Doctoral Thesis

Multi-Objective Shape Optimization of Radio-Frequency Cavities

Author(s): Kranjčević, Marija

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MULTI-OBJECTIVE SHAPE OPTIMIZATION OF RADIO-FREQUENCY CAVITIES

A thesis submitted to attain the degree of
DOCTOR OF SCIENCES of ETH ZURICH

presented by
MARIJA KRANJČEVIĆ,
M.Sc. in Applied Mathematics, University of Zagreb
born on 10.05.1992
citizen of the Republic of Croatia

accepted on the recommendation of
Prof. Dr. Peter Arbenz, examiner
Prof. Dr. Ralf Hiptmair, co-examiner
Dr. Andreas Adelmann, co-examiner
Prof. Dr. Ursula van Rienen, co-examiner

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Abstract

Radio frequency (RF) cavities are commonly used in particle accelerators to accelerate charged particle beams. The shape of the RF cavity determines the resonant electromagnetic fields and frequencies, which need to satisfy a variety of often conflicting requirements in order to stably and efficiently accelerate the beam. For example, the shunt impedance has to be maximized in order to reduce the power load, and the electric field on the cavity surface must not exceed a critical threshold in order to avoid discharges and excessive dark current in the RF cavity. However, cavities with a high shunt impedance often also have a high electric field on their surface.

Therefore, we formulate such problems as constrained multi-objective shape optimization problems and search for the Pareto front using a massively parallel implementation of a multi-objective evolutionary algorithm (EA). We focus on axisymmetric RF cavity shapes, and use a fast axisymmetric Maxwell eigen-solver for computing the necessary properties of both the fundamental mode and the higher order modes (HOMs). In particular, we solve two real-world RF cavity shape optimization problems.

The first problem is the optimization of the main RF cavity of the planned Swiss Synchrotron Light Source upgrade, called SLS 2.0, at the Paul Scherrer Institut, which aims to dramatically improve the synchrotron light quality. We use the multi-objective EA together with a constraint handling method to find good RF cavity shapes for SLS 2.0. Since it is planned to reuse the existing cavity, extended by a new type of absorber for the most troubling beam excited HOMs, this optimization is hypothetical. Nonetheless, we provide insight into the problem by computing the Pareto front approximation, and find a few good RF cavity shapes for which the beam interaction with the HOMs is already minimized. The objective function that corresponds to the interaction of the beam with the HOMs is, in its most natural formulation, discontinuous, which further supports the use of an EA.

The second problem we consider is the optimization of the superconducting RF cavity for the Z-pole operating mode of the lepton collider at the Future Circular Collider (FCC). The FCC is planned to collide beams with unprecedented luminosities and extend the research that is currently being conducted at the Large Hadron Collider (LHC). In particular, the circular lepton collider is planned to study the properties of Z, W and Higgs bosons, as well as top quark, using four different modes of operation over the years. In addition to optimizing the RF properties, we focus on finding a cavity shape that is robust with respect to geometric perturbations, which could arise, for example, from manufacturing inaccuracies or harsh operating conditions at cryogenic temperatures. In particular, the fundamental frequency should be robust because,
if it is detuned, additional power is needed to maintain the same accelerating electric field. In order to gain insight about the model, we first perform a global sensitivity analysis. We then use these results to reduce the search space, reformulate the problem, and devise an optimization strategy. In the end we show a good cavity for the Z-pole operating mode of the lepton collider at the FCC, which, for example, has a robust fundamental frequency, and the frequencies of the trapped dipole modes extremely close to each other which would simplify their damping with coaxial HOM couplers.

In both cases, in addition to the widely considered elliptical cavity shapes, we also explore the possibility of using a different type of geometry. The proposed approach could easily be applied to other types of geometries and other RF cavity shape optimization problems, with the underlying software used for computing the properties of arbitrary HOMs.
Zusammenfassung

Hochfrequenz (HF) Kavitäten werden üblicherweise in Teilchenbeschleunigern genutzt, um Pakete geladener Teilchen zu beschleunigen. Die Geometrie der HF Kavität bestimmt die Verteilung der elektromagnetischen Felder und die Resonanzfrequenzen, welche verschiedene Bedingungen erfüllen müssen, um die Teilchen stabil und effizient zu beschleunigen. Diese Bedingungen widersprechen sich oft gegenseitig. Zum Beispiel sollte die Shuntimpedanz möglichst gross sein, um die Verlustleistung zu minimieren und das elektrische Feld darf eine kritische Grenze nicht überschreiten, um Durchschläge und übermässigen Dunkelstrom in der Kavität zu vermeiden. Allerdings haben Kavitäten mit hoher Shuntimpedanz oft auch hohe elektrische Felder an der Oberfläche.

Deshalb formulieren wir solche Probleme als Optimierung mit mehreren Zielfunktionen mit Nebenbedingungen und suchen die Pareto-Front mit einer massiv parallelisierten Implementation eines multikriteriellen evolutionären Algorithmus (EA). Wir konzentrieren uns auf axialsymmetrische HF Kavitäten, und benutzen einen schnellen axialsymmetrischen Maxwell Eigenlöser, um die notwendigen Eigenschaften sowohl des Grundschwingungsmodes, als auch Modi höherer Ordnung (MHO) zu berechnen. Insbesondere lösen wir zwei praktische Optimierungsprobleme für Kavitätsgeometrien.

Das erste Problem ist die Optimierung der Hauptkavität der geplanten Erneuerung der Synchrotron Lichtquelle Schweiz, genannt SLS 2.0, am Paul Scherrer Institut. Durch den Umbau soll die Lichtqualität des Synchrotrons drastisch verbessert werden. Wir nutzten den multikriteriellen EA zusammen mit einer Bedingungsbehandlungsmethode, um eine gute Kavitätsgeometrie für SLS 2.0 zu finden. Da geplant ist, die bereits bestehenden Kavitäten wiederzuverwenden und mit einem neuen Dämpfer für die problematischsten, strahlangeregten MHO auszurüsten, ist diese Optimierung hypothetisch. Dennoch verschaffen wir uns dank der Pareto-Front Approximierung neue Erkenntnisse und finden ein paar gute Kavitätsgeometrien für welche die Strahlwechselwirkung mit den MHO bereits minimiert ist. Dass die Zielfunktion der Wechselwirkung zwischen Strahl und MHO in seiner natürlichen Form unstetig ist, begründet die Verwendung von EA zusätzlich.

