Design of Ray-Helmholtz Hybrid Solver using Numerical Microlocal Analysis and Its Computer Implementation

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Abstract

In this thesis, we present the design, computer implementation and verification of a Ray / Helmholtz hybrid solver for high frequency scattering problems.

The hybrid solver uses direct numerical simulations based on Helmholtz equation in the parts where the scatterer boundary shows a complicated local geometry and geometrical optics (GO) in the parts where the material and geometry is slowly varying. The hybridization reduces the computational cost and complexity at high frequencies. The domain decomposition method (DDM) is used to couple the models through a new numerical tool called "numerical microlocal analysis" (NMLA). A new approach of using NMLA for absorbing boundary conditions (ABC) is also discussed.

The solvers are implemented and validated in MATLAB. In the ABC part, a C++ FEM solver and a MATLAB solver are used together.

Keywords Wave Equation, Helmholtz Equation, Geometrical Optics, Domain Decomposition Methods, Boundary Decomposition Methods, Hybrid Solver
Sammanfattning

Design och datorimplementation av en strålgång/Helmholtz-hybridmetod baserad på numerisk mikrolokal analys

I denna avhandling presenterar vi en hybridmetod för högfrekventa spridningsproblem som kombinerar strålgång med lösning av Helmholtz ekvation. Vi diskuterar metodens design, implementation och validering.

Hybridmetoden använder direkt simulering av Helmholtz ekvation där spridarens geometri är komplicerad och geometrisk optik där material och geometri varierar långsamt. Hybridiseringen reducerar beräkningskostnaden och komplexiteten vid höga frekvenser. Modellerna kopplas ihop med hjälp av en domänuppdelningsmetod baserad på ett nytt numeriskt verktyg kallat ”numerisk mikrolokal analys” (NMLA). Vi diskuterar också hur NMLA kan användas för att implementera absorberande randvillkor (ABC).

Lösarna är implementerade och validerade i MATLAB. För ABC-delen används en FEM-lösare skriven i C++ kopplad till ett MATLAB-program.
# Contents

1 Introduction .............................................. 1
  1.1 Background, Aim and Scope .................................. 1
  1.2 Outline of Thesis ........................................... 2

2 Mathematical Theory ...................................... 3
  2.1 Time Harmonic Solutions of the Wave Equation ............... 3
  2.2 Geometrical Optics (GO) Approximation ...................... 4
  2.3 Numerical Microlocal Analysis (NMLA) of Harmonic Wavefields ........................................... 7
  2.4 Integral Equation Method .................................... 9

3 Numerical Methods ....................................... 13
  3.1 Implementation of NMLA ................................... 13
    3.1.1 Approximation of $\beta$ ray .............................. 13
    3.1.2 Finding $\phi$ from $B$ and $\theta$ .......................... 14
  3.2 Numerical Treatment of Integral Equation (MoM) .............. 14
    3.2.1 First Order Staircase Functions .......................... 15
    3.2.2 Second Order Hat Functions ............................... 16
    3.2.3 Computation of Scattered Field ............................ 16
  3.3 Domain and Boundary Decomposition Methods .................. 17
    3.3.1 Domain Decomposition Methods (DDM) ..................... 17
    3.3.2 Boundary Decomposition Methods (BDM) .................... 20
    3.3.3 Iteration Algorithm of DDM and BDM ...................... 20
  3.4 Construction of Absorbing Boundary Condition (ABC) ........... 22

4 Computer Implementation and Numerical Results ................. 25
  4.1 Introduction to Computer Implementation of Solvers ........... 25
  4.2 Verification of Solvers .................................... 26
    4.2.1 MoM Solver .............................................. 26
    4.2.2 NMLA Solver ............................................. 26
    4.2.3 GO Solver ............................................... 33
  4.3 BDM by MoM and NMLA ...................................... 38
  4.4 New Approach of ABC ...................................... 41

5 Conclusion ................................................. 47

Bibliography .................................................. 48
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Chapter 1

Introduction

1.1 Background, Aim and Scope

The wave equation plays a central role in many branches of science and engineering. It reads

\[ u_{tt} = c(x)^2 \cdot \Delta u, \quad x \in \Omega, \quad \Omega \subset \mathbb{R}^d, \]  

(1.1)

where \( c(x) \) is the local speed of wave propagation of the medium. With some variations, it occurs primarily in three fields: acoustics, elasticity, and electromagnetics. The acoustic wave equation describes the propagation of sound in a medium e.g. the air. The Maxwell equations describe the propagation of electromagnetic waves. The elastic wave equation describes compression and shear waves.

There are a number of direct numerical methods to solve the wave equation, such as finite differences (FD), finite element methods (FEM), integral equation methods, etc. When the essential frequencies in the wave field are relatively high, and thus the wavelengths are short compared to the overall size of the computational domain, direct simulation of the wave equation will be very costly. In direct numerical simulation, the accuracy of the solution is determined by the number of grid points or elements per wavelength. The computational cost of maintaining constant accuracy grows algebraically with frequency, and for sufficiently high frequencies a direct numerical simulation is no longer feasible. Then approximate models for wave propagation must be used. Geometrical optics (GO), is the asymptotic approximation obtained when the frequency tends to infinity. This model is much less costly at high frequencies. The classical derivation of GO can be found e.g. in the book by Whitham (1974) [1].

However, there are still cases where GO is not a sufficient model. For example when the geometry or the medium has a complicated fine scale structure, the asymptotic model GO may not be relevant or become too complex and intractable. Some modified GO approximate models, such as GTD [2], PTD, UTD, have been developed to add more correction terms to the GO method in specific cases. A more straightforward approach is to use direct numerical simulations based on (1.1) or Helmholtz equation in the part of the domain that shows a complicated local geometry while GO is used in other parts where the material and geometry is slowly varying. In these cases, one can use domain decomposition methods (DDM) with hybrid techniques to couple the models.

In DDM for partial differential equations the computational domain is split into several subdomains. The PDE is then solved independently in each subdomain with some simple boundary conditions. The result is communicated between the domains and the boundary conditions are updated accordingly. The PDE is solved again in each subdomain and the method continues...
iteratively until the solutions in the subdomains match at the boundaries. DDM are used in computational wave propagation either to reduce the cost and memory requirement (possibly after parallelization) or more simply to reduce the geometrically induced complexity of a problem.

In this thesis, we will combine the ideas of DDM with the asymptotic model, and use the latter in the subdomains where it is relevant, but use the full detailed model in the complicated subdomains. This could offer a real gain in cost/complexity. This thesis will investigate the use of a new numerical tool called "numerical microlocal analysis", jointly developed at NADA and INRIA (Rocquencourt, France) [3], to construct such a hybrid asymptotic domain decomposition method. The detailed wave model is the Helmholtz equation and the asymptotic model is geometrical optics.

The potential applications behind this thesis lie in computational electromagnetics, acoustics, optics and geophysics. As a concrete example, one can think of the problem shown in Figure 1.1. A small object of complicated geometry is attached on the large platform and thus it is a multi-scale problem. The small scale scattering problem can be the electromagnetic signature analysis for a small antenna. The large scale scattering problem can be the shape optimization of the large platform to achieve a small global electromagnetic signature, e.g. where to install the small antenna on a vehicle. Among other aspects, the numerical simulation of this problem will assist the design of such system to achieve better performance. Our hybrid solver is aiming at this kind of problems.

A new approach of absorbing boundary conditions (ABC) by using "numerical microlocal analysis" is also addressed in this thesis. The basic idea is to translate the numerical solutions into the form of rays. By finding the reflected rays from the boundary and killing them, the out-going rays will be absorbed at the boundary more efficiently. The algorithm is designed and embedded into a Finite Element Solver with ABC developed at INRIA.

The algorithm was implemented and verified in MATLAB. In the ABC part, a C++ FEM solver was used. The project was conducted in the NADA/INRIA "GOES" team (www-rocq.inria.fr/~benamou/goes.html). I thank Dr. Marc Durufle at INRIA for letting me use his FEM code in the ABC part of the project.

1.2 Outline of Thesis

In Chapter 1, we give brief background of the problem. In Chapter 2, the mathematical theories of geometrical optics, integral equations (MoM) and numerical microlocal analysis are formulated, while the corresponding numerical methods are stated in Chapter 3. In Chapter 4, we present a brief introduction to the computer implementation and some numerical results and analysis. General conclusions of the whole paper are given in Chapter 5.
Chapter 2

Mathematical Theory

2.1 Time Harmonic Solutions of the Wave Equation

We start by deriving the equations that are used in this paper. Equation (1.1) is the simplest equation for the discussion of two and three dimensional waves. In order to set up the problem, we must specify the domain in which we want to solve the equation, and give boundary conditions.

A complete set of data is obtained upon prescribing initial values for $u$ and its time derivative $u_t$. Up to a multiplicative constant corresponding to a choice of physical units, we have to solve

$$u_{tt} = c^2 \cdot \Delta u, \quad x \in \Omega, \quad t > 0,$$

$$u(0, x) = u_0(x), \quad x \in \Omega,$$

$$\frac{\partial u}{\partial t}(0, x) = u_1(x), \quad x \in \Omega,$$

$$u(t, x) \big|_{\partial \Omega} = 0, \quad \text{or} \quad \frac{\partial u}{\partial n}(t, x) \big|_{\partial \Omega} = 0,$$

(2.1)

where $\partial \Omega$ is the boundary of the domain $\Omega$.

