Reliable $hp$ finite element computations of scattering resonances in nano optics

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Tũũ atũjalaaka anasũ wakuaipa sutuma otta tũ atũjaakat antitsũ anaa wamũin wapushuwa’aya.

Shiasa tũũ jolotsũka sũnakaka waya maalia, sũntitka talataa wamũin.
La sabiduría nos da bienestar en la vida y el conocimiento nos trae progreso.

Wisdom leads us to well-being in life and knowledge brings us progress.

La estrella de la mañana nos iluminó al amanecer, y nos trajo alegría en la vida.

The morning star shined upon us at sunrise, and it filled our lives with joy.

Proverbs shared among the Wayúu, an indigenous tribe dwelling deep in La Guajira desert. Their communities gather around the northernmost tip of South America, washed by the Caribbean sea. The people of the sun, sand and wind, currently have to resist the unethical growth of the modern world in order to keep their traditions alive.

Translation from Wayuunaiki by Jose Cirilo Pushaina.
Figure 1: Scattered profile and resonances corresponding to a dielectric dimer with a thick coating of gold in TE polarization.
Abstract

Eigenfrequencies are commonly studied in wave propagation problems, as they are important in the analysis of closed cavities such as a microwave oven. For open systems, energy leaks into infinity and therefore scattering resonances are used instead of eigenfrequencies. An interesting application where resonances take an important place is in whispering gallery mode resonators.

The objective of the thesis is the reliable and accurate approximation of scattering resonances using high order finite element methods. The discussion focuses on the electromagnetic scattering resonances in metal-dielectric nano-structures using a Drude-Lorentz model for the description of the material properties. A scattering resonance pair satisfies a reduced wave equation and an outgoing wave condition. In this thesis, the outgoing wave condition is replaced by a Dirichlet-to-Neumann map, or a Perfectly Matched Layer. For electromagnetic waves and for acoustic waves, the reduced wave equation is discretized with finite elements. As a result, the scattering resonance problem is transformed into a nonlinear eigenvalue problem.

In addition to the correct approximation of the true resonances, a large number of numerical solutions that are unrelated to the physical problem are also computed in the solution process. A new method based on a volume integral equation is developed to remove these false solutions.

The main results of the thesis are a novel method for removing false solutions of the physical problem, efficient solutions of non-linear eigenvalue problems, and a new a-priori based refinement strategy for high order finite element methods. The overall material in the thesis translates into a reliable and accurate method to compute scattering resonances in physics and engineering.
Sammanfattning

Egenfrekvenser är viktiga vid analys av vågpropagering i slutna kaviteter, såsom exempelvis elektromagnetiska vågor i en mikrovågsugn. För öppna system läcker energi till oändligheten och därför används spridningsresonanser istället för egenfrekvenser. En intressant tillämpning där spridningsresonanser spelar en avgörande roll är i så kallade viskgallerier, där en svag viskning tydligt kan uppfattas från ett längre avstånd.


Med denna metod fås förutom bra approximationer till de sanna resonanserna även ett stort antal numeriska lösningar som inte är relaterade till det fysikaliska problemet. För att ta bort dessa falska lösningar utvecklas i avhandlingen en ny metod baserad på en volymsintegralkvation.

Huvudresultaten i avhandlingen är en ny metod för att ta bort falska lösningar, en ny effektiv metod att lösa icke-linjära egenvärdesproblem och en ny a-priori-baserad förfiningsstrategi för finita elementmetoder. Sammanfattningsvis ger avhandlingen ett tillförlitligt tillvägagångssätt att beräkna spridningsresonanser inom fysik och teknik med hög precision.
Resumen

En problemas de propagación de ondas, el concepto de las frecuencias propias es comúnmente estudiado debido a su importancia en el análisis de cavidades cerradas como lo son los hornos de microondas. Adicionalmente, para sistemas no acotados la energía se pierde por radiación al infinito y por ende las resonancias de dispersión se usan en vez de las frecuencias propias. Una aplicación interesante donde el concepto de resonancias es aplicado, es en los resonadores de modo de galería susurrante.

El propósito de la tesis es establecer una modelación confiable y precisa para realizar la aproximación de las resonancias de dispersión usando métodos de elementos finitos de orden superior. La discusión se centra en las resonancias de dispersión electromagnéticas en estructuras dieléctricas o metálicas nanométricas, usando el modelo de Drude-Lorentz para la descripción de las propiedades ópticas de los materiales. A su vez es de observar que un par de resonancia satisface una ecuación de onda reducida y una condición de onda saliente. En la tesis se reemplaza la condición de onda saliente por condiciones tipo Dirichlet-to-Neumann, o por capas perfectamente acopladas. Para ondas electromagnéticas y ondas acústicas, la ecuación de onda reducida es discretizada mediante el uso de elementos finitos, y el problema de resonancias resulta en un problema de valores propios no lineal.

Adicional a la correcta aproximación de resonancias naturales, un gran número de soluciones numéricas ilegítimas, sin relación con el problema físico, son obtenidas computacionalmente. Para la eliminación de éstas soluciones espurias, se ha desarrollado un nuevo método basado en la formulación de la ecuación integral de volumen. De ahí, que los resultados principales de la tesis deriven en un método novedoso para la eliminación de soluciones espurias al problema físico, métodos eficientes para la resolución de problemas de valores propios no lineales y en una nueva estrategia de refinamiento a-priori para métodos de elementos finitos de orden superior.

En general, el material de la tesis se traduce en un método preciso y confiable para el tratamiento computacional de resonancias de dispersión con aplicación a la física e ingeniería.
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1 Introduction

The history of the concept electromagnetic wave propagation has been very fruitful in the development of Physics and Engineering. One of the greatest technological leaps ever experienced took place after the grounds for propagation of electromagnetic waves were established by James Clerk Maxwell in his *Treatise on Electricity and Magnetism* in 1873. His contribution to the field was rapidly applied by Heinrich Hertz and Guglielmo Marconi and many others only few years later than Maxwell’s equations were postulated. Since then, society has heavily benefited from each new application in the field. The invention of radio transmitters opened the door for communications at higher frequencies, and this in turn to a myriad of discoveries and applications that we observe, and benefit from, on a daily basis. Examples range from convenient mobile phone communication, fast Internet access through optical fibers, tomography image reconstruction for surgical precision and reliability, accurate optical sensors, among many others.

Particularly, we model wave propagation through Partial Differential Equations, which carry important information that can be used in order to make reliable predictions in science and engineering. The information of complex physical phenomena can be decoded by finding solutions to these equations. Despite the fact that we understand the general theory of wave propagation to satisfactory levels, when it comes to practical applications, our human limitations force us to rely on computers to do the calculation for us. Ultimately, it becomes more evident with the increasing complexity of modern problems, that the combination of understanding a physical problem and being able to perform concrete computations, is what seems to be pushing forward the boundaries of scientific knowledge.

