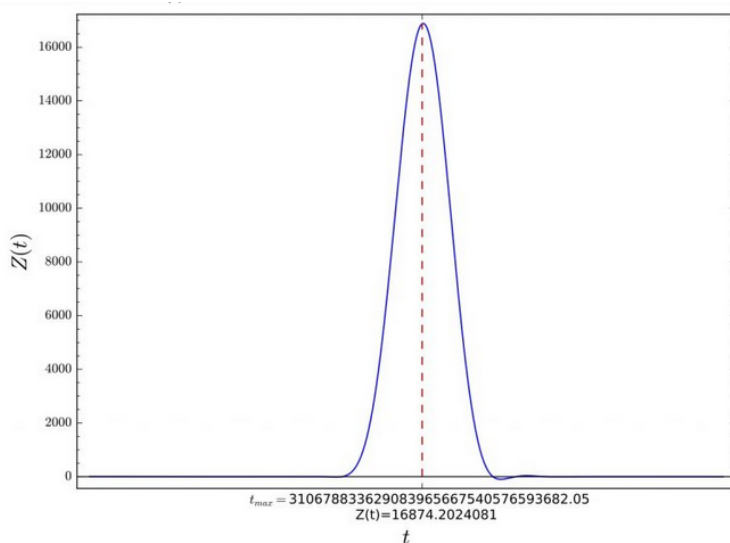


Figure 3: The largest value of the Riemann-Siegel Z function calculated by the Riemann Zeta Search Project.

The same paper [111] written by Bober and Hiary tells us that for a real number t , we can apply the Riemann–Siegel formula to write

$$Z(t) = 2\operatorname{Re} \left\{ e^{i\theta(t)} \sum_{n \leq \left(\frac{t}{2\pi}\right)^{1/2}} \frac{1}{n^{1/2+it}} \right\} + O(t^{-1/4}),$$

We then conclude that it is possible to compute $\zeta(1/2 + it)$ to sufficient accuracy in $\mathcal{O}(t^{1/2})$ time which is faster than the Euler–Maclaurin Summation formula .

Project 3. Calculating nontrivial zeros through the Odlyzko–Schönhage algorithm.

An extremely ambitious project would be to apply the Odlyzko–Schönhage algorithm. The Odlyzko–Schönhage algorithm was created to admit efficient evaluations of the Riemann–Siegel $Z(t)$ function in a range of the form $T \leq t \leq T + \Delta$, where $\Delta = \mathcal{O}(\sqrt{T})$. For t in this range, we write

$$Z(t) = \sum_{n=1}^{k_0-1} \frac{\cos(\theta(t) - t \log n)}{\sqrt{n}} + \operatorname{Re}(e^{-i\theta(t)} F(t)) + \sum_{n=k_1+1}^m \frac{\cos(\theta(t) - t \log n)}{\sqrt{n}} + R(t).$$

In the above expression, $R(t)$ is a remainder term and $F(t)$ is a complex function defined by

$$F(t) = F(k_0 - 1, k_1; t) := \sum_{k=k_0}^{k_1} \frac{1}{\sqrt{k}} e^{it \log k},$$

with $k_1 = \lfloor \sqrt{T/2\pi} \rfloor$ and k_0 a fixed, small integer. In practice, given an interval $[T, T + \Delta]$ and t in this range, the values of k_0 and k_1 are fixed in the computation of $Z(t)$. We choose k_0 to be small compared to the value of $T^{1/2}$. The most time consuming part of the evaluation of $Z(t)$ is the computation of $F(k_0 - 1, k_1; t)$. To this end, Odlyzko and Schönhage developed a technique dedicated to a fast evaluation of this sum.

To obtain fast evaluations of $F(t) = F(k_0 - 1, k_1; t)$ in the range $[T, T + \Delta]$, the Odlyzko–Schönhage algorithm is divided into two steps:

1. Multiple evaluations of $F(t)$ are handled on a well chosen regular grid of abscissa for t .
2. From these values, an interpolation formula obtains efficiently any value of $F(t)$ at a certain accuracy provided that t stays in our range.

In particular, Odlyzko handles multi-evaluations of $F(t)$ and multi-evaluations of derivatives of $F(t)$ on the regular grid. His implementation uses an interpolation formula (based on Chebyshev polynomials) for multi-evaluations of $F(t)$.

An existing implementation of the Odlyzko–Schönhage algorithm is included in the source code on [Jonathan Bober's website](#). However, this is difficult to follow. Using a preconditioner of time $\mathcal{O}(T^{1/2+\varepsilon})$, the Odlyzko–Schönhage algorithm can evaluate a single value of $\zeta(1/2 + it)$ for any $T < t < T + T^{1/2}$ to within $\pm t^{-c}$ in $\mathcal{O}(t^\varepsilon)$ operations on numbers of $\mathcal{O}(\log t)$ bits for any $\varepsilon > 0$. Therefore, it is the fastest and most competitive out of the three techniques. Writing (and documenting) a full implementation of the Odlyzko–Schönhage algorithm would be extremely valuable to practitioners in the mathematical sciences and engineering. It would be a good idea to implement this algorithm in C/C++ or Fortran.