Instead of the time-dependent wave equation, it is common to look for time harmonic solutions of the equation

$$u(x, t) = v(x) \cdot e^{-i\omega t}$$

(2.2)

where $\omega$ is a fixed frequency and $v$ satisfies the Helmholtz equation. Denoting by $v_d$ the Dirichlet boundary condition and by $v_n$ the Neumann boundary condition, (2.1) becomes

$$\Delta v + \omega^2 \eta^2 v = 0, \quad x \in \Omega, \quad \eta(x) = \frac{c_0}{c(x)},$$

$$v \big|_{\partial \Omega} = v_d, \quad \text{or} \quad \frac{\partial v}{\partial n} \big|_{\partial \Omega} = v_n,$$

(2.3)

where $\eta$ is called the index of refraction, $c(x)$ is the local wave velocity of the medium and $c_0$ is the reference velocity (e.g. the speed of light in vacuum). For simplicity we will henceforth let $c_0 = 1$. In this paper, we will work with Helmholtz equation (2.3). We consider the scattering problem where $\Omega$ is the exterior of a scatterer and $v_d$ is given by an incoming wave.
2.2 Geometrical Optics (GO) Approximation

We assume that \( v \) can be expanded in a so called WKB series,

\[
v = e^{i\omega \phi(x)} \sum_{m=0}^{\infty} A_m(x)(i\omega)^{-m}
\]

\[
= e^{i\omega \phi(x)}(A_0(x) + A_1(x)(i\omega)^{-1} + A_2(x)(i\omega)^{-2} + \cdots).
\]  

(2.4)

When the value of \( \omega \) is large, it is enough to keep the term \( A_0 \) and discard higher order terms. Substituting the series into (2.3), we get

\[
\Delta v + \omega^2 \eta^2 v = \omega^2 e^{i\omega \phi(x)} A_0(x)(- | \nabla \phi(x) |^2 + \eta^2)
\]

\[
+ \omega^1 i e^{i\omega \phi(x)}(\Delta \phi(x) A_0(x) + 2\nabla \phi(x) \cdot \nabla A_0(x))
\]

\[
+ \omega^0(\cdots) + \omega^{-1}(\cdots) + \cdots.
\]

We want the right hand side to be zero and thus equate coefficients of powers 2 and 1 of \( \omega \) to zero. We get the eikonal equation

\[
| \nabla \phi | = \eta,
\]

(2.5)

and the transport equation

\[
2\nabla \phi \cdot \nabla A_0 + \Delta \phi A_0 = 0.
\]

(2.6)

Equation (2.1) has solutions of the type \( u = \hat{A}(x, t)e^{i\omega \phi(x,t)} \) while (2.3) has \( v = A(x)e^{i\omega \phi(x)} \).

With consistent initial and boundary data, by (2.2) we get

\[
\hat{A}(x, t)e^{i\omega \phi(x,t)} = A(x)e^{i\omega \phi(x) - t),
\]

(2.7)

i.e. \( \hat{\phi}(t, x) = \phi(x) - t \). We note that, since the family of curves \( \{ x \mid \hat{\phi}(t, x) = \phi(x) - t = 0 \} \), parameterized by \( t \geq 0 \), describe a propagating wave front in (2.4), we often directly interpret the frequency domain phase \( \phi(x) \) as the travel time of a wave.

Let us introduce the bicharacteristic pair \( (x(t), p(t)) \) related to the Hamiltonian \( H(x, p) = c(x) | p | \), as

\[
\frac{dx}{dt} = \nabla_p H(x, p) = c(x) | p |, \quad x(0) = x_0,
\]

\[
\frac{dp}{dt} = -\nabla_x H(x, p) = - | p | \nabla c(x), \quad p(0) = p_0.
\]

(2.8)

In \( d \) dimensions the bicharacteristics are curves in \( 2d \)-dimensional phase space \( (x, p) \in \mathbb{R}^{2d} \). It follows immediately that \( H \) is constant along them, \( H(x(t), p(t)) = H(x_0, p_0) \). We are interested in solutions for which \( H \equiv 1 \). In this case the projections on physical space, \( x(t) \), are usually called rays, and we can reduce (2.8) to

\[
\frac{dx}{dt} = \frac{1}{\eta^2} p, \quad x(0) = x_0,
\]

\[
\frac{dp}{dt} = \frac{\nabla_p H}{\eta}, \quad p(0) = p_0, \quad | p_0 | = \eta(x_0).
\]

(2.9)
2.2. Geometrical Optics (GO) Approximation

Solving (2.9) is called ray tracing. It should be noted here that if $\eta = \text{const}$ the rays are just straight lines.

The eikonal equation (2.5) can be written as

$$H(x, \nabla \phi(x)) = 1,$$  \hspace{1cm} (2.10)

with $H$ as above. By differentiating (2.10) with respect to $x$, we get

$$\nabla_x H(x, \nabla \phi(x)) + D^2 \phi(x) \nabla_p H(x, \nabla \phi(x)) = 0.$$  \hspace{1cm} (2.11)

Here $D^2$ represents the Hessian. Then for any curve $y(t)$ we have the identity

$$\frac{d}{dt} \nabla \phi(y(t)) = D^2 \phi(y(t)) \frac{dy(t)}{dt}$$

$$- \nabla_x H(y(t), \nabla \phi(y(t))).$$

Taking $x(t)$ to be the curve for which the expression in brackets vanishes, we see that $(x(t), \nabla \phi(x(t)))$ is a bicharacteristic. By the uniqueness of solutions to (2.8), we therefore have that $p(t) \equiv \nabla \phi(x(t))$ if we take $p_0 = \nabla \phi(x_0)$. Hence, with this initialization, the rays are therefore always orthogonal to the level curves of $\phi$, since $|dx/dt|$ is parallel to $p = \nabla \phi$ by (2.9). The difference in phase between two points on the same characteristic signifies the time it takes for a wave to travel between them, i.e.

$$\phi(x(t)) - \phi(x(0)) = t.$$  \hspace{1cm} (2.12)

Assuming we know the phase $\phi(x_0)$ and $\nabla \phi(x_0)$ on a line $A$, we want to calculate the phase $\phi$ at another point $x_1$ on another line $B$ further away as in Figure 2.1.

![Figure 2.1: Computation of phase $\phi$ along the ray](image)

In this thesis, let $\eta \equiv 1$ for simplification such that the rays go along straight lines with the slope equal to $\nabla \phi(x_0)$, i.e. $\nabla \phi(x_0) = (\cos \theta / \sin \theta)$. By (2.12), we get

$$\phi(x_1) = \phi(x_0) + |x_1 - x_0| \quad x_1 = x_0 + |x_1 - x_0| \quad \nabla \phi(x_0).$$  \hspace{1cm} (2.13)

Next, we want to compute the amplitude $A$ at $x_1$ given $A(x_0)$. Note that, once $\phi$ is known, the transport equation (2.6) is a linear equation with variable coefficients. We are to solve this
Chapter 2. Mathematical Theory

equation for the amplitude $A$ along the rays. By the ray tracing formulation of GO in [6], we can directly start from:

$$A(x(t, x_0)) = A(x_0) \frac{\eta(x_0)}{\eta(x(t, x_0))} \sqrt{\frac{q(0, x_0)}{q(t, x_0)}}$$

(2.14)

where $x(t, x_0)$ is the ray at time $t$ starting in the point $x_0$ and $q = \det J$, $J$ is the Jacobian of $x$ respect to initial data, $J = D_{x_0}x(t, x_0)$.

From Figure 2.1, we have

$$x(t, x_0) = x_0 + t\begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} = x_0 + t\begin{pmatrix} \phi_x(x_0) \\ \phi_y(x_0) \end{pmatrix}$$

thus

$$q = \det(D_{x_0}x(t, x_0))$$

$$= \det\begin{pmatrix} 1 + t\phi_{xx} & t\phi_{xy} \\ t\phi_{xy} & 1 + t\phi_{yy} \end{pmatrix}$$

$$= (1 + t\phi_{xx})(1 + t\phi_{yy}) - t^2\phi_{xy}^2.$$

We are to eliminate the terms of $\phi_{xx}$ and $\phi_{xy}$ by using the fact that $\phi$ satisfies the eikonal equation

$$\phi_x^2 + \phi_y^2 = 1.$$

It gives after differentiation by $x$ and $y$,

$$\begin{cases} 
\phi_x \phi_{xx} + \phi_y \phi_{xy} = 0, \\
\phi_x \phi_{xy} + \phi_y \phi_{yy} = 0,
\end{cases}$$

then

$$\phi_x^2 \phi_{xx} - \phi_y^2 \phi_{yy} = 0,$$

$$\phi_{xx} = \frac{\phi_y^2 \phi_{yy}}{1 - \phi_y^2}.$$

And it gives

$$\phi_{xy} \phi_x \phi_{xy} \phi_y = \phi_y \phi_{yy} \phi_x \phi_{xx},$$

then

$$\phi_{xy}^2 = \phi_{xx} \phi_{yy}.$$

Finally, we get

$$q = 1 + t^2\phi_{xx} \phi_{yy} + t(\phi_{xx} + \phi_{yy}) - t^2\phi_{xy}$$

$$= 1 + t(\phi_{xx} + \phi_{yy})$$

$$= 1 + t\frac{\phi_{yy}}{1 - \phi_y^2}.$$
where \( t = |x_1 - x_0| \). This gives \( A(x_1) \) by (2.14). Finally we have solutions at points located at the new point \( x_1 \) as

\[
v(x_1) = A e^{i\omega \phi} = A(x_0) e^{i\omega \phi(x_1)} \sqrt{\frac{1}{1 + |x_1 - x_0|^2 \phi_{yy}(x_0)}},
\]

(2.15)

with \( \phi(x_1) \) given in (2.13). To calculate \( \phi_{yy} \), central differences can be used.