1.1 Resonances and dissipation of energy

A simplified model example where we model the propagation of waves is a tensioned guitar string. By plucking the string, waves of amplitude propagate and reflect to and fro from the end points where the string is fixed. If a harmonic forcing device is attached to the string, by fine-tuning the forcing frequency we can observe oscillations of the wire that experience maximum amplitudes for certain frequencies. The forcing frequencies that excite maximum peaks of amplitude are referred to as natural frequencies or eigenfrequencies. In this simple one-dimensional example, the natural frequencies are introduced due to confinement in the system, which in a tensioned string is due to fixing its ends to the guitar. A simple model for the problem corresponds to the so-called wave equation that we introduce in Section 2.1. In the mathematical model, fixing the end points of the string is equivalent to imposing homogeneous Dirichlet boundary conditions. These type of idealized problems are know in the literature as *closed cavities*. The the real eigenfrequencies $\omega_j$ and eigenmodes $u_j$ are obtained by simple methods for Sturm-Liouville problems [15,19,34].
The description of the waves on a string, initially at rest, is given as the superposition

\[ w(x,t) = \sum_j \alpha_j u_j(x)e^{-i\omega_j t}, \]

for some coefficients \( \alpha_j \). When no forcing is applied to a real guitar-string system, the amplitude of oscillation is observed to decay with time. This fact indicates that there exists losses, and energy is leaking out of the system slowly with time.

Damping of waves can be introduced to our model by allowing frequencies \( \omega_j \) to be complex valued and having negative imaginary parts. In such case, the amplitude \( w(x,t) \) from (1) decays exponentially with time resembling the observed physical phenomena. We say then that the guitar-string system is open, and waves can propagate to infinity. These new complex frequencies of the system are denoted resonances, and quasi-stationary modes are referred to as resonant modes or quasi-modes \([42]\). In higher dimensions, a closed cavity can be represented by a hard cylindrical structure as illustrated in Figure 2. Then, waves propagating inside the cylinder experience multiple reflections with the walls of the structure. For waves confined in the \((x,y)\)-plane the corresponding eigenfrequencies \( \omega_j \), are given by the roots of the Bessel function of first kind \([15, 19]\), which we plot by using circles in Figure 3. The black curves correspond to amplitudes of the waves when the system is forced with plane wave of frequency \( \omega \). Similarly as described for the string, we observe peaks of amplitude when \( |\omega - \omega_j| \) becomes small.

If waves are now allow to penetrate the walls of the cylinder, we obtain the scattering amplitudes as the red curve shown in the top panel of Figure 3. The corresponding complex resonances are given as the red bullets in the lower panel, which represents a section of the complex plane.
1.2 Scattering resonances of a dielectric resonator

A similar experiment is performed for the scattering of plane waves of frequency $\omega_s$ by a soft cylinder as depicted in Figure 2. The resulting scattering amplitudes follow the curve plotted in the top panel of Figure 4. The lower panel shows the scattering resonances of the problem, where the correspondence of scattering amplitudes and resonances is evident. In the red stars, we mark two resonances and show their scattering fields in Figure 5, which correspond to wave frequencies left) $\omega_s = \text{Re}\{\omega_j\} - h$, middle) $\omega_s = \text{Re}\{\omega_j\}$, and right) $\omega_s = \text{Re}\{\omega_j\} + h$ for a small value $h = 0.05$. The resulting scattering fields appear to be confined to the interface of the cylinder, and resemble the so-called Whispering-gallery-modes (WGM).

In Figure 6 we plot some of the resonance modes computed with a Perfectly Matched Layer for the infinite cylinder scatterer. Particularly, modes corresponding to exterior resonances show an exponential growth away from the resonator. Additionally, modes corresponding to interior resonances show confined waves that live in the interface of the resonator. Particular examples of interior resonances feature the well known WGM.

Figure 3: Top) Maximum wave amplitude vs. frequency of a closed cavity (black), and dielectric cavity (red). Bottom) Spectral window showing Dirichlet eigenvalues (∘) and resonances (○) for the same example excited by a planar wave.
Figure 4: Top) Scattered amplitudes $|u^s|$ corresponding to the scattering of the incident plane wave $u^i = e^{i\omega_s x}$ with frequency $\omega_s$, over a dielectric cylinder of infinite length. Bottom) Spectral window for the corresponding resonances.
Figure 5: Scattered field $(\text{Re} \, u^s)$ for $\omega_s - h, \omega_s, \omega_s + h$, small $h$ and $\omega_s \approx \text{Re}\{\omega_m\}$ for the resonances: top) $\omega_m = 4.807 - 0.019i$, and bottom) $\omega_m = 7.1089 - 0.0018i$. The scattering field becomes confined around the resonator for frequencies $\omega_s$ closer to shape resonances $\omega$.

Figure 6: Top) Exterior resonances: 5.01-0.26i, 5.87-0.24i, 8.19-0.26i and 9.82-0.27i. Bottom) Interior resonances: 4.80-0.019i, 6.542-0.0034i, 9.61-0.023i and 10.79-0.107i.
2 Wave problems

A wave equation models the propagation in space of a disturbance in some physical medium at equilibrium. Typical examples are the variation of density by sudden air compression (clapping) to which we refer as acoustic waves [14,19]. Another example of relevant importance in the thesis are electromagnetic waves. Then waves describe the propagation of a disturbance in the electric and magnetic fields which may have been emitted by a charge distribution undergoing acceleration at some earlier time $t_0$ [14,20].

2.1 The wave equation

The mathematical modeling of waves consists on assigning to each point $x \in \mathbb{R}^d$ in a $d$-dimensional space a value of a physical quality $\tilde{w}(x,t)$ (density, pressure) at time $t$, which is assumed real. For simplicity we work with complex quantities, for example $w(x,t)$, but we recover the physical quantity of interest by setting $\tilde{w}(x,t) := \text{Re}\{w(x,t)\}$.

The wave equation for $w(x,t)$ is formally introduced as

$$\frac{1}{c^2} \frac{\partial^2 w}{\partial t^2} - \Delta w = F,$$

for $x \in \Omega \subset \mathbb{R}^d$, $t \in (0,\infty)$,

(2)

where the term $F$ is denoted a source. In addition to the partial differential equation (2), it is necessary to specify initial conditions $w(x,0), \partial_t w(x,0)$ for $x \in \Omega$ at time $t = 0$. In the case where the domain $\Omega$ is compact, one needs to specify suitable boundary conditions at the boundary $\Gamma$, for example $w(x,t) = 0$, for $x \in \Gamma$, $t \in (0,\infty)$. In some cases, it is convenient to specify the behavior of waves at infinity. A typical example is the assumption that there are no sources at infinity, from where solutions to (2) are required to be outgoing.

One often encounters problems where the source has the harmonic time dependence $F(x,t) := f(x)e^{-i\omega t}$, for a fixed frequency $\omega \in \mathbb{R}$. Then it makes sense to look for harmonic solutions of the form $w(x,t) := u(x)e^{-i\omega t}$, from where the problem (2) transforms into

$$-\Delta u - \omega^2 n^2 u = f, \ x \in \Omega,$$

(3)

where similarly as for (2), the system is closed by specifying $u(x)$ for $x \in \Gamma$ as the boundaries of a compact domain, or by specifying the behavior of $u$ at infinity. In (3) we introduced the refractive index $n := 1/c$, which may depend on $\omega$. Equation (3) is known as the Helmholtz equation and governs the wave propagation phenomena in frequency domain. This problem has been widely studied in the literature, and is in the heart of the thesis.