Das zweite behandelte Problem ist die Optimierung einer supraleitenden HF Kavität für den Z-Pole Betriebsmodus des Lepton Colliders am Future Circular Collider (FCC). Im FCC sollen Elementarteilchen in noch nie dagewesener Leuchtkraft kollidieren und so die Forschung, die momentan am Large Hadron Collider (LHC) durchgeführt wird, erweitern. Insbesondere wird der ringförmige Lepton Collider entwickelt, um über die Jahre, in vier verschiedenen Betriebsmodi, Eigenschaften von Z, W und Higgs-Bosonen, sowie des Top-Quarks zu untersuchen. Zusätzlich zu der Optimierung der HF-Eigenschaften
berücksichtigen wir hier zusätzlich die Kavitätsgestaltung. Diese soll gegenüber Störungen der Geometrie möglichst unempfindlich sein. Solche Störungen können beispielsweise durch herstellungsbedingte Ungenauigkeiten oder durch harsche Betriebsbedingungen bei kryogenen Temperaturen hervorgerufen werden. Insbesondere die Grundfrequenz sollte stabil sein. Denn, wenn sie verstimmt ist, wird zusätzliche Leistung benötigt, um das gleiche elektrische Feld zu erzeugen. Um Einblicke in das Modell zu gewinnen führen wir zuerst eine globale Empfindlichkeitsanalyse durch. Dann verwenden wir diese Ergebnisse, um den Suchraum zu verkleinern, das Problem umzuformulieren und eine neue Optimierungsstrategie zu entwickeln. Zum Schluss präsentieren wir eine gute Kavität für den Z-Pol Betriebsmodus des Leptonen Colliders des FCC. Diese Kavität besitzt beispielsweise eine unempfindliche Grundfrequenz und die Frequenzen der eingeschlossenen Dipolmodi liegen extrem eng beieinander, was ihre Bedämpfung mit einer koaxialen MHO Auskopplung vereinfacht.

In beiden Fällen haben wir zusätzlich zu den häufig betrachteten elliptischen Kavitätsgestaltungen, auch andere Arten von Geometrien untersucht. Die vorgeschlagene Methode kann einfach auf andere Arten von Geometrien und andere HF Optimierungsprobleme, mit dem zugrundeliegenden Computerprogramm zur Berechnung der Eigenschaften von beliebigen MHO, angewandt werden.
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Particle accelerators are an indispensable tool for fundamental and applied research. They are used in areas such as particle physics, chemistry, biology, materials science and medicine.

Radio frequency (RF) cavities are widely used in particle accelerators. They are metallic chambers with a resonating electromagnetic field that is used to accelerate charged particles, from electrons and protons to heavy ions and uranium [54, 108].

For example, the Swiss Synchrotron Light Source (SLS) at the Paul Scherrer Institut (PSI) provides high brightness photon beams that are used for research in biology, chemistry and materials science. In the storage ring of SLS, four ELETTRA-type [36] RF cavities with resonant frequencies of 500 MHz compensate for the energy loss due to synchrotron radiation and focus the electron bunches in the longitudinal direction [20]. Other examples of standing-wave cavities at PSI include the four coupled RF cavities with resonant frequencies of 70 MHz that power the cyclotron of the PROSCAN facility for cancer treatment [83], and the RF cavities with resonant frequencies of 50 and 150 MHz at the HIPA facility that accelerate a proton beam in order to drive a spallation neutron source and a muon and pion source for fundamental research [85].

To efficiently accelerate the beam, the RF cavity has to satisfy a variety of requirements. First, accelerator physics requirements, such as longitudinal focusing, space limitations and the availability of power sources, usually define the desired resonant frequency, the voltage and the number of cavities. Second, the fundamental mode (FM), i.e., the mode with the lowest frequency, usually needs to satisfy many requirements, which are often conflicting. For example, the shunt impedance [103] has to be maximized in order to reduce the power load, and the electric field on the cavity surface should not exceed a critical threshold in order to avoid discharges and excessive dark current in the RF cavity. Third, the interaction of higher order modes (HOMs) with the beam should be minimized. Moreover, the cavity shape needs to be robust against geometric perturbations, which could arise from, e.g., harsh operating conditions at cryogenic temperatures or manufacturing inaccuracies. Also, overly complicated shapes should be avoided in order to enable manufacturing.
Since the resonant modes, electromagnetic fields and frequencies are determined by the shape of the RF cavity, the goal is to find a cavity shape, or shapes, that satisfy the above requirements. If the cavity shape is parameterized by a design vector \( \mathbf{d} = (d_1, \ldots, d_N)^T \), also called a design point, in some search space \( X \subset \mathbb{R}^N \), this can be formulated as a constrained multi-objective shape optimization problem

\[
\begin{align*}
\min & \quad F_i(\mathbf{d}), \quad i = 1, \ldots, n, \\
G_i(\mathbf{d}) & \leq 0, \quad i = 1, \ldots, k, \quad (1.1) \\
H_i(\mathbf{d}) & = 0, \quad i = 1, \ldots, l, \quad (1.2)
\end{align*}
\]

where \( F_1, \ldots, F_n : X \to \mathbb{R} \) are objective functions, and (1.1) and (1.2) are inequality and equality constraints, respectively, with

\[
G_1, \ldots, G_k, H_1, \ldots, H_l : X \to \mathbb{R}.
\]

For example, an objective function could be defined as the peak value of the electric field on the cavity surface, and the corresponding objective to have this value as small as possible. The requirement that the resonant frequency matches the desired value could either be formulated as an objective or as a constraint.

The outline of this chapter is as follows. In section 1.1 we will give an overview of related work on RF cavity shape optimization. In section 1.2 we will describe our approach to solving the constrained multi-objective RF cavity shape optimization problem. We will list the main contributions in section 1.3, and give an outline of the thesis in section 1.4.