### 2.3 Numerical Microlocal Analysis (NMLA) of Harmonic Wavefields

Given a solution of Helmholtz equation in a neighborhood of a fixed observation point, numerical microlocal analysis determines the number of crossing rays and their directions and complex amplitudes at the observation point. It relies on the intuitive idea that the solution locally behaves as an elementary plane wave when the wavelength is much smaller than the scale of variations in \( \eta \) characterizing the medium.

It is based on the GO approximation

\[
v(x) \simeq A(x) e^{i\omega \phi(x)}.\]

(2.16)

Assume \( A \) and \( \phi \) are smooth functions, a first order Taylor expansion around \( x_0 \) gives the local plane wave approximation

\[
v(x) \simeq B(x_0) e^{i\omega(x-x_0) \cdot \nabla \phi(x_0)}
\]

(2.17)

where we call \( B(x_0) = A(x_0) e^{i\omega \phi(x_0)} \) the complex amplitude.

Numerical microlocal analysis will compute \( B(x_0) \) and \( \nabla \phi(x_0) \) from \( v(x) \) in a neighborhood of the observation point \( x_0 \). In the case of several crossing waves, \( v \) is a sum of terms like in (2.17). Starting with 2D, we assume that there exists some integer \( N \) and some phase functions and complex amplitudes, \( \phi_n(x) \) and \( B_n(x) \), \( n = 1, \ldots, N \), such that

\[
v(x) \simeq \sum_{n=1}^{N} B_n(x) e^{i\omega(x-x_0) \cdot \nabla \phi_n(x_0)},
\]

(2.18)

when \( |x - x_0| \) is small.

We assume that the values of the solution around the point at which we look at are directly available, either in analytic or numerical form. Let \( x_0 \) be a point in space and \( v \) a solution to the Helmholtz equation in the neighborhood of \( x_0 \). We consider the Helmholtz solution for wave number \( \omega \) on a circle of radius \( \frac{\alpha}{\omega \eta(x_0)} \) around the point \( x_0 \) and define

\[
U_\alpha(s) := v(x_0 + \frac{\alpha}{\omega \eta(x_0)} s)
\]

where \( \alpha \) is a constant and \( s \) is unit vector along the circle. We denote by \( d_n(x) \) the direction of propagation of the rays \( \nabla \phi_n(x) = \eta(x) d_n(x) \).

Using the Taylor expansions

\[
\phi_n(x) = \phi_n(x_0) + \nabla \phi_n(x) \cdot (x - x_0) + \cdots
\]

\[
= \phi_n(x_0) + \eta(x_0) d_n(x_0) \cdot (x - x_0) + \cdots
\]

\[
A_n(x) = A_n(x_0) + \cdots
\]
and (2.18), we have
\[ U_\alpha(\hat{s}) \simeq U^{ray}_\alpha(\hat{s}) := \sum_{n=1}^{N} B_n(x_0)e^{i\alpha \hat{s} \cdot \hat{d}_n(x_0)}, \tag{2.19} \]
where \( B_n(x_0) = A_n(x_0)e^{i\omega \phi_n(x_0)} \) is the complex amplitude of ray \( n \) at \( x_0 \).

We introduce the angle notation: \( \theta_n = \theta(\hat{d}_n) \) and \( \theta(\hat{s}) \) such that
\[ \hat{s} = \begin{pmatrix} \cos \theta(\hat{s}) \\ \sin \theta(\hat{s}) \end{pmatrix}, \quad \hat{d}_n = \begin{pmatrix} \cos \theta_n \\ \sin \theta_n \end{pmatrix}. \]
The 2D Jacobi-Anger expansion is
\[ e^{i\alpha \hat{s} \cdot \hat{d}_n} = e^{i\alpha \cos(\theta_n - \theta(\hat{s}))} = \sum_{\ell=-\infty}^{\ell=\infty} i^\ell J_\ell(\alpha)e^{-i\ell(\theta_n - \theta(\hat{s}))}, \]
where \( J_\ell(\alpha) \) is the Bessel function of order \( \ell \). Inserting the Jacobi-Anger expansion into (2.19), we get
\[ U^{ray}_\alpha(\hat{s}) = \sum_{\ell=-\infty}^{\ell=\infty} \left( \sum_{n=1}^{N} B_n(x_0)i^\ell J_\ell(\alpha)e^{-i\ell(\theta_n - \theta(\hat{s}))} \right). \]
We truncate the sum to \( |\ell| \leq L(\alpha) \) where
\[ L(\alpha) = \alpha + C_1 \alpha^\frac{2}{3} + C_2 \log(\alpha + \pi), \tag{2.20} \]
for some suitable constants \( C_1 \) and \( C_2 \).

We let \( F \) be the Fourier transform with inverse \( F^{-1} \) and \( D_\alpha \) be truncation operator
\[ (D_\alpha \gamma)_{\ell} := d^2_\ell \gamma_{\ell}, \quad d^2_\ell = \begin{cases} \frac{2\pi}{2\ell(\alpha) + 1} \frac{1}{i^\ell J_\ell(\alpha)}, & |\ell| \leq L(\alpha), \\ 0, & \text{otherwise}, \end{cases} \tag{2.21} \]
and define
\[ \beta_\alpha(\hat{s}) := F^{-1} D_\alpha FU^{ray}_\alpha. \tag{2.22} \]
Then we obtain
\[ \beta_\alpha(\hat{s}) = \sum_{n=1}^{N} \frac{B_n}{2L(\alpha) + 1} \sum_{\ell=-L(\alpha)}^{\ell=L(\alpha)} e^{-i\ell(\theta_n - \theta(\hat{s}))}. \tag{2.23} \]
By analyzing (2.23), we can show that for a fixed \( \hat{s} \)
\[ \lim_{\alpha \to \infty} \beta_\alpha(\hat{s}) = \begin{cases} B_n, & \hat{s} = \hat{d}_n, \\ 0, & \text{otherwise}. \end{cases} \]
Thus we can expect the above filtering procedure to give as output a function \( \beta_\alpha(\hat{s}) \), defined on the circle or sphere in 3D, which has sharp peaks in the directions of propagation of the rays when \( \alpha \) is large enough.
2.4 Integral Equation Method

In this section, we show how to rewrite Helmholtz equation (2.3) as an integral equation. This formulation will later be used when we solve Helmholtz in the domain where GO is not suitable. We consider the problem in Figure 2.2, where an incoming wave \( v^{\text{inc}} \) is scattered off an object. Outside the object the material is constant, \( \eta = 1 \). The total field can be written as \( v = v^{\text{inc}} + v^{\text{sc}} \) where \( v^{\text{sc}} \) is the scattered field. The \( v^{\text{inc}} \) naturally satisfies

\[
\Delta v^{\text{inc}} + \omega^2 v^{\text{inc}} = 0, \quad x \in \Omega.
\] (2.24)

To solve (2.3), with zero Dirichlet condition, \( v_d = 0 \), we therefore only need to solve

\[
\Delta v^{\text{sc}} + \omega^2 v^{\text{sc}} = 0, \quad x \in \Omega,
\]

\[
v^{\text{sc}} = -v^{\text{inc}}, \quad x \in \partial \Omega.
\] (2.25)

Henceforth, we drop the superscript ‘sc’.

\[\text{Figure 2.2: Computational domain}\]

The following integral expression is called a single layer potential

\[
v(x) = \int_{\partial \Omega} G(x, y) \sigma(y) ds(y),
\] (2.26)

while the following integral expression is called a double layer potential

\[
v(x) = \int_{\partial \Omega} \frac{\partial G(x, y)}{\partial n_y} \gamma(y) ds(y),
\] (2.27)

where \( x, y \in \mathbb{R}^2 \), and \( G(x, y) \) is the Green’s function satisfying

\[
\Delta G + \omega^2 G = -\delta(x - y),
\] (2.28)

with \( \delta \) the Dirac delta-function. For exterior wave problems in 2D, \( G \) must be the zeroth order Hankel function of the first kind, i.e.

\[
G(x, y) = \frac{1}{4i} H_0^{(1)}(\omega | x - y |).
\]
The potentials in (2.26) and (2.27) satisfy the Helmholtz equation in $\Omega$ and the outgoing radiation condition at infinity. The single layer potential is continuous with respect to the variable $x$ when crossing the boundary $\partial \Omega$ where its value is

$$v(x) = \int_{\partial \Omega} G(x, y)\sigma(y)ds(y), \quad x \in \partial \Omega. \tag{2.29}$$