In a more general setting, $F$ may be represented by several harmonic components. The linearity of the differential operator in (2) acting on $w$, allow us to find solutions
of problem (2) as a superposition of individual contributions. This is, we write
\[ w(x, t) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x, \omega) e^{-i\omega t} d\omega, \]
and we say that \( u(x, \omega) \) and \( f(x, \omega) \) are Fourier components at frequency \( \omega \) of \( w(x, t) \) and \( F(x, t) \) respectively.

### 2.2 Maxwell’s equations in matter

For the discussion of propagation of electromagnetic waves, we assume non-magnetic materials with constant permeability \( \mu_0 \), and introduce the macroscopic Maxwell equations

\[
\nabla \cdot \mathbf{D} = \rho_{\text{free}}, \quad \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0, \tag{5a}
\]
\[
\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{H} = \mathbf{J}, \tag{5b}
\]

for the macroscopic electric \( \mathbf{E} \) and magnetic \( \mathbf{H} \) fields, displacement \( \mathbf{D} \), and magnetic induction \( \mathbf{B} \) fields. The sources are the free charge \( \rho_{\text{free}} \), and current \( \mathbf{J} \) densities. If we consider a fixed frequency \( \omega \), then it is a standard practice to consider time harmonic fields \( \mathbf{E}(x, t) = \mathbf{E}(x, \omega)e^{-i\omega t} \), and similarly for all the other fields \( \mathbf{D}, \mathbf{H}, \mathbf{B} \), and sources.

In the time harmonic setting, Maxwell equations (5) acquire the form

\[
\nabla \cdot \mathbf{D} = \rho, \quad \nabla \times \mathbf{E} - i\omega \mathbf{B} = 0, \tag{6a}
\]
\[
\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{H} + i\omega \mathbf{D} = \mathbf{J}. \tag{6b}
\]

We assume materials that are locally homogeneous and isotropic, and use the following constitutive relations and Ohm’s law

\[
\mathbf{D} = \varepsilon(x, \omega)\mathbf{E}, \quad \mathbf{B} = \mu_0 \mathbf{H}, \quad \text{and} \quad \mathbf{J} := \sigma(x, \omega)\mathbf{E}, \tag{7}
\]

where the conductivity \( \sigma \) and permittivity \( \varepsilon \) are allowed to be functions of space and frequency. From Maxwell’s equations (6b) and (6d), and relations (7) we can obtain decoupled wave equations for the fields \( \mathbf{E}, \mathbf{H} \). This is done by introducing the relative complex permittivity \( \varepsilon \), and by taking the curl of (6b) and (6d) and combining the outcome. The result are the so-called master equations

\[
\nabla \times \nabla \times \mathbf{E} - \left( \frac{\omega}{c} \right)^2 \varepsilon \mathbf{E} = 0, \tag{8a}
\]
\[
\nabla \times \left( \frac{1}{\varepsilon} \nabla \times \mathbf{H} \right) - \left( \frac{\omega}{c} \right)^2 \mathbf{H} = 0, \tag{8b}
\]
where the complex relative permittivity $\epsilon$, discussed below, accounts for the description of the dielectric and metals in the optical regime [32]. In a more general setting and using the linearity of Maxwell’s equations, the fields can be obtained in time domain as the superposition of solutions in frequency domain

$$
\mathbf{E}(x,t) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathbf{E}(x,\omega)e^{-i\omega t} d\omega,
$$
$$
\mathbf{E}(x,t) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathbf{E}(x,\omega)e^{i\omega t} dt,
$$

and similarly for the $\mathbf{H}$ fields.

2.2.1 Infinite length along the $z$-axis

Now we consider a dielectric cylinder with infinite length along the $z$-axis as shown in Figure 2. In the case that $\epsilon = \epsilon(x, y, \omega)$ is independent of $z$, the particular symmetry of the problem suggests the following explicit separation of variables

$$
\mathbf{E} := \mathbf{E}(x, y)e^{ik_3 z} \quad \text{and} \quad \mathbf{H} := \mathbf{H}(x, y)e^{ik_3 z}.
$$

If the propagation of waves is restricted to the $x$-$y$ plane, then $k_3 = 0$ and no propagation takes place along $z$, from where electromagnetic fields become independent from the $z$ coordinate. In such conditions, the master equations (8) are posed as equivalent 2D scalar problems by choosing appropriate polarizations [8].

**Transverse Magnetic (TM) polarized waves:** In the case where the fields have the explicit form $(0, 0, E_3)^T$, $(H_1, H_2, 0)^T$, then from (8a) and (10) we obtain the equivalent problem

$$
- \Delta E_3 - \left( \frac{\omega}{c} \right)^2 \epsilon E_3 = 0, \quad x \in \mathbb{R}^2.
$$

**Transverse Electric (TE) polarized waves:** Similarly, for fields with the explicit form $(E_1, E_2, 0)^T$, $(0, 0, H_3)^T$, from (8b) and (10) we obtain the equivalent problem

$$
- \nabla \cdot \left( \frac{1}{\epsilon} \nabla H_z \right) - \left( \frac{\omega}{c} \right)^2 H_3 = 0, \quad x \in \mathbb{R}^2.
$$

By using the suggested cylindrical symmetry, the three dimensional vector problems in (8) are reduced to the equivalent two dimensional scalar problems (11), and (12). Once the transverse component in (11), or (12) is found, equations (6b) and (6d) allow us to recover the solution for the $\mathbf{E}$ and $\mathbf{H}$ fields.

Sometimes, for convenience of the presentation, the square of the refractive index $n^2 := \epsilon(x, \omega)$ is used instead of the relative permittivity function.
2.3 Compact notation and definitions

After proper scaling of the problems (11) and (12), we use for convenience in the exposition, the following compact notation

\[ -\nabla \cdot (\rho \nabla u) - \omega^2 \eta u = 0, \tag{13} \]

where \( u := E_3, \rho := 1, \eta := \epsilon \) for the TM-case and \( u := H_3, \rho := 1/\epsilon, \eta := 1 \) for the TE-case.

In most of the thesis the following conventions are used. Some of the definitions in this section are illustrated in Figure 8. First, we refer to the physical domain \( \Omega_a := B(0, a) \), as the open ball of radius \( a \) with boundary \( \Gamma_a \), and write its complement as \( \Omega_a^+ := \mathbb{R}^d \setminus \Omega_a \). For given positive values \( \epsilon_{\text{min}}, \epsilon_{\text{max}} \), the relative permittivity \( \epsilon \) is assumed to satisfy \( 0 < \epsilon_{\text{min}} \leq |\epsilon(x)| \leq \epsilon_{\text{max}} \), for all \( x \in \Omega_a \). The relative permittivity and refractive index are set to attain the constant values \( \epsilon_{\infty}, n_0 \) for \( x \in \Omega_a^+ \), respectively. The region \( \Omega_r := \text{supp} (\epsilon - \epsilon_{\infty}) \) is then a compact set that we use to define the so-called resonators, and the air region in \( \Omega_a \) is defined as \( \Omega_0 := \mathbb{R}^d \setminus \Omega_r \).