1.1 Related work

The first RF cavities were designed by analytically solving the eigenvalue problem that arises from Maxwell’s equations, and then using perturbation corrections \[55\] and mode matching techniques. The design of modern RF cavities still usually starts from simplified cavity shapes which possess symmetries, such as axisymmetric cavity shapes. With the help of some intuition from perturbation theory, the geometry is then iteratively optimized using computer programs, such as SUPERFISH \[46\] for axisymmetric cavities, and FemaXX \[42\] or commercially available codes like HFSS\(^1\) and Microwave Studio\(^2\) for fully three-dimensional (3D) cavities, i.e., 3D cavities that are not necessarily axisymmetric.

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\(^1\)ANSYS\(\textregistered\) HFSS, https://www.ansys.com/Products/Electronics/ANSYS-HFSS

\(^2\)CST Microwave Studio\(\textregistered\), https://www.cst.com/products/cstmws
1.2 Our approach

The corners of cylindrical cavity shapes, for which the solution is known analytically [55], were rounded, first with circle arcs and then, in order to enhance performance, ellipse arcs [61]. Such elliptical cavities are still a widely considered type of geometry [4, 13, 57, 68, 87, 88], though other types of geometries have occasionally been considered, such as, for example, the axisymmetric cavity shapes where the cross section boundary is defined by a Bézier spline [77], or a non-uniform rational B-spline [41].

For example, in [87, 88] the peak magnetic field on the cavity surface was minimized while other figures of merit were kept fixed. In [68] a Pareto front approximation between the peak electric and magnetic field on the surface of the cavity was obtained by analyzing over a thousand cavity shapes.

Another way of dealing with a multi-objective optimization problem is scalarization, i.e., converting it into a single-objective optimization problem, usually with the help of some predetermined weights. Approaches that employ scalarization and gradient-based methods for RF cavity shape optimization problems where the frequency of the accelerating mode has to match a given target frequency and one or a few properties of the electromagnetic field of the fully 3D cavity shape need to be optimized have been published in [4–6].

1.2 Our approach

In this section we will describe our approach to solving constrained multi-objective RF cavity shape optimization problems. In each of the subsections, we will first give a brief overview of the available methods and then justify our decision to use a specific one.

1.2.1 Multi-objective optimization

Two distinct approaches to solving multi-objective optimization problems are:

1. reducing the multi-objective optimization problem to a single-objective optimization problem,

2. handling the multiple objectives simultaneously.

Another way nonlinear multi-objective optimization methods can be classified is by considering the involvement of an expert in the problem domain, called a decision maker [69].

- No preference methods. The decision maker is not involved, i.e., no preference information is given. An example is the method of global criterion [109, 111], where all objective function are considered to be
1 Introduction

equally important, but a good reference solution should still be given, and the method reduces the problem to a single-objective optimization problem, i.e., this method belongs to (1).

- **A priori methods.** The decision maker gives the preference information at the beginning, after which a solution that best satisfies this information needs to be found. Examples include lexicographic ordering, goal programming [22], and the weighted sum method, which belong to (1).

- **A posteriori methods.** The decision maker chooses from a set of candidate solutions. When searching for the set of candidate solutions, one needs to be able to compare the quality of two design points, as well as a good description of optimality. A widely used description is the Pareto optimality. A point \( d_1 \) Pareto dominates another point \( d_2 \) if it is not worse than \( d_2 \) in any of the objectives, and it is strictly better in at least one objective. A point is Pareto optimal if it is not Pareto dominated by any other point in the design space. For example, multi-objective evolutionary algorithms [30, 89] belong to this category, as well as to (2).

- **Interactive methods.** The search for the solution is iterative, and the decision maker states preference in each iteration.

Since the objective functions are often conflicting, and since reducing the problem to a single-objective optimization problem often requires a priori knowledge about preference, we decide to handle the objectives simultaneously. There are many, mostly stochastic, methods that handle multiple objectives simultaneously. They are typically easy to implement and parallelize, but it can be quite challenging to find good parameters for a specific problem. Furthermore, it is not guaranteed that the found solutions will be optimal. Most of these are a posteriori methods, and most of them model stochastic processes from nature. Popular examples include evolutionary algorithms, simulated annealing [60], particle swarm optimization [58], ant colony optimization [35], and artificial immune system [29].

Evolutionary algorithms are probably the most popular, and they have already been successfully applied in the area of particle accelerator physics. For example, in [12] an evolutionary algorithm (EA) was used to optimize a high brightness dc photoinjector, and [52, 70] presented a massively parallel multi-objective optimization tool combined with beam dynamics simulation, which employed an EA as the optimization method. Other advantages of EAs include their ability to escape local optima, and their suitability for dealing with possibly discontinuous objective functions.
Therefore, we decide to use the massively parallel implementation of a multi-objective EA from [52,70] to search for the set of Pareto optimal points. In this way we can explore a wide search space and find new, potentially interesting RF cavity shapes that can then be analyzed by an expert.

**Gradient-based multi-objective optimization**

Optimization methods that use gradient information and handle the multiple objectives separately have also been suggested [37]. However, the benefit of using them is not as clearly established as in the single objective optimization problems [16]. A preliminary optimization with the approach from [37] improved all of the objective function values simultaneously, but it was very expensive, and both the improvement in the objective function values and the change in the design parameters were quite small. Still, the method is interesting and further work in this direction could lead to better results.

**1.2.2 Forward solver**

We focus on standing-wave RF cavities. The resonant electromagnetic fields and frequencies can be computed by solving time-harmonic Maxwell’s equations. Different approximation methods, e.g., the finite difference method [95], the boundary element method, the finite integration technique [99,100] or the finite element method can be used to solve time-harmonic Maxwell’s equations in order to compute the necessary electromagnetic fields and frequencies [56,72]. We opt for the mixed finite element method because of its flexibility for modeling the problem in terms of domain approximation, avoidance of spurious modes, favorable previous results and available implementations, both for the fully 3D [42] and the axisymmetric case [23]. The fully 3D solver is parallel and based on the Trilinos package [49], while the axisymmetric solver is serial. We will give the details in chapter 2.