Its normal derivatives have discontinuities when crossing $\partial \Omega$. Their limit values on both sides of $\partial \Omega$ are

$$\frac{\partial v}{\partial n}\big|_{\text{int}}(x) = \frac{\sigma(x)}{2} + \int_{\partial \Omega} \frac{\partial G(x, y)}{\partial n_x}\sigma(y)ds(y),$$

$$\frac{\partial v}{\partial n}\big|_{\text{ext}}(x) = -\frac{\sigma(x)}{2} + \int_{\partial \Omega} \frac{\partial G(x, y)}{\partial n_x}\sigma(y)ds(y). \tag{2.30}$$

The double layer potential has a discontinuity when crossing $\partial \Omega$. The corresponding limit values on both sides of $\partial \Omega$ are

$$v_{\text{int}}(x) = -\frac{\gamma(x)}{2} + \int_{\partial \Omega} \frac{\partial G(x, y)}{\partial n_y}\gamma(y)ds(y),$$

$$v_{\text{ext}}(x) = \frac{\gamma(x)}{2} + \int_{\partial \Omega} \frac{\partial G(x, y)}{\partial n_y}\gamma(y)ds(y). \tag{2.31}$$

Its normal derivative is continuous when crossing $\partial \Omega$.

$$\frac{\partial v}{\partial n} = \int_{\partial \Omega} \frac{\partial^2 G(x, y)}{\partial n_x \partial n_y}\gamma(y)ds(y), \quad x \in \partial \Omega. \tag{2.32}$$

Any solution to Helmholtz equation can be expressed as a combination of single and double layer potentials:

$$v(x) = \int_{\partial \Omega} G(x, y)\sigma(y)ds(y) - \frac{\partial G(x, y)}{\partial n_y}\gamma(y)ds(y).$$

When such expression satisfies the corresponding boundary conditions, it solves the exterior Dirichlet (or Neumann) problems. Consider now the integral evaluated for points $e$ and $i$ just outside and inside $\partial \Omega$. By (2.29) to (2.32), we can show that the jumps in function value $v$ and $\partial v/\partial n$ are

$$v_e - v_i = \gamma,$$

$$\frac{\partial v_e}{\partial n} - \frac{\partial v_i}{\partial n} = \sigma.$$

Define the scattered field to be continuous across $\partial \Omega$. This is possible whenever the interior Helmholtz problem with Dirichlet condition has a unique solution. This holds when $-\omega^2$ is not an eigenvalue of the Laplace operator inside $\partial \Omega$. Thus we have $\gamma = 0$ and the final integral equation becomes

$$-v^{\text{inc}}(x) = \int_{\partial \Omega} G(x, y)\sigma(y)ds(y), \quad x \in \partial \Omega, \tag{2.33}$$

where $v^{\text{inc}}(x)$ is the incoming wave. Similarly we can formulate the integral equation for Neumann BC. In this thesis we choose to work with Dirichlet BC.

The problem in (2.33) is a Fredholm integral equation of the first kind for $\sigma$ with kernel $G$. First kind equations with smooth kernels are often ill-posed in the sense that short wavelength
perturbations to $\sigma(y)$ are smoothed by the integration. The converse of this statement is that short wavelength components of the left hand side are strongly magnified. Such problems have to be regularized by filtering out short wavelength noise. However, our kernel $G$ is weakly singular and $\sigma(y)$ contributes strongly to $v^{inc}(x)$. The problem of determining $\sigma(y)$ from $v^{inc}(x)$ is reasonably well conditioned. There remains to discretize the integral equation to produce a finite linear system of equations. It is described in Chapter 3.
Chapter 3

Numerical Methods

3.1 Implementation of NMLA

In our numerical algorithm of NMLA, we firstly compute a numerical approximation of $\beta_{\alpha}^{\text{ray}}(\hat{s})$ on a uniform discretization of the unit circle, possibly including a Tichonov regularization procedure which can get rid of the small values of the Bessel functions in (2.21). Secondly, we analyze the numerical results $\beta_{\alpha}^{\text{ray}}(\hat{s})$ to find a preliminary set of ray directions and amplitudes. Finally, we post-process the results via a nonlinear optimization procedure to get more accurate results.

3.1.1 Approximation of $\beta_{\alpha}^{\text{ray}}$

Introduce a uniform grid $\theta_m$ with $M = 2L(\alpha) + 1$ points on the unit circle,

$$\theta_m = m \Delta \theta, \quad \Delta \theta = \frac{2\pi}{M}, \quad m = 0, \ldots, M - 1.$$ 

Then let $U_m$ be the grid function that samples the given solution at the grid points. By (2.22) in Section 2, we get

$$\{\beta_m\} \simeq 2\pi \text{FFT}^{-1} \left\{ \frac{\text{FFT}(U_m)}{(2L(\alpha) + 1)J_\ell(\alpha)} \right\}. \quad (3.1)$$

Note that $L(\alpha)$ in (2.20) only relies on the constants $C_1, C_2$ and $\alpha$. So the number of unknowns and evaluations of the solution are independent of $\omega$. Therefore also the cost of NMLA is independent of $\omega$.

If the truncation $M$ is too large the exponential decay of Bessel function $J_\ell(\alpha)$ can lead to very small coefficients that impair the precision of the formula. In addition, we can not guarantee that Bessel functions $J_\ell(\alpha)$ are not zero for all $\ell$ values. A simple solution is to use a Tichonov type regularization. Let $\hat{U}_\ell$ be the Fourier transform of $U_m$. We propose the regularized version of (3.1),

$$\beta_m^{\epsilon} = 2\pi \text{FFT}^{-1} \left\{ \frac{\hat{U}_\ell(2L(\alpha) + 1)J_\ell(\alpha)}{i\ell(2L(\alpha) + 1)^2J_\ell(\alpha)^2 + 4\epsilon \pi^2)} \right\}, \quad (3.2)$$

where $\epsilon$ is a small constant. This expression remains bounded even where $J_\ell(\alpha)$ is zero or close to zero.
The precision of our method is limited by the size of the observation circle around \( x_0 \) and this may be a severe restriction. So we use a post-processing procedure where the data obtained from the spectral inversion is used as initial data for a routine that tries to fit the expansion directly to the sampled solution values. This is done by nonlinear minimization of the residual. The standard Gauss-Newton minimization algorithm is used. For a more detailed description, see [3].

### 3.1.2 Finding \( \phi \) from \( B \) and \( \theta \)

We often want to calculate the amplitude \( A \), phase \( \phi \) and ray direction \( \nabla \phi \) along a curve. By NMLA, we can only calculate the angle \( \theta \) and complex amplitude \( B \) of rays. The amplitude is easily obtained from

\[
A = |B|, \tag{3.3}
\]

and the gradient by

\[
\nabla \phi = \begin{pmatrix} \phi_x \\ \phi_y \end{pmatrix} = \eta(x_0) \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix}.
\]

However, finding \( \phi \) is more difficult. Since it is multiplied by \( \omega \) in (2.16), it is also important to compute it with an accuracy of at least \( O(1/\omega^2) \). Suppose we want to find \( \phi \) on a line in sample points \( x_n = n \Delta x \). Given

\[
B(x_n) = A(x_n) e^{i \omega \phi(x_n)}, \tag{3.4}
\]

then the phase \( \phi(x_n) \) is only determined up to \( 2\pi/\omega \) increments:

\[
\frac{1}{\omega} \arg B(x_n) = \phi(x_n) + \ell \frac{2\pi}{\omega} + O\left(\frac{1}{\omega^2}\right), \quad \ell \in \mathbb{Z}. \tag{3.5}
\]

The error term comes from the fact that \( B(x_n) \) is accurate up to order \( O(1/\omega) \).

Suppose that we already have computed \( \phi(x_{n-1}) \), \( \nabla \phi(x_{n-1}) \) and \( \nabla \phi(x_n) \). We can then extrapolate from previous points by Taylor expansion:

\[
\phi(x_{n-1}) + \frac{1}{2} \Delta x [\phi_x(x_{n-1}) + \phi_x(x_n)] = \phi(x_n) + O(\Delta x^3 + \frac{\Delta x}{\omega}), \tag{3.6}
\]

since \( \nabla \phi(x_{n-1}) \) and \( \nabla \phi(x_n) \) have accuracy \( O(1/\omega) \). If \( \Delta x \ll \omega^{-\frac{1}{2}} \) this estimate of \( \phi(x_n) \) is enough to find right \( \ell \) in (3.5):

\[
\ell = \arg \min_{\ell} \frac{1}{\omega} \arg B(x_n) + \ell \frac{2\pi}{\omega} - \phi(x_{n-1}) - \frac{1}{2} \Delta x [\phi_x(x_{n-1}) + \phi_x(x_n)] . \tag{3.7}
\]

Higher order extrapolation gives \( \Delta x \ll \omega^{-\frac{1}{2}} \). By using the right \( \ell \) in (3.5) we get \( \phi(x_n) \) with accuracy \( O(1/\omega^2) \).