Finally, in the case when \( \Omega_r \) can be separated into disjoint resonators, they are labeled as \( \Omega_m \in \Omega_r \), by using the index \( m = 1, 2, \ldots, N_r \). Then, by using the characteristic function \( \chi_{\Omega_m} \) corresponding to \( \Omega_m \), we write the region occupied by all the resonators as \( \Omega_r := \bigcup_{m=1}^{N_r} \Omega_m \).

2.3.1 Electromagnetic material properties

In electromagnetics, the material properties of metals are characterized by the complex relative permittivity function \( \epsilon \), which changes rapidly at optical frequencies \( \omega \)
The most common accurate material model is the Drude-Lorentz model

\[ \epsilon_{metal}(\omega) := \epsilon_{\infty} + \sum_{j=0}^{N_p} \frac{f_j \omega_p^2}{\omega_j^2 - \omega^2 - i\omega\gamma_j}, \tag{14} \]

where \( \epsilon_{\infty} \geq 1 \) and \( f_j, \omega_p, \omega_j, \gamma_j \) are non-negative [8]. Figure 7 illustrates the resulting \( \epsilon_{metal} \) from employing model (14), and using parameters corresponding to Silver [22]. Then, the permittivity function for material properties that are piecewise constant in \( \Omega \), can be written in the form

\[ \epsilon(x, \omega) := \sum_{m=0}^{N_r} \epsilon_m(\omega) \chi_{\Omega_m}(x), \quad x \in \Omega, \quad \omega \in \mathcal{D}, \tag{15} \]

where the dependencies on \( \omega \in \mathbb{C} \) in \( \epsilon_m \) for \( m = 0, 1, \ldots, N_r \), are of Drude-Lorentz type (14). In addition, graded material properties are also considered in the thesis, meaning that \( \epsilon \) can also be a continuous function for \( x \in \Omega \).
3 The exterior Helmholtz problem

In this section problems involving wave propagation in free space (unbounded domains) are described. The main assumption is that there are no sources outside $\Omega_a$, and that no waves are reflected from infinity. In this setting, the problems from Section 2 require an outgoing wave condition, that is described below in short.

Most of the numerical methods for the discretization of partial differential equations are designed for dealing with bounded domains. Then, it becomes necessary to truncate the domain for the use of the finite element method introduced in Section 4. Among several methods, two popular methods are used in this thesis for resonance computations. The Perfectly Matched Layer (PML) [5, 24], and the Dirichlet-to-Neumann maps (DtN) [6], which are both used in the thesis. However, for simplicity of the exposition we present only the DtN in this introductory chapter.

3.1 Scattering of monochromatic planar waves

Let $u$ denote a solution of the Helmholtz problem (3) and split the total wave as $u = u^i + u^s$. The incoming wave is assumed as the planar wave $u^i = e^{im_0 \omega x}$, which satisfies $-\Delta u^i - \omega^2 n_0^2 u^i = 0$. The total wave $u$ in TM polarization satisfies

$$-\Delta (u^i + u^s) - \omega^2 n^2(u^i + u^s) = 0; \quad n(x, \omega) = \begin{cases} n(\omega), & x \in \Omega_r \\ n_0, & \text{otherwise} \end{cases}.$$ 

We formulate the scattering problem as: Find $u^s$ for given $\omega \in \mathbb{R}$ and $f \in L^2(\Omega_r)$, such that

$$-\Delta u^s - \omega^2 n_0^2 u^s = 0, \quad x \in \Omega_0, \quad -\Delta u^s - \omega^2 n^2 u^s = f, \quad x \in \Omega_r,$$

$$f(\omega, x) = \omega^2(n^2 - n_0^2)e^{im_0 \omega x}.$$ 

The scattered wave $u^s$ is required to satisfy an outgoing wave condition, which is described in the following section.
The problem in (16) corresponds to the electromagnetic version (11) in TM polarization with \( u := E_3 \). The scattering problem for TE polarization (12) can be defined similarly. In compact notation, the scattering problem is formulated as: For given \( \omega \in \mathbb{R} \), and \( f \in L^2(\Omega_r) \), find \( u \) such that
\[
-\nabla \cdot (\rho \nabla u) - \omega^2 \eta u = f, \quad x \in \Omega_a,
\]
with \( u \) outgoing.  

### 3.2 Outgoing radiation condition

The Sommerfeld radiation condition serves as a means to identify outgoing solutions from Helmholtz problems. The condition is written for \( x \in \mathbb{R}^d \) and \( \omega \in \mathbb{R} \) as
\[
\lim_{r \to \infty} r^{d-1} \left( \frac{\partial}{\partial r} - i\omega n_0 \right) u(x) = 0.
\]

An appropriate outgoing condition for the full electromagnetic 3D vector case exists and it is denoted the Silver-Müller radiation conditions [19].

An important drawback of condition (18) is that it is only valid for real frequencies \( \omega \). However, it is possible to derive an exact outgoing condition that does work for complex frequencies.

#### 3.2.1 Outgoing condition for \( d = 1 \)

The Helmholtz equation in one dimension reads
\[
-\frac{d^2 u}{dx^2} - \omega^2 u = 0,
\]
which formally has the solutions \( \{e^{i\omega x}, e^{-i\omega x}\} \). The condition (18) at a point \( x = a > 0 \), becomes
\[
u'(a) - i\omega u(a) = 0,
\]
which is satisfied for every \( a > 0 \) by \( u = e^{i\omega x} \). Then, we say that \( e^{i\omega x} \) is an outgoing solution of (19). This result suggests that the condition (20) can be used as a boundary condition for practical purposes. Additionally, we see that the outgoing solution in time \( w(x,t) = u(x,\omega)e^{-i\omega t} = e^{i\omega(x-t)} \), results in a wave that propagates in the positive axis away from the origin.

#### 3.2.2 Outgoing condition for \( d = 2 \)

In the two dimensional case, nontrivial solutions to the Helmholtz equation
\[
-\Delta u - \omega^2 u = 0,
\]
are found by the use of separation of variables in polar coordinates \( (r,\theta) \) [15, Ch. 5], [19, Sec. 2.1]. The radial part of \( u \) is given in terms of the Hankel functions
\( \{H_m^{(1)}(\omega r), H_m^{(2)}(\omega r)\}, \ m \in \mathbb{Z} \) \[11, \text{Ch. 10}. \] For large \( r \), the use of the formulas \[11, \text{Sec. 10.2}\]

\[
H_m^{(1)}(\omega r) \approx \sqrt{2/(\pi \omega r)} e^{i(\omega r - \frac{1}{2} m \pi - \frac{3}{4} \pi)}, \tag{22}
\]

\[
H_m^{(2)}(\omega r) \approx \sqrt{2/(\pi \omega r)} e^{-i(\omega r - \frac{1}{2} m \pi - \frac{3}{4} \pi)},
\]

verifies that only \( H_m^{(1)}(\omega r) \) satisfies the condition (18). Similarly as for the one-dimensional case, it is clear from (22) that \( H_m^{(1)}(\omega r)e^{-i\omega t}, \ m \in \mathbb{Z} \) is a radial wave traveling away from the origin.