**1.2.3 Shape parameterization and meshing**

The EA requires many function evaluations. Since a function evaluation requires the solution of time-harmonic Maxwell’s equations, and since the fully 3D solver is computationally intensive, in this thesis we will focus on axisymmetric RF cavity shapes. Cavities with coaxial coupling [82] intrinsically satisfy the axisymmetry condition. In cases where the axisymmetry condition is broken by, for example, a coupler or a damper, a fully 3D solver needs to be used. However, at the expense of increased computational cost, the same optimization method could still be employed. Furthermore, as we will illustrate
in chapter 2, the figures of merit of the close-to-axisymmetric shapes and their axisymmetric approximations are quite close, so an optimized axisymmetric cavity could be used as a starting point in a fully 3D optimization.

Two common approaches for parameterizing admissible shapes using a finite number of parameters are the following [47, 81]. First, the positions of the boundary nodes of a mesh can be taken as the design variables [39, 66]. This is an intuitive, easy to implement approach where the geometry changes are limited only by the number of design variables. However, the number of design variables often becomes very large which leads to a difficult and expensive optimization problem. Furthermore, additional constraints are often needed in order to ensure the regularity of the boundary [47]. Second, the domain boundary can be defined by a curve whose parameters are taken to be the design variables. Examples include polynomials [74, 79], Bézier curves, B-spline curves [18], non-uniform rational B-splines [86], cubic splines [97], lines and conic sections. In general, this results in fewer design variables.

We opt for the second approach and consider geometry types that are close to the RF cavity shapes which are known to be good, such as elliptical cavities. A parameterization of an elliptical cavity with a non-symmetric cross section is illustrated in Fig. 1.1. The geometry is axisymmetric, so it is enough to define half of its cross section. This can be done with eight geometric parameters:

\[ R_{eq}, \quad R_i, \quad l, \quad L, \quad A_L, B_L, A_R, B_R \]

We will often fix some of the geometric parameters to a specific value, and consider the rest to be design variables. For example, if the parameters \( L, l \) and \( R_i \) are fixed, a design point is

\[ d = (d_1, \ldots, d_5) = (R_{eq}, A_L, B_L, A_R, B_R)^T. \]

In chapters 2-4 we will also describe different types of geometries.

Once a parameterization is defined, a design point determines the RF cavity cross section, which can then be meshed. A mesh is called structured if all of its interior nodes have the same number of adjacent elements [47]. Otherwise, the mesh is called unstructured. Structured meshes are usually simpler and faster.
1.2 Our approach

Figure 1.1: An axisymmetric geometry type, with half of the cross section parameterized by $L$, $l$, $R_{eq}$, $R_i$, $A_L$, $B_L$, $A_R$, and $B_R$. The curved part of the boundary consists of four ellipse arcs of $90^\circ$.

to generate, but the size of its elements cannot vary rapidly, so, for the same problem, a structured mesh may need more elements than an unstructured one. Furthermore, it might be difficult to create a structured mesh if the domain has a complicated shape.

Since we want to be able to create and mesh various shapes, we opt for unstructured meshes. A common example of unstructured meshes are triangular meshes. Since it is open-source, widely used, written in C++ (like the EA implementation from [52, 70]), and it supports the creation of a wide variety of geometry types using, for example, lines, ellipses and non-uniform rational B-splines, we decide to use the Gmsh [43] C++ API to create unstructured triangular meshes.

1.2.4 Sensitivity analysis

Local sensitivity analysis (SA) estimates the local impact of an input parameter by computing the partial derivative of the model output with respect to the input parameter, in a specific point [91]. On the other hand, global SA studies the computational model by determining how different input parameters influence the model output [3, 91, 94]. This makes it possible to classify the parameters as important, relatively important or unimportant. For example, the unimportant input parameters can be fixed to a nominal value in order to
reduce the number of parameters, and the computational cost.

Global SA comprises many techniques and metrics \([19, 53]\). For example, screening techniques, such as the Morris method \([27]\), regression-based methods, which require linearity or monotonicity \([53]\), and variance-based methods, which can be applied to non-linear and non-monotonic models \([91, 94]\).

Variance-based methods decompose the variance of the model output into a sum of contributions of each input parameter, or their combinations. The variance-based sensitivity indices, also called Sobol’ indices \([92]\) can be computed directly, using a Monte Carlo simulation \([94]\). Since this requires a large number of model runs, whenever a model evaluation is computationally costly, metamodeling approaches are used instead. The computational model is replaced by a metamodel, also called a surrogate model, which is far less computationally expensive and has a clear internal structure. The Sobol’ indices of the computational model are then approximated by the Sobol’ indices of the surrogate model, which can either be computed using a Monte Carlo simulation, or using the known internal structure of the surrogate model.

The surrogate model is commonly computed using the polynomial chaos (PC) expansion, which is based on the polynomials that are orthogonal with respect to the probability distribution of the input parameters. The Sobol’ indices can then be computed analytically from the PC expansion coefficients \([3, 48, 84, 94]\). Furthermore, this can be computed using the Uncertainty Quantification Toolkit (UQTk) \([33, 34]\).

Therefore, we will use UQTk to compute the polynomial surrogate and the PC-based Sobol’ indices. We will use this information to identify and neglect the unimportant, i.e., the non-influential, geometric parameters. We will also identify the influential geometric parameters in order to better formulate the optimization problem and improve the optimization method.

1.2.5 Real-world problems

In this thesis we will solve the following real-world axisymmetric RF cavity shape optimization problems.

SLS 2.0

PSI is currently elaborating an upgrade proposal for SLS, called SLS 2.0 \([93]\), for dramatically improved synchrotron light quality. We will use the multi-objective EA combined with a constraint handling method to find good RF cavity shapes for SLS 2.0. Since it is planned to reuse the existing ELETTRA-type \([36]\) cavity, extended by a new type of absorber for the most troubling beam excited HOMs, our optimization will be hypothetical. Nonetheless, we
1.3 Contributions

will provide insight into the problem by computing a Pareto front approximation, and find a few good RF cavity shapes for which the beam interaction with the HOMs is already minimized. This will be presented in chapter 3.

**FCC-ee-Z**

The Future Circular Collider (FCC) [14] is planned to collide beams with unprecedented luminosities and extend the research that is currently being conducted at the Large Hadron Collider (LHC). FCC would comprise three colliders: a lepton collider (FCC-ee), a hadron collider, and a lepton-hadron collider. FCC-ee is planned to study the properties of Z, W and Higgs bosons, as well as top quark, using four different modes of operation over the years.