### 3.2 Numerical Treatment of Integral Equation (MoM)

In this section we show how to solve the integral equation (2.33) numerically. We will use the collocation method which proceeds by approximating \( \sigma(y) \) by a linear combination of a number of selected basis functions,

\[
\sigma(y) = \sum_{n=1}^{N} \sigma_n f_n(y). \tag{3.8}
\]
Selecting a number of field points \( y_k \) just on \( \partial \Omega \) \( k = 1, \ldots, M \) and requiring that the equation be satisfied exactly at these points we obtain:

\[
b_k = -v^{inc}(y_k) = \sum_{n=1}^{N} \sigma_n \int_{\partial \Omega} f_n(y) G(y - y_k) dy,
\]

or

\[
A_{s} = b, \quad A = \{a_{kn}\}, \quad s = \{\sigma_n\}, \quad b = \{b_k\}, \quad a_{kn} = \int_{\partial \Omega} f_n(y) G(y - y_k) dy,
\]

where \( M \) is usually chosen equal to \( N \) but may also be taken greater than \( N \) to provide some over-determination in ill-conditioned cases. In this thesis, we use the discretization of \( M = N \).

### 3.2.1 First Order Staircase Functions

The simplest basis functions are constructed by replacing the curve \( \partial \Omega \) by a polygon with vertices \( y'_k \), and edges \( \Delta y_k = y'_{k+1} - y'_k \). We take \( f_k = 1 \) over edge \( k \) and 0 elsewhere. The square pulse basis functions give a staircase representation of \( \sigma(y) \). The points \( y_k \) are usually chosen as the midpoints of the edges:

\[
y_k = \frac{y'_{k+1} + y'_k}{2}.
\]

The integrals in (3.10) are evaluated exactly, if possible, or by numerical quadrature. The simplest scheme is to use a one point rule for all integrals except for \( k = n \), the self-contribution of element \( k \), which becomes the diagonal element of the coefficient matrix \( A \). There is a logarithmic singularity in this integral and we choose to use the first few terms in the Taylor expansion of \( G \) around \( y_k \). For small value \( z \) we have:

\[
H_0^2(z) = J_0(z) - iY_0(z) \\
\simeq 1 - i \frac{2}{\pi} \ln \left( \frac{1}{2} z \right) + \gamma + O(z^2 \ln z), \quad \gamma = 0.557215664 \cdots,
\]

\[
G(z) = \frac{1}{4i} H_0^2(z) \simeq \frac{1}{4i} - \frac{1}{2\pi} (\gamma - \ln 2) - \frac{1}{2\pi} \ln z.
\]
By exact integration of the first terms and let \( h_k = |\Delta y_k| \), \( \delta = \frac{1}{4\pi} - \frac{1}{4\pi}(\gamma - \ln 2) \), we get
\[
a_{kk} \simeq \delta h_k - \frac{1}{\pi}\left(\frac{h_k}{2}\ln\frac{h_k}{2} - \frac{h_k}{2}\right).
\] (3.12)

### 3.2.2 Second Order Hat Functions

![Figure 3.2: Hat functions](image)

We replace the curve \( \partial \Omega \) by a polygon with vertices \( y_k \), and edges \( \Delta y_k = y_{k+1} - y_k \). As Figure 3.2, we take basis functions to be hat functions \( f_k = 1 \) at \( y_k \) and 0 at \( y_{k+1} \) and \( y_{k-1} \), i.e.
\[
f_k(y) = \begin{cases} 
  y - y_{k-1}, & y \in [y_{k-1}, y_k], \\
  y_{k+1} - y, & y \in [y_k, y_{k+1}], \\
  y_{k+1} - y, & y \in [y_{k+1}, y_k].
\end{cases}
\]

Again, there is singularity at the diagonal elements of the coefficient matrix \( A \). By exact integration with an approximated \( G \), we have
\[
a_{kk} \simeq \frac{1}{8}(\delta + \frac{1}{16\pi})(h_k^2 + h_{k+1}^2) - \frac{1}{16}(h_k^2 \ln\frac{h_k}{2} + h_{k+1}^2 \ln\frac{h_{k+1}}{2})
\] (3.13)

### 3.2.3 Computation of Scattered Field

Using the fact that \( \gamma = 0 \) in our case, the scattered field can be written as
\[
v(x) = \int_{\partial \Omega} G(x - y)\sigma(y)ds(y).
\] (3.14)

The potential source \( \sigma \) is approximated by (3.8), then we have
\[
v(x) = \sum_{k=1}^{N} \sigma_k \int_{\partial \Omega} f_k(y)G(x - y)ds(y).
\] (3.15)

In case of staircase functions, the integral term in (3.15) can be approximated by one point rule as \( G(\omega | x - y_k |)h_k \). The final formula becomes
\[
v(x) = \sum_{k=1}^{N} \sigma_k G(\omega | x - y_k |)h_k.
\] (3.16)
3.3 Domain and Boundary Decomposition Methods

The idea of domain decomposition methods (DDM) is to split the domain into smaller sub-domains and solve a sequence of similar sub-problems on these sub-domains. The numerical methods applied in each sub-domains can be the same or different from each other. The boundary conditions are adjusted iteratively.

As a test case, we will divide the domain into two sub-domains. Domain $\Omega_1$ contains the smaller object possibly with a complicated geometry of the boundary, such as an antenna, and domain $\Omega_2$ contains much bigger and smooth object, such as an aircraft. More sub-domains can be treated similarly. For simplicity, we start with two sub-domains in this thesis.

Even though the geometry of boundary $\partial \Omega_1$ could be very complicated, the computational cost by direct numerical simulation is affordable since the object is assumed to be small. In $\Omega_1$, we will therefore solve Helmholtz equation by an integral equation methods, e.g. MoM. In $\Omega_2$, the object is rather big and thus direct numerical simulation is not feasible. We will use the asymptotic method, geometrical optics there. On the boundary $\Gamma$ between $\Omega_1$ and $\Omega_2$, the numerical tool NMLA will be used to communicate information.

Basically, there are two approaches for this case: DDM and BDM.

3.3.1 Domain Decomposition Methods (DDM)

One approach to DDM was proposed by Jean-David Benamou and Bruno Despres (1997) [4]. We denote $v_1$ and $v_2$ the solutions of $v$ in $\Omega_1$ and $\Omega_2$ respectively. On the crossing boundary $\Gamma$, they impose the mixed (or "Robin") boundary condition

$$\frac{\partial}{\partial n_1} v_1 + i\omega v_1 |_{\Gamma} = -\frac{\partial}{\partial n_2} v_2 + i\omega v_2 |_{\Gamma}.$$  (3.17)
Chapter 3. Numerical Methods

We solve the sub-problem in $\Omega_1$ with zero impedance boundary conditions on boundary $\Gamma$ as the first step to get $v_1$. Then we solve the sub-problem in $\Omega_2$ with (3.17) as boundary condition on boundary $\Gamma$ to get $v_2$. Then we iterate till convergence. It can be formally described as

\[
\Delta v_1^0 + \omega^2 v_1^0 = 0 \quad \text{in} \quad \Omega_1, \tag{3.18}
\]
\[
\frac{\partial}{\partial n_1} v_1^0 + i\omega v_1^0 = 0 \quad \text{on} \quad \Gamma,
\]

and for $n > 0$,

\[
\Delta v_i^{n+1} + \omega^2 v_i^{n+1} = 0 \quad \text{in} \quad \Omega_i, \quad i = 1, 2, \tag{3.19}
\]
\[
\frac{\partial}{\partial n_i} v_i^{n+1} + i\omega v_i^{n+1} = -\frac{\partial}{\partial n_{3-i}} v_{3-i}^n + i\omega v_{3-i}^n \quad \text{on} \quad \Gamma.
\]

Figure 3.4: The incoming and reflected waves

The boundary condition (3.17) in fact implies that:

\[
\frac{\partial}{\partial n_1} W + i\omega W |_{\Gamma} = 0, \tag{3.20}
\]

where $W = v_1 - v_2$. Consider the waves in a small circle as in Figure 3.4. Assume the incoming wave is $W^{\text{in}} = \alpha e^{i\omega r \cdot \theta_0} e^{i\omega r \cdot \theta}$ and the reflected wave is $W^{\text{ref}} = \beta e^{i\omega r \cdot \theta'}. \theta'$ is the angle $\theta' = \pi - \theta$ and $W = W^{\text{in}} + W^{\text{ref}}$. We want $W$ to satisfy (3.20). Thus we get

\[
\left(\frac{\partial}{\partial n_1} + i\omega\right) W
\]
\[
= \left(\frac{\partial}{\partial n_1} + i\omega\right) \left(\alpha e^{i\omega r \cdot \theta_0} e^{i\omega r \cdot \theta} \right) + \beta e^{i\omega r \cdot \theta'}
\]
\[
= \left(\frac{\partial}{\partial n_1} + i\omega\right) \left(\alpha e^{i\omega(-x \cos \theta - y \sin \theta)} e^{i\omega(x \cos \theta' + y \sin \theta')} \right) + \beta e^{i\omega r \cdot \theta'}
\]
\[
= \left(\frac{\partial}{\partial n_1} + i\omega\right) \left(\alpha e^{i\omega(-x \cos \theta - y \sin \theta)} \right) + \beta e^{i\omega(-x \cos \theta + y \sin \theta)}
\]
\[
= \{n_1 \text{ and } y \text{ are in the same direction}\}
\]
\[
= \alpha i\omega(1 - \sin \theta) e^{i\omega(-x \cos \theta - y \sin \theta)} + \beta i\omega(1 + \sin \theta) e^{i\omega(-x \cos \theta + y \sin \theta)}.
\]
3.3. Domain and Boundary Decomposition Methods