The exact representation of outgoing waves is written as the superposition of the outgoing solutions discussed above

\[
u(r, \theta) = \sum_{m=-\infty}^{\infty} \hat{u}_m H_m^{(1)}(\omega r) e^{im\theta}, \text{ for } x \in \Omega^+_a,
\tag{23}
\]

where the complex coefficients \( \hat{u}_m \) are unknown.

In the three dimensional case \((d = 3)\), a similar argumentation can be used.

### 3.3 Dirichlet to Neumann Maps

In this section we describe a technique that allow us to truncate open domains by using an exact representation of outgoing waves. The Dirichlet-to-Neumann map, or DtN in short, can be then used as boundary condition. For simplicity, the DtN is presented for the Helmholtz equation (17) in TM polarization, and we use \( n_0 = 1 \). By using the splitting

\[
u(x) := \begin{cases} 
u_a, & x \in \Omega_a, \\ \nu_0, & x \in \Omega^+_a, \end{cases}
\tag{24}
\]

the problem (17), is formulated as

\[
-\Delta \nu_a - \omega^2 n^2 \nu_a = f, \quad x \in \Omega_a, \\
\nu_a = \nu_0, \quad x \in \Gamma_a, \\
\nabla \nu_a \cdot \mathbf{n} = \nabla \nu_0 \cdot \mathbf{n}, \quad x \in \Gamma_a, \\
-\Delta \nu_0 - \omega^2 \nu_0 = 0, \quad x \in \Omega^+_a, \\
\nu_0 \equiv \text{outgoing}, \quad x \in \Omega^+_a,
\tag{25}
\]

where \( \mathbf{n} \) is the normal vector pointing outwards from \( \Omega_a \).

If we assume that \( \nu_0 \) is known as given data on \( \Gamma_a \), then we can use the series representation (23) to relate the coefficients \( \hat{u}_m \) in terms of \( \nu_a \). For this, the use of the condition \( \nu_a(a) = \nu_0(a) \) leads to

\[
\hat{u}_m = \frac{1}{2\pi H_m^{(1)}(\omega a)} \int_0^{2\pi} \nu_a(a, \theta) e^{-im\theta} d\theta.
\tag{26}
\]
The use of (26) and the compatibility condition $\nabla u \cdot n = \nabla u_0 \cdot n$, results in

$$G(\omega)u := \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \omega \frac{H_m^{(1)}(\omega a)}{H_m^{(1)}(\omega a)} e^{im\theta} \int_0^{2\pi} u(a, \theta') e^{-im\theta'} d\theta'. \quad (27)$$

It becomes clear that we can reformulate (25) and (17), into the problem

$$-\nabla \cdot (\rho \nabla u) - \omega^2 \eta u = f, \quad x \in \Omega, \quad \rho \nabla u \cdot n = G(\omega)u, \quad x \in \Gamma. \quad (28)$$

The operator $G(\omega)$ is known in the literature as the DtN map, and in practical applications, we truncate the infinite series until $|m| = l$ and obtain the truncated operator $G^l(\omega)$. For further details on DtN maps see [19, sec 3.2].

### 3.4 The scattering resonance problem

The resonance problem is formulated through the use of the DtN map, by letting $\mathcal{D} = \{ z : H_m^{(1)}(za) = 0, m \in \mathbb{Z} \}$. Then the problem is formally:

For $\omega \in \mathbb{C} \setminus \mathcal{D}$, find pairs $(\omega, u)$ such that

$$-\nabla \cdot (\rho \nabla u) - \omega^2 \eta u = 0, \quad x \in \Omega, \quad \rho \nabla u \cdot n = G(\omega)u, \quad x \in \Gamma. \quad (29)$$

Alternatively, resonances can be defined through the use of volume integral equations as done below.

#### 3.4.1 Lippmann-Schwinger formulation of resonances

A scattering resonance can be defined as a complex number $\omega$ for which the Lippmann-Schwinger equation

$$T(\omega)u := u - K(\omega)u = 0, \quad (30)$$

has a non-zero solution $u$. The integral operator $K$ in (30) is for TM/TE waves given by

$$TM : K(\omega)u := \omega^2 \int_{\Omega} \Phi(x, y) (\epsilon - 1) u dy, \quad TE : K(\omega)u := \nabla \cdot \int_{\Omega} \Phi(x, y) \left( \frac{1}{\epsilon} - 1 \right) \nabla u dy. \quad (31)$$

Here, $\Phi(x, y)$ is known as the outgoing Green function in free space for the Helmholtz equation [26,27] given by

$$\Phi(x, y) = \begin{cases} \frac{i}{2\omega} e^{i\omega|x-y|}, & d = 1 \\ \frac{i}{4} H_0^{(1)}(\omega|x-y|), & d = 2 \\ e^{i\omega|x-y|}, & d = 3 \end{cases} \quad (32)$$

Solutions of problem (30) are automatically outgoing. In acoustics the case is equivalent to the TM polarization.
4 Discretization and resulting nonlinear eigenvalue problem

For the discretization of the equation in (29), we use the Finite Element Method (FEM), which provides an effective and flexible framework for the discretization of Partial Differential Equations (PDE). The main idea of the method is to introduce a triangulation $\mathcal{T}(\Omega)$ of simple shapes denoted elements, that cover the computational domain $\Omega$. Each element, is assigned a local polynomial basis $P_p$ on $\mathbb{R}^d$ with elements of degree $\leq p$. Global basis functions $\{\varphi_j\}_{j=1}^N$ are defined by tailoring together the local basis functions at element edges. In this way, we can represent solutions to PDEs over the entire domain as piecewise polynomial functions.

In our computations the FE mesh is designed such that the permittivity function $\epsilon$ is continuous in each element $K_j$. We set $h_j$ as the length of the largest diagonal of each element $K_j$, and denote by $h$ the maximum mesh size $h := \max_j h_j$. Then, solutions of the equation (29), are approximated by $u_h \in S_h(\Omega)$, with finite element space defined as

$$S_h(\Omega) := \{u \in H^1(\Omega) : u|_{K_j} \in P_p(K_j) \text{ for } K_j \in \mathcal{T}\}, \quad (33)$$

and the $L^2$-inner product, $L^2$-norm, and Hilbert space as

$$(u,v)_{\Omega} := \int_{\Omega} u \overline{v} \, dx, \quad \|u\| := \sqrt{(u,u)}, \quad \text{and} \quad H^1(\Omega) := \{u : \|u\|^2 + \|\nabla u\|^2 < \infty\}, \quad (34)$$

respectively.