Project 4. Parallelizing the code for projects (1)-(2).

A computer science student (or someone interested in high performance computing) could write a parallel implementation of the Euler-Maclaurin Summation formula or the Riemann–Siegel formula described above. They would need access to supercomputing resources (through the university or a national lab). This would be a good project for an engineering student who is interested in learning more about number theory.

Project 5. Investigating Montgomery’s pair correlation conjecture and the distribution of spaces between zeros.

As people became more interested in finding zeros of the Riemann zeta function, they started to use statistical tools to find relationships between zeros. In 1973, Hugh Montgomery and Freeman Dyson discovered that there is an interesting relationship between the spaces of consecutive zeros of the Riemann zeta function and the spaces of eigenvalues generated from a random matrix. This is known as Montgomery’s pair correlation conjecture [67, 125]. The conjecture states that the pair correlation between pairs of zeros of the Riemann zeta function (normalized to have unit average spacing) is

$$1 - \left(\frac{\sin(\pi u)}{\pi u} \right) + \delta(u).$$

Here $\delta(u)$ represents the normalized spacing between zeros. In the 1980s, Andrew Odlyzko started investigating statistical properties of the zeros of $\zeta(s)$. He used the Cray X-MP supercomputer to analyze the distribution of the spacings between non-trivial zeros. Part of this work was motivated by the fact that Odlyzko was interested in creating a faster and more powerful algorithm than the Riemann-Siegel formula (which was why the Odlyzko-Schönhage algorithm was created). Odlyzko found that distribution of zeros agrees with the distribution of spacings of GUE random matrix eigenvalues in random matrix theory.

Writing a nontrivial zero as $\rho = \frac{1}{2} + i\gamma_n$, Odlyzko let the normalized spacings be

$$\delta_n = \frac{\gamma_{n-1} - \gamma_n}{2\pi} \log \left(\frac{\gamma_n}{2\pi} \right).$$

Given that the Odlyzko-Schönhage algorithm can compute $\zeta(1/2 + it)$ in an average time of t^ϵ steps, Odlyzko was able to compute millions of zeros around heights of 10^{20} . This provided evidence supporting the relationship between the distribution of zeros of the Riemann zeta function and the distribution of spacings of GUE random matrix eigenvalues. In particular, Odlyzko noticed that as more zeros are sampled, the more closely their distribution approximates the shape of the GUE random matrix. A visualization of this is included in Figure 4 on the next page.

A student interested in statistics and computer programming could review the numerics done by Odlyzko [16] and write their own code. On the other hand, a student more inclined towards pure mathematics can study the distribution of spaces between zeros [94, 81] and the relationship between the Riemann zeta function and prime numbers.

Remark: All of these student projects are centered around numerical aspects of the Riemann zeta function. It would be interesting to implement an application of the theory developed by the finite difference or finite element methods. I spent a summer working at the Cold Regions Research and Engineering Laboratory (CRREL) where I was introduced to the Elmer FEM multiphysical software [101]. The open source software supports many physical models including the Heat equation, Navier-Stokes equations, Helmholtz equation, and many more. A student interested in mechanical engineering or application based mathematics could spend a semester or an entire year working on a physical model in Elmer.

Pair Correlation Function

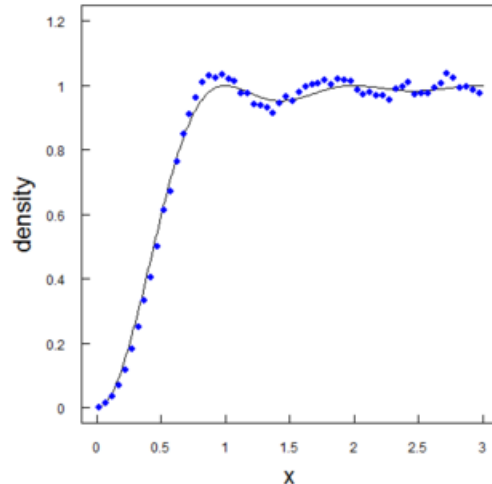


Figure 4: The real line describes the two-point correlation function of the random matrix of type GUE. Blue dots describe the normalized spacings of the non trivial zeros of Riemann zeta function, for the first 10^5 zeros.

Future Work

Through my current research interests are somewhat narrow, I hope to get involved in more projects and learn more about modern applications of PDE theory. I would like to improve my skills in high performance computing and implement more ambitious projects in parallel computing. I would also like to communicate more with other mathematicians as I tend to do most of my work alone. In the next several years, I hope to continue collaboration with undergraduates, graduate students, faculty, and professionals at national labs. I am interested in the numerics of the water wave problem and will investigate computer implementations of the shallow-water equations, the numerics of turbulent flows, and many others.

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