When \( r \to 0 \), i.e. \( r \) is on \( \Gamma \), \( x \to 0, y \to 0 \), we get

\[
\alpha i \omega (1 - \sin \theta) + \beta i \omega (1 + \sin \theta) = 0,
\]

\[
\alpha = -\frac{1 + \sin \theta}{1 - \sin \theta} \beta.
\]

Discretize the small circle on \( \Gamma \) into \( M \) equal intervals as in Figure 3.5. Considering \( W = v_1 - v_2 \)

\[
W = \sum_{k=1}^{M} B_{1,k} e^{i \omega \cdot \vec{s} \cdot \vec{\theta}_k} - \sum_{k=1}^{M} B_{2,k} e^{i \omega \cdot \vec{s} \cdot \vec{\theta}'_k} = \sum_{k=1}^{M} B_{k} e^{i \omega \cdot \vec{s} \cdot \vec{\theta}_k}, \tag{3.21}
\]

where \( B_k = B_{1,k} - B_{2,k} \), \( B_{1,k} \) and \( B_{2,k} \) are the complex amplitudes corresponding to the solutions \( v_1 \) and \( v_2 \), \( \vec{s} \theta_k \) is the unit vector on the direction \( \theta_k \).

In the iteration (3.19), the values \( v_{k-1}^3 \) are known, i.e. \( B_{3-k,k} \) are known. Only \( B_{i,k} \) are the unknowns. To solve them, we need \( M \) equations. Take the \( M/2 \) direction pairs \( \theta_k \) and \( \theta'_k = -\theta_k \) as in Figure 3.5. By (3.21), we get

\[
B_k = -\frac{1 + \sin \theta_k}{1 - \sin \theta_k} B_{k'}, \tag{3.22}
\]

where \( B_k, B_{k'} \) are defined in (3.21) corresponding to the directions of \( \theta_k \) and \( \theta'_k \). Since \( k = 1, \cdots, M/2, \) we get \( M/2 \) equations for \( B_{i,k} \). There are \( M/2 \) more equations needed to solve the system.

As a simple case, we can assume that there is no object in \( \Omega_2 \) and thus there will be no rays coming back to \( \Omega_1 \). Then \( B_{1,k} \) corresponding to the left going rays will be zeros and we get \( M/2 \) more equations. The system is then closed and can be solved. In other cases, we need to solve the GO equations in \( \Omega_i \) to get the incoming rays in terms of the outgoing. This gives an additional \( M/2 \) equations which close the system.
3.3.2 Boundary Decomposition Methods (BDM)

The second approach is BDM proposed and analysed by e.g. Mikhael Balabane [5]. It gives the scattered wave as a sum of contributions, each due to a part of the boundary of the scatterer. The algorithm is proved to converge with geometric speed to the solution. It was used in industrial software such as Aeospatiale-EADS for aircrafts and satellites (code ECHO) [5].

We state more precisely the computational problems we are to solve. In contrast to the case of DDM, we use the following notation: let the scatterer \( K = K_1 \cup K_2 \subset \mathbb{R}^2 \) be a compact set, a union of two non-intersecting compact sets. Let \( \Omega = K^c \) be the complementary set of \( K \) in \( \mathbb{R}^2 \) and \( \Omega_i = K_i^c \) so that \( \Omega = \Omega_1 \cap \Omega_2 \). See Figure 3.6.

\[
\begin{align*}
\Delta v_i + \omega^2 v_i &= 0 \quad \text{in} \quad \Omega_i, \quad i = 1, 2, \\
v_i \mid \partial \Omega_i &= v^{inc} \mid \partial \Omega_i - \sum_{i' \neq i} v_{i'} \mid \partial \Omega_i.
\end{align*}
\]

(3.23)

One can compute \( v_i \) by \( v_i = \sum_{n=0}^{\infty} v^n_i \) where \( v^n_i \) solves the following sequence of Helmholtz equations in \( \Omega_i \):

\[
\begin{align*}
\Delta v^0_i + \omega^2 v^0_i &= 0 \quad \text{in} \quad \Omega_i, \quad i = 1, 2, \\
v^0_i \mid \partial \Omega_i &= v^{inc} \mid \partial \Omega_i.
\end{align*}
\]

(3.24)

and, for \( n \neq 0 \),

\[
\begin{align*}
\Delta v^n_i + \omega^2 v^n_i &= 0 \quad \text{in} \quad \Omega_i, \quad i = 1, 2, \\
v^n_i \mid \partial \Omega_i &= -\sum_{i' \neq i} v^{n-1}_{i'} \mid \partial \Omega_i.
\end{align*}
\]

(3.25)

3.3.3 Iteration Algorithm of DDM and BDM

To show the iteration algorithm, we divide the work into several steps as in Figure 3.7 where one can see how the problem in \( \Omega_2 \) is solved with NMLA.
1. Compute the scattering problem for $\Omega_1$.
2. Use NMLA to calculate the rays on the crossing boundary.
3. Propagate these rays into $\Omega_2$. By the GO method, we solve the sub-problem in $\Omega_2$ and get the rays reflected from $\partial \Omega_2$ on the crossing boundary $\Gamma$.
4. Update the boundary conditions for the $\Omega_1$.

Note that the grid points on $\Gamma$ only need to resolve the phase and amplitude, not the wavelength. Step 2 and step 3 are the same for DDM and BDM methods. However, there are differences in step 1 and step 4. The differences between DDM and BDM are the following:

- DDM uses Robin conditions on $\Gamma$ and Dirichlet conditions on $\partial \Omega_1$. BDM only uses Dirichlet conditions on $\partial \Omega_1$.
- In DDM, only boundary conditions on $\Gamma$ is updated by using (3.19). In BDM, boundary conditions on $\partial \Omega_1$ is updated by propagating rays from $\Gamma$ onto $\partial \Omega_1$.

The steps 1-4 are iterated till convergence. The convergence of both approaches have been proven in [4] and [5] in the ideal scattering where the subproblems are solved exactly. The approach of DDM requires a solver with Robin boundary condition on $\Gamma$. In this paper, we will follow the approach of BDM which is simpler to implement.
3.4 Construction of Absorbing Boundary Condition (ABC)

In this thesis, we propose a new approach of ABC by using NMLA. We translate the Helmholtz solutions at the outer boundary into rays. The artificially reflected rays at the outer boundary can then be found. By forcing these reflected rays to be zero, "killing" them, the outgoing rays are absorbed by the boundary more efficiently. We embedded this algorithm into a FEM solver developed by Dr. Marc Durufle at INRIA. The result is compared with the original ABC approach of FEM solver.

The FEM solver solves the system (3.26) in 2D or 3D. In the case of 2D, the computational domain is shown in Figure 3.8.

\[-\omega^2 \rho v - \text{div}(\mu \nabla v) = f \quad \text{in} \quad \Omega,
\]
\[v = 0, \quad \text{or} \quad \frac{\partial v}{\partial n} = 0 \quad \text{on} \quad \partial \Omega_1,
\]
\[\frac{\partial v}{\partial n} + i\omega v = 0 \quad \text{on} \quad \partial \Omega_2.\]

By taking \(\rho = 1, \mu = 1, f = 0\), it solves Helmholtz equation (2.3) with ABC on \(\partial \Omega_2\). To deal with the ABC, the FEM solver uses the following iteration algorithm:

1. Solve the Helmholtz equation with zero Robin condition on \(\partial \Omega_2\):

\[\Delta v^0 + \omega^2 v^0 = 0 \quad \text{in} \quad \Omega,
\]
\[\frac{\partial}{\partial n} v^0 + i\omega v^0 = 0 \quad \text{on} \quad \partial \Omega_2,
\]
\[v^0 = -v^{\text{inc}} \quad \text{on} \quad \partial \Omega_1.
\]

2. Calculate the potential \(v^0_{\text{pot}}\) and its derivative \(\frac{\partial}{\partial n} v^0_{\text{pot}}\) on \(\partial \Omega_2\) by (3.27). The integral is taken along a curve \(\Gamma\) which can be taken as \(\partial \Omega_1\) or any closed curve between \(\partial \Omega_1\) and \(\partial \Omega_2\).