Many of the details related to discretization of PDEs with FE can be found, for example, in [28, 37], and important implementation details in [36]. The flexibility of the FEM allows for many features that have been used in the thesis, as for example: the computation with high polynomial degrees, flexible quadrature rules for numerical integration, easy parametrization of complex geometries by using curvilinear elements and transfinite interpolation [40,41].

4.1 Assembly of the FE matrices

From the discussion in the last section, we introduce FE basis functions $\{\varphi_1, \ldots, \varphi_N\}$ as the basis for $S_h(\Omega^h_a)$. Then, the FE representation formula and entries in the finite element matrices corresponding to equation (29), become

$$u_h = \sum_{j=1}^{N} \xi_j \varphi_j, \quad A_{ij} = (\rho \nabla \varphi_j, \nabla \varphi_i)_{\Omega^h_a}, \quad M_{ij} = (\eta \varphi_j, \varphi_i)_{\Omega^h_a}, \quad (35)$$

for $\xi \in \mathbb{C}^N$. The matrix eigenvalue problem is then: Find the eigenpairs $(\omega, \xi)$ such that

$$F(\omega) \xi := (A - \omega^2 M + Q)(\omega) \xi = 0, \quad (36)$$
where the corresponding matrix valued function \( Q(\omega) \) arises from the respective formulation DtN-FE [7], or PML-FE [5].

In the case where \( \epsilon(\omega, x) \) is given as a piecewise function, we write (36) as
\[
F(\omega) \xi := \left( \sum_{m=0}^{N_r} \{ \rho_m(\omega) \tilde{A}_m - \omega^2 \eta_m(\omega) \tilde{M}_m \} + Q(\omega) \right) \xi = 0, \quad (37)
\]
with matrices \( \tilde{A}_{mj} = (\nabla \phi_j, \nabla \phi_i)_{\Omega_h}, \quad \tilde{M}_{mj} = (\phi_j, \phi_i)_{\Omega_h}, \quad m = 0, 1, \ldots, N_r. \)

### 4.2 Pseudospectra computations

Computations of the pseudospectra provide insight into the behavior of the resolvent \((F^h)^{-1}\). In these computations, we use that \( \sigma_\delta(F^h) \) is the set of all \( z \in \mathbb{C} \) such that
\[
\sigma_{\min} F^h(z) < \delta, \quad (38)
\]
where \( \sigma_{\min} F^h(z) \) denotes the smallest singular value of \( F^h(z) \) [39, Def. 2.10].

### 4.3 Numerical sorting of resonances

In this section we present a discrete form of (30) that allow us to identify resonances from spurious solutions once we have computed FE solutions \((\omega_h^m, u_h^m)\) to (36) or to (37). The resulting expression for the sorting scheme is a discrete form of the condition \( \| \chi_a T(\omega) \chi_a u \| < \delta \), where \( u_h \) is a FE solution restricted to \( \Omega_a \). Then, a discretization for the Lippmann-Schwinger equation (30) is written in the form
\[
T(\omega) u_h = u_h - K(\omega) u_h, \quad u_h := \sum_{j=1}^{N} \xi_j \phi_j, \quad \text{with} \quad \| u_h \|_{L^2(\Omega_a)} = 1. \quad (39)
\]

The details of the Galerkin discretization (39), are given in [5, 6].

**Definition 1. Pseudospectrum indicator:** The computed eigenvalue \( \omega_h \) belongs, for given \( \delta > 0 \), to the \( \delta \)-pseudospectrum \( \sigma_\delta(T^h) \) if the eigenpair \((\omega_h, u_h)\) satisfies \( \| T^h(\omega_h) u_h \|_{\Omega_a} < \delta \). Then, for a given domain \( \Omega_a \supseteq \Omega_r \), we define the pseudospectrum indicator as
\[
\delta^h(\Omega_a) := \| T^h(\omega_h) u_h \|_{\Omega_a}. \quad (40)
\]

We aim to measure whether or not the computed eigenpair \((\omega_h, u_h)\) is related to a physical scattering resonance pair, but naturally, very bad approximations exhibit also large \( \delta^h \) values.

### 4.4 Software and packages

We have greatly benefited from the excellent readily available libraries for scientific computations. For the \( hp \)-FE environment and fast assembly routines we relied on the
deal.II library [3], for the computational linear algebra platform, PETSc [33] was used, and for computation of large nonlinear eigenvalue problems and pseudospectra we used SLEPc [18].
5 Summary of Papers

In this Section we give brief summaries of the four papers that compose this thesis. In papers I and IV we develop a technique used to identify true FE approximations of scattering resonance pairs. In paper II we present an efficient procedure for approximation of resonances when a DtN is used as an outgoing wave condition. We describe the specialized solution strategy for the arising nonlinear eigenvalue problem and illustrate its effectiveness. In paper III we study pollution errors in Helmholtz problems for complex frequencies. We derive estimators of the pollution error and develop a-priori $hp$-FE strategies. The novel $hp$-FE strategy significantly reduces the preasymptotic phase compared to classical FE approaches.

5.1 Paper I

This paper centers on the finite element approximation of scattering resonances for Helmholtz problems in exterior domains. Particularly, the subject of spectral instability and related problems arising in the computation are discussed for one dimensional problems. The PML and DtN formulations are used for the truncation of the computational domain.

Numerical computations result in approximations to resonances and in additional non-physical solutions that in the paper are called spurious solutions. These spurious solutions that are present for moderately large FE spaces are very common in practical
computations. It is possible to prove convergence for the DtN-FE and PML-FE. Hence, no spurious solutions exist if the FE space is large enough and the PML layer is thick enough [24]. However, the rate of convergence depends critically on resolvent norms that may be very large.

The paper presents a detailed characterization of the spurious eigenvalues for the PML-FE formulation. The complex plane is split into feasible and non-feasible searching regions for approximations to resonances. Additionally, a novel DtN-PML formulation is introduced which permits to compute accurate newton approximations to the PML eigenvalues.

The origin of unphysical eigenvalues in scattering resonance computations is spectral instability, which is common for non-normal operators [10,39]. Spectral instability is known to be less problematic with volume integral equations compared with formulations based on differential operators. The Lippmann-Schwinger (LS) formulation is independent of the parametrization of the domain outside the resonator.

The left panels in Figure 9 give, in colored contours, pseudospectrum computations (38) for a benchmark problem. In (a) for the DtN-FE formulation and in (b) for the LS formulation. From the spectral window shown in the figure, it can be seen that the LS formulation has the same number of eigenvalues as there are exact scattering resonances. It also exhibits a resolvent norm that grows rapidly only close to the eigenvalues, an is well-behaved away from the spectrum. On the contrary, the DtN-FE shows a larger number of eigenvalues than the number of exact scattering resonances shown in the spectral window. Additionally, its resolvent norm can get large even away from the spectrum. The case for the PML (not shown) is similar and more pronounced than for the DtN.