We will optimize the superconducting RF cavity for the Z-pole operating mode of the FCC-ee (FCC-ee-Z). In addition to optimizing the RF properties, we will focus on finding a cavity shape that is robust with respect to geometric perturbations, which could, for example, arise from manufacturing inaccuracies or perturbations during operation [17, 26, 44, 106]. We will use the results of a global SA to reformulate the problem, reduce the search space, and devise an optimization strategy. In the end we will show a good cavity for the FCC-ee-Z. This will be done in chapter 4.

### 1.3 Contributions

The major contributions of this thesis are the following.

- **A fast and stable forward solver.** We combine and extend existing codes in order to solve axisymmetric Maxwell’s equations. We parallelize the serial parts and find good parameters. Furthermore, we implement the fast calculation of many figures of merit, the creation of various cavity shapes, as well as some visualization capabilities. The resulting code can be used to compute the properties of the FM, as well as arbitrary HOMs.

- **Insight into the problem.** We perform a global SA in order to determine the relative influence of each design parameter and gain insight into the problem.

- **Optimization method.** We combine the forward solver with a massively parallel implementation of an EA in order to optimize the multiple objectives simultaneously. We find good parameters, compare different constraint handling methods and use the results of the global SA to devise a better optimization method.
1 Introduction

- Solving real-world problems. We find good cavity shapes for two real-world problems. We consider different objective functions and types of geometries, and optimize the cavities with respect to both the properties of the FM and the HOMs.

1.4 Thesis outline

In chapter 2 we will describe the forward solver, i.e., the evaluation of the vector objective function $F(d) = (F_1(d), \ldots, F_n(d))^T$ in a given design point $d = (d_1, \ldots, d_N)^T$ by solving time-harmonic Maxwell’s equations in half of the cross section of the axisymmetric RF cavity shape determined by $d$. Afterwards, in chapter 3, we will describe the use of a multi-objective EA, combined with a constraint handling method, for solving constrained multi-objective optimization problems. We will first determine good options and parameters on a few simple problems, and then hypothetically solve a real-world RF cavity shape optimization problem for the planned SLS upgrade, SLS 2.0. In chapter 4 we will perform a global SA, and use the results to reformulate the problem, reduce the search space and devise an optimization strategy. We will then find a good and robust cavity for the FCC-ee-Z. Finally, in chapter 5, we will give a summary of each of the chapters, as well as some ideas for possible future work. For the sake of clarity, we will give the auxiliary information in Appendix A.

Throughout the thesis we will use abbreviations whenever possible, so we also give a list of abbreviations at the end of the thesis, on page 121. Furthermore, after each term, symbol or abbreviation whose meaning might not be immediately apparent, we will give a reference to the place in the text where additional information can be found, in brackets. Similarly, after statements where the reasoning might not be completely clear, we will give a reference to auxiliary definitions or statements used to draw the conclusions. Moreover, we color-code the tables: the colors orange, red and blue refer to the information on the design variables, objective functions and ‘other’, respectively.

We ran the simulations and optimizations on the Euler cluster\(^3\) of ETH Zürich, either using Intel Xeon E5-2680 V3 (12 cores @ 2.5 GHz, cache size 30 MB) or Intel Xeon Gold 6150 (18 cores @ 2.7 GHz, cache size 24.75 MB), with gcc 4.8.2, Gmsh 2.12.0, and Trilinos 12.6.1.

\(^3\)https://scicomp.ethz.ch/wiki/Euler
In this chapter we will describe the forward solver, i.e., the evaluation of the vector objective function \( \mathbf{F} = (F_1, \ldots, F_n)^T \) in a design point \( \mathbf{d} = (d_1, \ldots, d_N)^T \) that determines an RF cavity shape [cf. section 1.2.3]. The entire process is illustrated in Fig. 2.2. We consider axisymmetric RF cavity shapes, in which case the 3D cavity shape is described by (half of) its cross section. This is illustrated in Fig. 2.1, where the cylinder in the top left corner is determined by the light gray rectangle, parameterized by the radius \( R \) and length \( L \). A more complicated axisymmetric cavity shape, determined by \( L, l, R_{eq}, R_i, A_L, B_L, A_R, B_R \), is shown in Fig. 1.1. In the following we will call these variables geometric parameters. Either all or some of these (with the rest fixed to a specific value) will be considered as design variables in the optimization. In sections 2.1–2.4 we will present our approach to solving time-harmonic Maxwell’s equations in axisymmetric domains. Afterwards, in section 2.5, we will describe the calculation of some figures of merit. In chapters 3 and 4 we will use these figures of merit to define the objective functions.

Figure 2.1: An axisymmetric RF cavity with a cylindrical shape, called the pillbox cavity (top left), and half of its cross section \( \Omega_p \) (bottom right). \( \partial \Omega_p \) denotes the boundary of \( \Omega_p \), and the axes are oriented such that the particles travel horizontally.
2.1 Maxwell’s equations in axisymmetric domains

In this section we will give time-harmonic Maxwell’s equations in a 3D domain (Problem 1) and describe the simplification in case the domain is axisymmetric, which leads to the formulation of Problem 3.

We first define the following boundary conditions (BC):

- perfectly electrically conducting (PEC) BC - the electric field is perpendicular to the surface (i.e., denoting the surface normal by \( \mathbf{n} \), \( \mathbf{e} \times \mathbf{n} = 0 \)), and the magnetic field is parallel,

- perfectly magnetically conducting (PMC) BC - the electric field is parallel to the surface (\( \mathbf{e} \cdot \mathbf{n} = 0 \)), and the magnetic field is perpendicular.
2.1 Maxwell’s equations in axisymmetric domains

We assume PEC BC [cf. (2.2)]. We also assume that there is vacuum inside the cavity, and that there are no external fields, sources or charges. A time-harmonic approach for the electric and magnetic field leads to the following form of Maxwell’s equations [42, p.16].