\[v^0_{\text{pot}} \mid \partial \Omega_2 = \int_{\Gamma} \frac{\partial G}{\partial n} v^0 + \frac{\partial v^0}{\partial n} G ds. \] (3.27)
3. Solve the Helmholtz equation with boundary values on $\partial \Omega_2$ updated using $v_{pot}^0$:

$$\Delta v^1 + \omega^2 v^1 = 0 \text{ in } \Omega,$$

$$\frac{\partial}{\partial n} v^1 + i\omega v^1 = \frac{\partial}{\partial n} v_{pot}^0 + i\omega v_{pot}^0 \text{ on } \partial \Omega_2,$$

$$v^1 = -v^{inc} \text{ on } \partial \Omega_1.$$  

Then iterate: Solve the Helmholtz equation

$$\Delta v^{n+1} + \omega^2 v^{n+1} = 0 \text{ in } \Omega,$$

$$\frac{\partial}{\partial n} v^{n+1} + i\omega v^{n+1} = \frac{\partial}{\partial n} v_{pot}^n + i\omega v_{pot}^n \text{ on } \partial \Omega_2,$$

$$v^{n+1} = -v^{inc} \text{ on } \partial \Omega_1,$$

where

$$v_{pot}^n | \partial \Omega_2 = \int_\Gamma \frac{\partial G}{\partial n} v^n + \frac{\partial v^n}{\partial n} G ds. \quad (3.28)$$

To embed our ABC algorithm into the FEM solver, we replace the value of $v^n$, $\partial v^n/\partial n$ on $\Gamma$ by $v_{ABC}^n$, $\partial v_{ABC}^n/\partial n$ in (3.28), i.e.

$$v_{pot}^n | \partial \Omega_2 = \int_\Gamma \frac{\partial G}{\partial n} v_{ABC}^n + \frac{\partial v_{ABC}^n}{\partial n} G ds, \quad (3.29)$$

where $v_{ABC}^n$, $\partial v_{ABC}^n/\partial n$ are calculated on $\Gamma$ by our algorithm of “killing” reflected rays described below:

1. From NMLA, we compute the rays interpretation of $v^n$ on the small circle around the point $x_0$ on $\Gamma$ as

$$v^n(x_0 + \frac{\alpha}{\omega} \hat{s}) \simeq \sum B_k e^{i\alpha \hat{s} \cdot \hat{d}_k}. \quad (3.30)$$

2. We set

$$v_{ABC}^n(x_0 + \frac{\alpha}{\omega} \hat{n}) = \sum_{\hat{d}_k \cdot \hat{n} > 0} B_k e^{i\alpha \hat{s} \cdot \hat{d}_k}, \quad (3.31)$$

where $\hat{n}$ is the outward normal of $\Gamma$. 

Chapter 4

Computer Implementation and Numerical Results

In this chapter, we first explain the computer implementation of the solvers in brief. Then we show the test results of the MoM solver, the NMLA solver and the GO solver respectively. The test cases are designed such that the algorithms can be verified by comparing numerical results with exact results, or studying the convergence rate. After having verified these solvers separately, we show numerical result of hybrid solver by BDM, NMLA and MoM. The numerical results of the ABC part are also given and discussed.

4.1 Introduction to Computer Implementation of Solvers

Based on the numerical algorithms formulated in Chapter 2 and Chapter 3, the computer programs of MoM, NMLA and GO solvers were implemented in MATLAB. The hybrid solver of BDM, NMLA and MoM was also written in MATLAB. During the test of solvers, we found that the MATLAB program is not very efficient and the scale of the problem can not be large. For efficiency, these solvers should be translated into C++ and be parallelized in later work. The BDM algorithm is naturally suitable for parallelization and thus the computational cost of hybrid solver can be reduced dramatically.

In the ABC part, we used the FEM solver of Dr. Marc Durufle at INRIA, France. The program was written in C++ under Linux. To run the solver, the mathematics packages MUMPS, METIS, SELDON and a mesh generator APNO2MESH need to be installed. To embed our ABC algorithm into the FEM solver, we made some changes to the FEM program. To perform NMLA on $\Gamma$ in Figure 3.8, the solutions on small circles around points on $\Gamma$ are needed. We thus modified the original FEM solver to output these values into a data file. The MATLAB NMLA solver reads solutions from the data file. After performing NMLA and having killed the reflected rays, the updated potentials are written into another data file. The C++ FEM program will read these new potentials and use them in the next iteration. Note that the iteration procedure is now designed to be controled manually for the sake of convenience. After the FEM program outputs the data, it will wait till our ABC algorithm finishes and returns a signal from the keyboard. The iteration procedure can be designed to be automatic by calling a script file in the C++ FEM program to run the MATLAB program. Preferably, all the programs should be implemented in C++ to avoid such problems.
4.2 Verification of Solvers

4.2.1 MoM Solver

As the first test case, we take the scatterer as a unit circle. The frequency \( \omega = 2\pi \). The incident wave is taken as a plane wave from the left hand side. The scatterer is discretized by 10 points/wavelength. The staircase base functions are used. Figure 4.1(a) shows the real part of the scattered field. Figure 4.1(b) shows the real part of total field.

![Figure 4.1: Scattered and total field by a unit circle](image)

The exact solution of this test case is

\[
v^{sc}(r, \phi) = \sum_{m=-\infty}^{+\infty} i^m J_m(\omega R)e^{im\phi} H_2^m(\omega r),
\]

where \( r, \phi \) are cylinder coordinates, and \( R \) is the radius of the scatterer.

In our MoM solver, the staircase functions are expected to provide first order convergence while the hat functions provide second order. We can study the convergence rates of them by analyzing the errors at various grid point densities. We take the sample points on the line where \( y = -3 \) and \( x \in [-3, 3] \). The number of grid points on the scatterer is taken as 40, 80, 160 and 320. The results are shown in Figure 4.2 to Figure 4.6. From Figure 4.3, we can see that the order of convergence using staircase functions approaches 1. From Figure 4.6, we can see that the order of convergence using hat functions approaches 2. They agree with our expectation.

4.2.2 NMLA Solver

As the test case of the NMLA solver, we take the scatterer to be a thin plate, see Figure 4.7. For high frequencies, the diffracted wave is given by geometrical theory of diffraction (GTD). The amplitude of each diffracted ray is proportional to the amplitude of the inducing ray and a diffraction coefficient \( D \). The coefficient \( D \) depends on the directions of the inducing and diffracted rays, on the frequency and on the local boundary geometry and the index of refraction. In a two-dimensional homogeneous medium, the diffraction coefficient \( D \) of a half plane is

\[
D(\theta_d, \theta_{inc}, \omega) = \frac{e^{i\pi/4}}{2\sqrt{2\pi} \cos \frac{\theta_d - \theta_{inc}}{2}} \pm \frac{1}{\cos \frac{\theta_d + \theta_{inc}}{2}},
\]

The exact solution of this test case is

\[
v^{sc}(r, \phi) = \sum_{m=-\infty}^{+\infty} i^m J_m(\omega R)e^{im\phi} H_2^m(\omega r),
\]
4.2. Verification of Solvers

Figure 4.2: Convergence of solutions using staircase functions

Figure 4.3: Convergence of the errors using staircase functions
Figure 4.4: Convergence of the solutions using hat functions

Figure 4.5: Magnified part of the solutions using hat functions
4.2. Verification of Solvers

Figure 4.6: Convergence of errors using hat functions

with the definition of the angles as in Figure 4.7. The expression for the diffracted wave is then

\[ v_d = \frac{v_{inc}}{\sqrt{r}} D(\theta_d, \theta_{inc}, \omega) e^{i\omega r}, \]  

(4.3)

where \( r \) is the distance to the tip of the halfplane.

Figure 4.7: Diffracted rays

To solve the field by MoM, we take the size of the scatterer as rectangle of width 20 wavelengths and height 1 wavelength and the frequency \( \omega = 20\pi \). The scatterer is discretized by 10 points/wavelength. Let the incident wave be a plane wave hitting the rectangle from the right, i.e. \( \theta_{inc} = \pi \). The staircase basis functions are used. By NMLA, we calculate the rays interpretation at sample points that are uniformly distributed on the line \((x = 5, y \in [-5, 5])\)
as in Figure 4.9. Figures 4.10 to 4.13 compare the incoming and diffracted rays of NMLA and exact solutions at sample points.

![Scattered field](image)

**Figure 4.8: Scattered field**

![Rays solution at sample points by NMLA](image)

**Figure 4.9: Rays solution at sample points by NMLA**

From Figure 4.11 and Figure 4.10, we see that the incoming rays by NMLA match the exact solution quite well. Figure 4.12 and Figure 4.13 show that the angles of the diffracted rays obtained by NMLA have little error while the amplitudes have bigger error. The exact amplitudes are calculated from the MoM solution. The exact angles are the angles of the vectors connecting sampling points and the right corner of the scatterer.
4.2. Verification of Solvers

Figure 4.10: Amplitudes of incoming rays by NMLA and exact solutions

Figure 4.11: Angles of incoming rays by NMLA and exact solutions
Figure 4.12: Amplitudes of diffracted rays by NMLA and exact solutions

Figure 4.13: Angles of diffracted rays by NMLA and exact solutions
GTD is a high frequency approximation and thus it works more correctly for higher frequencies. To check this, we calculate the diffraction coefficients of increasing frequencies and compare them with the NMLA solution. From Figure 4.14, we can see that the GTD and NMLA solutions agree better when the frequency is higher. It matches our expectation.