Despite the positive features of the LS formulation, the direct computation of resonances with a volume integral equation is demanding since it results in a nonlinear eigenvalue problem, matrices are full, and each solver iteration requires a matrix assembly. Alternatively, we can instead determine if a computed eigenvalue numerically is in an $\epsilon$-pseudospectrum of the integral operator and the corresponding vector is an $\epsilon$-pseudomode. The results and reliability of this approach is observed in Figure 9, where it is shown in panel (c) the result of applying the filtering test by computing (40). Then, from the computed eigenpairs $(\omega^h_m, u^h_m)$, only approximations to true resonance pairs have a small pseudospectrum indicator $\delta_m$, and those eigenvalues not converging to exact resonances exhibit large values.

Finally, the general idea with the filtering scheme is to detect spurious solutions in the DtN and PML formulations, by testing test each computed pair and obtain a pseudospectral indicator $\delta_m$. Then we sort all computed pairs from the smallest to the largest value of $\delta_m$, and finally we choose a user defined tolerance $\delta_{TOL}$, and drop all pairs with $\delta > \delta_{TOL}$.

Numerical simulations indicate that the presented test can distinguish between spurious eigenpairs and true eigenpairs also in complicated cases when the spurious solutions mix with true approximations of resonances.
Figure 10: FE error convergence for a benchmark problem in 2D: Left) p-FE error convergence versus $\nu_{\text{max}}$ and right) p-FE error convergence with fitting curve (black): $\alpha_0 = 1.22 \times 10^5$, $\beta_0 = 0.4081$.

5.2 Paper II

The paper introduces an efficient procedure for the numerical approximation of resonances in exterior domains. The Helmholtz equation (11) in TM polarization, is discretized by using FE methods for given non-dispersive refractive index $n(x)$. The resulting matrix problem is formulated as the nonlinear eigenvalue problem (NEP) in (36), where the nonlinearity arises from the use of a DtN map. Even though our differential operator (28) is linear in $\omega^2$, the DtN operator $G(\omega)$ in (27) depends in a nonlinear way on the eigenvalue $\omega$. In our case $F(\omega)$ in (36) is meromorphic in $\mathbb{C}$, with poles in the region of interest given by scaled roots of Hankel functions.

In this work a new computational approach is presented to accurately approximate resonances, based on a high order FE method combined with a specialization of the tensor infinite Arnoldi method (TIAR). The class for Infinite Arnoldi methods can be interpreted as Krylov methods for a dynamically increasing companion linearization of an approximation of the problem [4,17,21]. The particular companion linearization arises from the Taylor expansion of $F(\omega)$ with respect to the spectral parameter $\omega$. In this way, the algorithm generates a Hessenberg matrix and the eigenvalues of this matrix correspond to eigenvalue approximations of the NEP. The last argument implies that a large number of derivatives is required in TIAR, from where the paper shows how the spectral derivatives are computed, and how the algorithm is designed to exploit the particular structure of the NEP.

A procedure to compute derivatives of the Hankel functions is used to specialize TIAR to (36). The method uses a formula involving Toeplitz matrices, and computes a given number of derivatives using only matrix-vector operations. The advantage is that the approach appears to be relatively insensitive to round-off errors.
In particular, we show that the new specialization of TIAR together with a $p$-FE strategy is an efficient and reliable tool for resonance calculations with the DtN map. Exponential convergence of the discretization error is obtained by selecting a large enough $\nu_{\max}$ in the truncation of DtN terms and then enhancing the polynomial order of the FE. The error for proposed FE+TIAR strategy with respect to $\nu_{\max}$ and with respect of the degrees of freedom $N$ is presented in Figure 10 corresponding to a standard benchmark. In the left panel we see that by increasing $\nu_{\max}$ then eigenvalue errors converge to its minimum value. Once the eigenvalue error has converged, further increase of $\nu_{\max}$ does not increase the error, even though more derivatives are computed in the solution routine.

The direct application of the solution strategy works well for some regions of the complex plane, but unfortunately not for the entire complex plane. For a given shift $\mu$, the the radius of convergence depends on properties of the matrix-valued function (36). TIAR is designed for problems which are analytic in a large domain, and convergence cannot be guaranteed for eigenvalues outside the convergence disk for the power series expansion at $\mu$. Therefore, a pole cancellation technique, is introduced in order to increase the radius of convergence for computation of eigenvalues that lie close to the poles of the matrix-valued function. By doing this, the NEP is transformed into a new problem with some of the poles removed.

Numerical computations show that the algorithm is efficient with respect to CPU-time. In particular, the CPU-time is for large problems dominated by a precomputation of the LU-factorization. The overall conclusion is that a higher order FE combined with TIAR is an efficient strategy for numerical approximation of resonances in exterior domains.

5.3 Paper III

In this paper, we work with open systems where the optical material properties of resonators consist of frequency dependent and lossy materials. These are modeled by the Drude-Lorentz model given in (14).

It is well known that the accuracy of a finite element approximation of the Helmholtz problem $-\Delta u - \omega^2 u = f$ deteriorates with increasing frequency $\omega \in \mathbb{R}$. A major problem is that the discrete frequency of the FE solution is different from the frequency of the exact solution. This effect called pollution has been studied intensively. Particularly, for a uniform mesh size $h$ the asymptotic error estimates for linear elements [19, Sec. 4.4.3] yield the condition $\omega^2 h < 1$, which for large $\omega$ results in prohibitively expensive meshes. The dispersion analysis presented in [1,19,38] yields pre-asymptotic estimates of the form $\omega h < 1$, which is a significant improvement. Additionally, it was realized that higher order elements are advantageous to reduce the pollution effect. However, the minimal dimension of a finite element space such that the relative eigenfunction error is below 100% is unknown even in the self-adjoint case with analytic coefficients (see [35, Remark 6.1]).

Resonances in our setting are approximated by the eigenvalues of a rational matrix-valued function in the neighborhood of a shift value $\mu$ in the complex plane. As we
work with scattering resonances, the resulting eigenvalues are complex. The natural step is then to extend the dispersion analysis in [1, 19, 38] to the case with a complex frequency $\omega$. Particularly, the derived expressions from [1] can be analytically continued to the complex plane, where attention is paid to the identification of possible branch cuts and poles of the different expressions when deriving extensions of the estimates in [1]. The results in paper III rely on the references [11, 29, 30], where many of the details of working with Bessel functions of complex argument are addressed.

The paper then moves to the subject of a-priori $hp$-strategies for non-self-adjoint eigenvalue problems with piecewise constant coefficients. The main contribution of the paper is presented in two a-priori refinement strategies based on the derived dispersion analysis on the finite element space. Then, for given $\omega \in \mathbb{C}$, the FE eigenfunctions restricted to a particular element, must satisfy the conditions for superexponential decay of the error on an extended mesh. In this way, the element wise polynomial
degrees $p_j$ and maximum element diameters $h_j$ must satisfy certain conditions that allow for their easy computation. As an illustration, a typical element-wise polynomial distribution is depicted in the left panel of Figure 11.