Problem 1. Given \( \Omega \subset \mathbb{R}^3 \) an open bounded domain with a Lipschitz continuous boundary \( \Gamma \), find \( e : \Omega \rightarrow \mathbb{R}^3 \) and \( \lambda \in \mathbb{R} \) such that

\[
\begin{align*}
\text{curl}(\text{curl}(e)) &= \lambda e, & \text{in } \Omega, \\
\text{div}(e) &= 0, & \text{in } \Omega, \\
e \times n &= 0, & \text{on } \Gamma,
\end{align*}
\]

(2.1)

where \( n \) is the surface normal.

Denoting \( e = (e_x, e_y, e_z)^T \), the \text{div} and \text{curl} operators are defined as

\[
\text{div}(e) = \partial_x e_x + \partial_y e_y + \partial_z e_z
\]

and

\[
\text{curl}(e) = (\partial_y e_z - \partial_z e_y, \partial_z e_x - \partial_x e_z, \partial_x e_y - \partial_y e_x)^T.
\]

(2.3)

Remark 1. Problem 1 has a solution only for some \( \lambda > 0 \) [23, pp.12,25,235]. The corresponding eigenfrequency is given by \( \omega = \sqrt{\lambda c} \), where \( c \) is the speed of light in vacuum\(^1\). The corresponding function \( e \) is often called the eigenfield.

The formulation in Problem 1, called the strong formulation, is often too difficult to solve directly. Therefore, the strong formulation equations are multiplied with appropriate test functions, and the resulting expressions integrated over the relevant domain. This leads to the formulation in Problem 2, called the weak formulation, which can be solved numerically using the finite element method [cf. section 2.3]. The function spaces are defined in Appendix A.1, Definition 4. The details can be found in [23, pp.20-26].

Problem 2. Let \( \Omega \subset \mathbb{R}^3 \) be an open bounded domain with a Lipschitz continuous boundary \( \Gamma \). Find \( e \in H_0(\text{curl}; \Omega) \) and \( \lambda \in \mathbb{R} \) such that for all test functions \( \delta \in H_0(\text{curl}; \Omega) \)

\[
\int_{\Omega} \text{curl}(\delta)^T \text{curl}(e) \, d\Omega = \lambda \int_{\Omega} \delta^T e \, d\Omega,
\]

and that for all \( \psi \in H_0^1(\Omega) \)

\[
\int_{\Omega} \text{grad}(\psi)^T e \, d\Omega = 0.
\]

(2.4)

\(^1c = 299,792,458 \text{ m/s} [96]\)
Denoting a point in $\Omega$ by $(x, y, z)^T$, the gradient in (2.4) is

$$\text{grad}(\psi) = (\partial_x \psi, \partial_y \psi, \partial_z \psi)^T.$$  \hfill (2.5)

**Remark 2.** The PEC BC (2.2) is enforced implicitly by $e \in H_0(\text{curl}; \Omega)$ [cf. Definition 4]. (2.4) corresponds to the divergence freeness condition (2.1).

In the following we will assume that $\Omega$ is axisymmetric. We will denote half of its cross section by $\Omega_p$ and refer to it simply as ‘the cross section’. We will denote the set of points on the boundary of $\Omega_p$ that are also located on the axis of rotation by $\Gamma_0$, and the rest of the boundary by $\Gamma_p$. This is illustrated in Fig. 2.1.

We denote the electric field in cylindrical coordinates by $\hat{e}$. Then

$$e(x) = U(\theta)\hat{e}(r),$$  \hfill (2.6)

where $r = (r, \theta, z)^T$, $x = (x, y, z)^T = (r \cos \theta, r \sin \theta, z)^T$ and

$$U(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$  

In order to allow only meaningful field descriptions in cylindrical coordinates, for a fixed $z \in \mathbb{R}$ the following uniqueness condition has to hold

$$e(0, 0, z) = U(\theta)\hat{e}(0, \theta, z), \quad \forall \theta \in [0, 2\pi].$$  \hfill (2.7)

The Fourier expansion in the azimuthal direction separates the meridian coordinates $r$ and $z$ from the azimuthal coordinate $\theta$ ($r_p = (r, z)^T$)

$$\hat{e}(r, \theta, z) = \sum_{m=0}^{\infty} \left[ c_e^{(m)}(r_p) \cos (m \theta) + s_e^{(m)}(r_p) \sin (m \theta) \right].$$  \hfill (2.8)

The number $m \in \mathbb{N}_0$ is called the azimuthal mode number,

$$c_e^{(m)} = (c_e^{(m)}(r_p), c_e^{(m)}(r_p), c_e^{(m)}(r_p))^T \quad \text{and} \quad s_e^{(m)} = (s_e^{(m)}(r_p), s_e^{(m)}(r_p), s_e^{(m)}(r_p))^T.$$  

Defining

$$w(r_p) = \begin{cases} (c_e^{(0)}(r_p), c_e^{(0)}(r_p), c_e^{(0)}(r_p))^T & \text{if } m = 0, \\
(c_e^{(m)}(r_p), s_e^{(m)}(r_p), c_e^{(m)}(r_p))^T & \text{if } m \in \mathbb{N}, \end{cases}$$  \hfill (2.9)

one arrives at the Fourier expanded weak formulation in cylindrical coordinates (Problem 3). The definitions of the function spaces are in Appendix A.1, Definition 5. For readability, we write $\langle a, b \rangle$ for $a^T b$. The details can be found in [23, pp.27-36].
2.1 Maxwell’s equations in axisymmetric domains

Problem 3. Let \( \Omega \subset \mathbb{R}^3 \) be an open bounded axisymmetric domain with a Lipschitz continuous boundary. Also, let \( \Omega_p \subset [0, \infty) \times \mathbb{R} \) be its cross section, and \( m \in \mathbb{N}_0 \) a fixed azimuthal mode number [cf. (2.8)]. Find \( w \in \mathring{H}_0(\text{curl}; \Omega_p) \) (\( w = (w_r, w_\theta, w_z)^T \)) and \( \lambda \in \mathbb{R} \) such that for all test functions \( v \in \mathring{H}_0(\text{curl}; \Omega_p) \) (\( v = (v_r, v_\theta, v_z)^T \)) and \( v_p = (v_r, v_z)^T \)

\[
\int_{\Omega_p} \frac{1}{r} \langle m v_p + \text{grad}_p(rv_\theta), m w_p + \text{grad}_p(rw_\theta) \rangle \, d\Omega_p \\
+ \int_{\Omega_p} r \langle \text{curl}_p(v)_p, \text{curl}_p(w_p) \rangle \, d\Omega_p
\]

\[
= \lambda \int_{\Omega_p} r \langle v_p, w_p \rangle + r \langle v_\theta, w_\theta \rangle \, d\Omega_p,
\]

and that for all \( \varphi \in \mathring{H}^1_0(\Omega_p) \)

\[
\int_{\Omega_p} r \langle \text{grad}_p(\varphi), w_p \rangle - m \langle \varphi, w_\theta \rangle \, d\Omega_p = 0.
\]