Figure 4.14: Diffraction coefficients of increasing frequencies

4.2.3 GO Solver

To check our GO solver, we calculate the case in Figure 4.15. Assuming we know the solution at the line $A$, we calculate the solution at the line $B$ by a GO solver. The method of propagating the rays from the line $A$ to the line $B$ by GO is described in Section 3.
As the first step, we compute the scattered field by MoM. We then compute the ray representation of the solution on the line $A$ by NMLA. The scattered field is shown in Figure 4.16. The ray representation on the line $A$ is shown in Figure 4.17 to Figure 4.19.

As the second step, we find the phase $\phi$ from $B$ as described in Section 3.1.2. Figure 4.20 shows the calculated $\phi$ on sample points on the line $A$. We compare the real part of the NMLA solution and the exact solution computed by MoM at the line $A$ in Figure 4.21.
4.2. Verification of Solvers

Figure 4.18: Amplitude of the solution by NMLA

Figure 4.19: Angle of the solution by NMLA
Figure 4.20: Phase of the solution

Figure 4.21: NMLA solution and exact solution
As the third step, we calculate the solution on the line $B$ by the GO solver. We compare the solution on the line $B$ by GO with that of directly using NMLA at the line $B$. Note that there is no analytical expression for the scattered field for this case. The results are compared in Figure 4.22 and 4.23. We then use the MoM solver to directly compute the numerical solution at the line $B$ to serve as exact solution. We compare the GO solution and exact solution at the line $B$ in Figure 4.24.

Figure 4.22: Amplitudes of GO and NMLA solutions

Figure 4.23: Phases of GO and NMLA solutions
4.3 BDM by MoM and NMLA

For the first test case, we assume the big object is in fact the entire right halfplane. This can be seen as an approximation of the case when the big object is rather close to the small one. Thus we can simplify the domain like in Figure 4.25.

By the MoM solver and the NMLA solver, we can calculate the ray solution on the boundary $\Gamma$. We need to reflect the rays back to the object $\partial \Omega_1$ by the GO solver. It is shown in Figure 4.26. Since the boundary condition is set to $v = 0$ on $\partial \Omega_2$, the reflected rays from $\Omega_2$ which incident on $\partial \Omega_1$ can be calculated by mirroring $\partial \Omega_1$ in $\Gamma$, introducing a mirrored scatterer with boundary $\partial \Omega_1'$, see Figure 4.27. Because the phase changes on $\partial \Omega_2$ when the rays are reflected, we reverse the sign of incoming waves at the mirrored object. In fact we do not even need to use the GO solver for this problem. We can directly do NMLA on $\partial \Omega_1'$. 

Figure 4.24: Real part of GO and exact solutions

Figure 4.25: Test case of DDM
4.3. BDM by MoM and NMLA

Figure 4.26: Reflection of the rays

Figure 4.27: Simplification by mirroring object
By the mirrored object, we calculate the reflected rays on $\partial \Omega_1$ from the boundary $\Gamma$. We take the frequency $\omega = 40$ and the number of grid points $p = 300$ on $\partial \Omega_1$. The NMLA solution on $\partial \Omega'_1$ mirrored on $\partial \Omega_1$ is shown in Figure 4.28. The error between the real parts of the ray solution and the MoM solution is shown in Figure 4.29.

![Figure 4.28: Reflected rays after one iteration](image)

![Figure 4.29: Error between GO and MoM solution](image)

To guarantee the accuracy of the MoM solution, we usually discretize the scatterer by no less than 5 points per wavelength. When the frequency is high, the number of grid points becomes large. In a direct BDM iteration, one would compute the field in each grid point on $\partial \Omega'_1$ using (2.26). Since $p \sim \omega$, this would cost $O(\omega^2)$ flops. However the amplitudes and angles
of the NMLA solution on the boundary usually vary smoothly. To save computational cost, we take a coarse grid on the boundary $\partial \Omega_1$ and calculate angles and amplitudes by polynomial interpolation. Since this grid size can be taken independent of $\omega$, the cost is reduced to $O(\omega)$.

There is a special treatment for angles since there might be $2\pi$ jumps in their values. The angle values can therefore be discontinuous. Before we interpolate the angles, we process all angle values by the algorithm described below:

Assume we have angle values $\theta_1, \cdots, \theta_M$. We let $\theta_1^{\text{proc}} = \theta_1$ and for $k > 1$ we set

$$\theta_k^{\text{proc}} = \theta_k + 2\pi \ell, \quad \ell = \text{argmin}_{\ell \in \mathbb{Z}} [\theta_k - \theta_{k-1}^{\text{proc}} + 2\pi \ell]. \quad (4.4)$$

Then iterate with next angle $\theta_{k+1}$. By this processing, the $2\pi$ jumps in the angle values are eliminated. A example is shown in Figure 4.30.

![Figure 4.30: Pre-processing of $\theta$](image)

We have now finished the first iteration. The boundary condition on $\partial \Omega_1$ will be modified by adding the reflected ray solution. We then compute the solutions in $\Omega_1$ by MoM with updated boundary conditions on $\partial \Omega_1$. Then we iterate till convergence as described in Section 3.3.3. The potentials on $\partial \Omega_1$ are shown in Figure 4.31 after iteration 1, 2, 3, 4. We can see that the potentials converge very quickly. Already after one iteration, they have approached the exact solution closely. Since we do not have the analytical solution for this case, the exact solution is calculated by MoM as in Figure 4.27 using two scatterers illuminated by an incoming field with different signs.

### 4.4 New Approach of ABC

We consider the problem in Figure 4.33. The computational domain $\Omega$ is bounded by $\partial \Omega_1$ and $\partial \Omega_2$. On the boundary $\partial \Omega_1$, we apply Dirichlet boundary condition. On the boundary $\partial \Omega_2$, we apply the absorbing boundary condition. $\Gamma$ is the internal boundary for the integral representation of values on $\partial \Omega_2$. The incident wave is coming from the left side. The frequency is $\omega = 100$. The size of scatterer is taken as 24 wavelength. To perform NMLA on $\Gamma$, we let the FEM solver output the solutions on the small circles in Figure 4.33.
At the first step, where $\frac{\partial v}{\partial n} + i\omega v = 0$ on $\Gamma$, the solution is shown in Figure 4.34.

By NMLA, we get the rays interpretation on the internal boundary $\Gamma$ as in Figure 4.35 and Figure 4.36. Figure 4.37 shows the error between NMLA results and original FEM solution on $\Gamma$. From Figure 4.36, we can clearly see the reflected rays in the top right corner. They are reflected by the outer boundary $\partial \Omega_2$. In fact, We chose the special shape of scatterer and boundaries as in Figure 4.33 in order to highlight the artificial reflections from $\partial \Omega_2$ that an ABC will have.

To improve the ABC, we kill those reflected rays in the top right corner of Figure 4.36. The potentials on the internal boundary $\Gamma$ will be modified accordingly, i.e. the values of the reflected rays are subtracted. We then use the integral representation to calculate the values on the outer boundary $\partial \Omega_2$ again. This concludes the first iteration.
4.4. New Approach of ABC

Figure 4.33: Computational domain

Figure 4.34: Scattered field at the first step
Chapter 4. Computer Implementation and Numerical Results

Figure 4.35: The first ray at the first step

Figure 4.36: The second ray at the first step
We then use the FEM solver to compute the field with the updated boundary values. The field of the second iteration is shown in Figure 4.38. By NMLA, we again calculate the rays interpretation on the internal boundary $\Gamma$. The scattered rays are shown in Figure 4.39. There are very few reflected rays in the up right corner. They are not presented in the figure.

We use the converged solution as the exact solution. We calculate the Euclidian norm of the error after the second iteration. Our algorithm gives 0.65. Without killing reflected rays, the
norm of the error is 0.62. They are rather close. Although our algorithm converge rather quickly, it does not converge faster than the current FEM solver from Marc Durufle. The algorithm of the integral representation in the current FEM solver described in Section 3.4 can kill the reflection as well. Thus our algorithm does not show an advantage when comparing with it. When our algorithm is used in another situation, it might present faster convergence rate, however.
Chapter 5

Conclusion

In this thesis, we constructed a Ray/Helmholtz hybrid solver by DDM/BDM. In the domain where the object has a complicated geometry, an integral equation solver is used. Even when the frequency is quite high, the computational cost is affordable since the domain is small. In the domain with a big object, we use a GO solver instead. On the common boundary, we use the NMLA tool to communicate data. By different processing algorithms on this common boundary, we can realize DDM or BDM. For both cases, systematic algorithms are formulated. Considering that BDM is simpler to implement, we chose BDM to test our algorithms and gave numerical results. The numerical results showed that our algorithms converge to the exact solutions very rapidly. The complexity of the problem is also reduced. The numerical solvers are written in MATLAB. The hybrid solver is naturally suitable to be parallelized. The computational cost can be decreased dramatically after translation into C++ and parallelization.

A new approach of ABC was also tested. By NMLA, we translated the Helmholtz solutions into ray representation. The reflected rays are killed directly. Thus the outgoing rays are being absorbed very efficiently. This algorithm was tested numerically. In this part, we used a combination of MATLAB and C++ programs communicating via data files. The results showed fast convergence. However, it is not faster than the original approach in the FEM solver since the integral representation in the FEM solver can kill reflections as well. At present, we use an adhoc way to find the reflected rays from apriori knowledge of the rays distribution. There are some work left to make it work with more general cases.
Bibliography