The proposed computational approach combines a novel $hp$-FEM strategy, based on dispersion analysis for complex frequencies, with a fast implementation of the nonlinear eigenvalue solver NLEIGS. Numerical computations illustrate that the pre-asymptotic phase is significantly reduced compared to standard uniform $h$ and $p$ strategies. Some examples for TM and TE polarizations are shown in the right panel of Figure 11. Moreover, the efficiency of the strategy grows with the refractive index contrast, which makes the new strategy highly attractive for metal-dielectric structures. The $hp$-refinement strategy together with the efficient parallel code result in highly accurate approximations and short runtimes on multi processor platforms.

Finally, the a-priori strategy for enriching the finite element space developed in this paper can in principle also be combined with an a-posteriori based strategy such as [13, 16].

### 5.4 Paper IV

In paper IV a sorting scheme is considered for the removal of spurious scattering resonant pairs in two-dimensional electromagnetic problems and in three-dimensional acoustic problems, when approximations of scattering resonances are computed with finite elements. The strategy is motivated by spectral stability properties of the
Lippmann-Schwinger type of volume integral equation \([25,31]\), and can be applied to configurations with graded material properties as well as piece-wise constant material properties.

In paper I a Lippmann-Schwinger (LS) type of integral equation was used for removing spurious solutions in a one-dimensional setting. The corresponding discretization of the LS formulation \((30)\), has a kernel \(\Phi(x,y)\) \((32)\) that is continuous, but has a jump in the derivative at points \(x = y\). The integration interval can always be split and by using Gauss-type of quadratures, numerical convergence for the quadrature error is experienced to high order.

The effective application of these ideas for problems with \(d = 2, 3\) turn out to be more challenging, and require further considerations that are addressed in the paper. Namely, in higher dimensions the kernel is weakly singular \([9, \text{Sec. 2.3}]\), which makes the integration in \((30)\) more demanding.

It is possible to overcome this difficulty by employing specialized quadrature rules. For example, in the references \([23]\), \([12]\), and \([2]\), specialized quadratures rules were applied to scattering problems. For eigenvalue computations the singularity is a greater challenge than for a source problem.

The paper discusses the computational costs related with the computation of \((30)\) and the pseudospectrum indicator \(\delta^h(\Omega_a)\) given in \((40)\). Simple estimations for higher space dimensions show that the computational and storage costs become extremely high for discretizations of volume integral equations. Furthermore, the evaluation of \(\delta^h_m(\Omega_a)\) results in sorting schemes that are far more expensive than the solution of the NEP \((36)\). The result is an effective and inexpensive strategy for testing the computed pair \((\omega^h, \xi)\), which has low memory requirements, utilizes an already assembled FE mesh, re-uses the pre-computed FE environment, and has a fully parallelizable algorithm. Furthermore, all eigenvalues in the spectral window are computed only once, and the proposed sorting indicator \(\tilde{\delta}\) is computed on each computed eigenpair.

The results of the application of the new sorting scheme to particular benchmarks are illustrated in Figure 12. In the panel on the left, a DtN-FE is used for the computation of the scattering resonances on a square dielectric configuration, which is non-dispersive. Reference eigenvalues are marked with dots and computed eigenvalues are marked with circles, which are colored by the sorting indicator \(\tilde{\delta}_m\). It is clear that the value for \(\delta\) increases with \(\text{Re}\{\omega}\), as expected from for the FE discretization error of non-dispersive Helmholtz problems \([1, 5, 19]\). Additionally, eigenvalues with small indicator values appear very close to the exact eigenvalues of the problem.

On the right panel of Figure 12, a PML-FE is used for testing the eigenvalues of a dispersive benchmark problem. The bottom panel is a close up window showing the indicator values \(\tilde{\delta}_m\) for an accumulation of eigenvalues. As expected, the value \(\tilde{\delta}_m\) increases when approaching a critical value. This behavior is expected since close to a critical point the resulting eigenfunction oscillates more rapidly, which implies that the FE error increases. Additionally, the DtN-FE produces better approximations to scattering resonances than the PML-FE, with lower values on the indicator \(\tilde{\delta}_m\).

The results in Figure 12 not only illustrate the reliability of the identification of true approximation to resonances by using the proposed sorting strategy, but they
also show its simplicity, flexibility, and large coverage in the complex plane. Particularly, correct approximations to scattering resonances are easily identified from the overwhelming rest of computed eigenvalues.

Numerical experiments on a broad range of benchmarks illustrate that the sorting scheme can be used to give valuable information on the location of true resonances at low computational cost. Finally, the results in the paper present a sorting scheme, based on the Lippmann-Schwinger equation, for the removal of spurious scattering resonant pairs in $\mathbb{R}^d$ Helmholtz problems.
References


Acknowledgements

My sincere and deep gratitude goes first to my advisor Christian Engström. I am thankful for the opportunity, guidance and inspiration you have provided in my time as your student. Thank you for the thorough supervision, patience and kindness you showed along my learning process.

I would like to express my sincere thanks to Eddie Wadbro for numerous discussions and relevant advise in my endeavor as a computational scientist. Thanks to the Computational design optimization group for offering a rich environment for academic discussions.

I am very grateful for the opportunity to have collaborated in joint work with Elias Jarlebring, Jose Roman and Carmen Campos. I enjoyed the scientific discussions held during the development of the projects. Thank you for the fruitful joint work.

I want to express my gratitude to Alejandro Hurtado for his support and guidance on my early career. Thanks also to the FISINFOR team for the kick-start. Many thanks to Andrée Falgin for his contributions on the meshing routine used in this thesis, the personal encouragement and for being a great pal all these years!

Thanks to all the colleagues at the UMIT research lab and the department of Mathematics at Umeå University for a stimulating academic environment. Special thanks to Anna Ivarsson, Lisa Hed, and Peter Anton for your guidance and kindness.

I would like to thank to the organizer of the UNIVERSUM proceedings on very many topics of life, Dr. Edward Cabezas, for having me as an invited speaker, and I am also grateful with its participants Mahmoud, Abel, and the respected delegation from the Animal Science community: Merko, Marko, and Degong. Thanks for making my time as a doctoral student more enjoyable.

The doctoral studies were partly supported by the Swedish Research Council under Grant No. 621-2012-3863, the department of Mathematics and UMIT research lab at Umeå University, for what I am grateful.

My deepest appreciation and love goes to you Tara, thank you for your unconditional love and support all these years. Thank you for adding meaning and beauty to my life.

Juan Carlos Araújo Cabarcas
Umeå, May 2019
List of papers

This thesis consists of an introductory chapter and the following papers*:


III. Juan C. Araújo C., Carmen Campos, Christian Engström, and Jose E. Roman, Computation of scattering resonances in absorptive and dispersive media with applications to metal-dielectric nano-structures, Submitted for journal publication.

IV. Juan C. Araújo C. and Christian Engström, Removal of spurious solutions encountered in Helmholtz scattering resonance computations in $\mathbb{R}^d$, Submitted for journal publication.

*The published papers have been re-typeset to match the style of the thesis and contain minor differences from the published versions.