The operator \( \text{curl}_p \) is defined as [cf. (2.3)]

\[
\text{curl}_p(g_p) = \partial_r g_z - \partial_z g_r,
\]

and, for a scalar function \( h : \Omega_p \rightarrow \mathbb{R} \), \( \text{grad}_p \) is defined as

\[
\text{grad}_p(h) = (\partial_r h, \partial_z h)^T.
\]

Remark 3. (2.11) corresponds to the divergence freeness condition (2.4).

Remark 4. The choice of the function space \( \mathring{H}_0(\text{curl}; \Omega_p) \) ensures that the solution satisfies the uniqueness condition corresponding to (2.7) [23, §3.5].

Note that in Problem 3 the azimuthal mode number \( m \in \mathbb{N}_0 \) is fixed. We can see from (2.8) that when \( m = 0 \), the electric field in cylindrical coordinates \( \mathbf{\hat{e}} \) does not depend on the azimuthal coordinate \( \theta \), i.e., the field is axisymmetric [cf. Fig. 2.8]. When \( m \in \mathbb{N} \), a solution \( w \) of Problem 3 corresponds to two eigenfields [23, p.35]

\[
\mathbf{\hat{e}}_1^{(m)}(r, \theta, z) = \begin{pmatrix} c^{(m)}_{e,r}(r_p) \cos(m\theta) \\ s^{(m)}_{e,\theta}(r_p) \sin(m\theta) \\ c^{(m)}_{e,z}(r_p) \cos(m\theta) \end{pmatrix},
\]

\[\text{(2.13)}\]
2 Forward solver

and

\[ e^{(m)}_2(r, \theta, z) = \begin{pmatrix}
-c^{(m)}(r_p) \sin(m \theta) \\
\frac{s^{(m)}(r_p)}{r_p} \cos(m \theta) \\
-c^{(m)}(r_p) \sin(m \theta)
\end{pmatrix} \begin{pmatrix}
(*) \\
\hat{e}^{(m)}_1(r, \theta + \pi/(2m), z)
\end{pmatrix}, \]

where \((*)\) denotes \(\sin(-x) = -\sin(x), \cos(-x) = \cos(x), \cos(x) = \sin(x + \frac{\pi}{2})\). These two fields correspond to the same \(\lambda^{(m)}\) [cf. Table 2.3], and the set of all solutions can be obtained by unifying the solutions for all \(m \in \mathbb{N}_0\). In practice, one is usually interested in the smallest eigenfrequencies of Problem 1 [cf. Remark 1], so only the problems [cf. Problem 3] corresponding to the few smallest \(m\) need to be considered. In the optimizations in chapters 3 and 4, it will suffice to consider \(m \in \{0, 1\}\).

To sum up, in order to solve time-harmonic Maxwell’s equations in a given axisymmetric RF cavity shape \(\Omega \subset \mathbb{R}^3\), we can solve Problem 3 in its cross section \(\Omega_p \subset [0, \infty) \times \mathbb{R}\), for a few of the lowest \(m \in \mathbb{N}_0\). Since exact solutions of Problem 3 are usually not available (an exception is the pillbox cavity from Fig. 2.1), we compute approximate solutions numerically. We follow [23, §4.3] and opt for the mixed finite element method. One of the benefits of this approach is the separation into meridian and azimuthal coordinates. Meridian coordinates \(r_p = (r, z)^T\) are approximated using two dimensional Nédélec basis functions, and the azimuthal coordinate \(\theta\) is approximated using slightly modified scalar Lagrange basis functions [cf. section 2.3]. Other benefits include avoiding the computation of non-physical solutions (also called spurious modes), and ease of incorporating curl conformity conditions [cf. \(\mathcal{H}(\text{curl}; \Omega_p)\), Definition 5] and BC [cf. \(\mathcal{H}_0(\text{curl}; \Omega_p)\), p.12]. Lastly, another very important reason for us is the availability of a very good serial implementation [23, 24] for constructing the finite element matrices for Problem 3.

In the following section we will describe the meshing of \(\Omega_p\) (i.e., the spatial discretization), and in section 2.3 the discretization of the function spaces \(\mathcal{H}_0(\text{curl}; \Omega_p)\) and \(\mathcal{H}_1^0(\Omega_p)\).

2.2 Spatial discretization

The 2D cross section \(\Omega_p \subset [0, \infty) \times \mathbb{R}\) is first (approximately) subdivided into mutually disjoint (and not too distorted) polygons, usually triangles and quadrilaterals [23, §4.2]. This is called spatial discretization, or meshing. Since our domain \(\Omega_p\) usually has a complicated shape [cf. Fig. 1.1], we use unstructured triangular meshes. We create these using the Gmsh [43] C++ API since
it is open source, written in C++, widely used, and it supports the creation of various shapes using, e.g., lines, circle arcs, and non-uniform rational B-splines. A mesh of the cross section of the pillbox cavity from Fig. 2.1 is shown in Fig. 2.3. In case the cross section $\Omega_p$ has a curved boundary, as is, for example, the case in Fig. 1.1, a mesh will only be an approximation of $\Omega_p$.

Figure 2.3: An unstructured triangular mesh of the pillbox cavity from Fig. 2.1.

We consider the sets of all triangles, vertices and edges in the mesh to be ordered and denote them by $T$, $V$ and $E$, respectively. We denote the $i$-th triangle in $T$ by $T_i$, the $i$-th vertex in $V$ by $V_i$, and the $i$-th edge in $E$ by $E_i$. Furthermore, we denote the total number of triangles, vertices and edges by $|T|$, $|V|$ and $|E|$, respectively. The set $V$ consist of pairs of coordinates $(r,z)$, each corresponding to a vertex in the mesh. The set $E$ consists of pairs of indices $(i,j)$, where the pair $(i,j)$ corresponds to the edge between $i$-th and $j$-th vertex in $V$. A triangle $T_i$ is represented as a pair $(T^v_i, T^e_i)$, where $T^v_i = (T^v_{i,1}, T^v_{i,2}, T^v_{i,3})$ and $T^e_i = (T^e_{i,1}, T^e_{i,2}, T^e_{i,3})$ are triples of the indices of $T_i$’s vertices and edges, respectively. The triple of vertex indices $T^v_i$ is ordered counterclockwise, starting from the vertex with the smallest $r$ (Fig. 2.4, left). If there are two such vertices, the one with the smaller $z$ is taken to be the start vertex (Fig. 2.4, right). The edge indices then satisfy

$$E_{T^e_{i,1}} = (T^v_{i,1}, T^v_{i,2}), \quad E_{T^e_{i,2}} = (T^v_{i,1}, T^v_{i,3}) \quad \text{and} \quad E_{T^e_{i,3}} = (T^v_{i,2}, T^v_{i,3}).$$

For use in the next section, we also define the sets of indices [cf. Fig. 2.1]

\[
\begin{align*}
V_{\Gamma_0} &= \{i \in \{1, \ldots, |V|\} : V_i \in \Gamma_0\} \\
V_{\Gamma_p} &= \{i \in \{1, \ldots, |V|\} : V_i \in \Gamma_p\} \\
E_{\Gamma_0} &= \{i \in \{1, \ldots, |E|\} : E_i = (j,k) \quad \text{and} \quad V_j, V_k \in \Gamma_0\} \\
E_{\Gamma_p} &= \{i \in \{1, \ldots, |E|\} : E_i = (j,k) \quad \text{and} \quad V_j, V_k \in \Gamma_p\}
\end{align*}
\]
2 Forward solver

and

\[ T_{i,0} = \{ i : T_{i,2}^e \in \Gamma_0 \}. \]

Note that, in case the triangle \( T_j \) has an edge on the rotation axis, the index of that edge will always be stored at \( T_{j,2}^e \) [cf. Fig. 2.4, right].

In general, the cross section \( \Omega_p \) is approximated by (\( \overline{T_i} \) is the closure of \( T_i \))

\[ \Omega_{p,T} = \bigcup_{i=1}^{\lvert T \rvert} \overline{T_i}, \tag{2.15} \]

so the integrals over \( \Omega_p \) [cf. (2.28)] can be approximated as

\[ \int_{\Omega_p} \approx \int_{\Omega_{p,T}} = \sum_{i=1}^{\lvert T \rvert} \int_{\overline{T_i}}. \tag{2.16} \]

Figure 2.4: Ordering of vertex and edge indices.

2.3 Mixed finite element method

In this section we will describe the discretization of Problem 3 using the mixed finite element method (FEM), which leads to the generalized (matrix) eigenvalue problem (GEVP) in Problem 4.

Even though in [23] both linear and quadratic basis functions are used, in both cases the approximated domain boundary consists of straight line segments, so the advantage of quadratic basis function is lost if the domain has a curved boundary [cf. Fig. 2.10]. Therefore, with the exception of Fig. 2.6,
2.3 Mixed finite element method

Fig. 2.10 and Table 2.2, which we use to illustrate the comparison between these two cases, and the artificial optimization problem in section 3.3, in the rest of the thesis we will only use linear basis functions, i.e., a first order approximation. Moreover, as stated in section 2.2, we will always use triangular meshes, so we will only describe how the linear basis functions are defined for triangles. The description of linear and quadratic basis functions for triangles and rectangles can be found in [23, pp.43-74]. A second order approximation employing both linear and quadratic basis functions and curvilinear elements could also be used. In order to do this, the integration of the bilinear forms (2.28) would have to be performed differently than in the existing implementation from [23], e.g., according to [23, §5.4]. Since the results we get using the first order approximation are already sufficiently accurate, we refrain from doing this.

Linear Lagrange basis functions restricted to the reference triangle (Fig. 2.5, left) are \( \left( \rho = (\rho, \zeta)^T \right) \)

\[
N_1^\Delta (\rho) = 1 - \rho - \zeta, \quad N_2^\Delta (\rho) = \rho, \quad \text{and} \quad N_3^\Delta (\rho) = \zeta. \tag{2.17}
\]

Denoting \( \text{grad}_\rho (N_i^\Delta) = (\partial_\rho N_i^\Delta, \partial_\zeta N_i^\Delta)^T \) [cf. (2.5)], linear Nédélec basis functions on the reference triangle are

\[
N_1^\Delta = N_1^\Delta \text{grad}_\rho (N_2^\Delta) - N_2^\Delta \text{grad}_\rho (N_1^\Delta),
\]

\[
N_2^\Delta = N_1^\Delta \text{grad}_\rho (N_3^\Delta) - N_3^\Delta \text{grad}_\rho (N_1^\Delta), \tag{2.18}
\]

\[
N_3^\Delta = N_2^\Delta \text{grad}_\rho (N_3^\Delta) - N_3^\Delta \text{grad}_\rho (N_2^\Delta).
\]

For a triangle \( T_i \) with vertices \( V_{T_{i,j}} \), \( j = 1, 2, 3 \) and

\[
B = (V_{T_{i,2}} - V_{T_{i,1}}, V_{T_{i,3}} - V_{T_{i,1}})
\]

the affine mapping

\[
\rho \rightarrow B \rho + V_{T_{i,1}}
\]

maps the reference triangle (Fig. 2.5, left) to \( T_i \). Its inverse

\[
\rho_p \rightarrow B^{-1}(\rho_p - V_{T_{i,1}})
\]

can be used to define the corresponding functions on \( T_i \) in the following way (\( f^\Delta \) denotes one of the restrictions to the reference triangle, and \( f \) the corresponding function on \( T_i \))

\[
f(\rho_p) = f^\Delta \left( B^{-1}(\rho_p - V_{T_{i,1}}) \right).
\]
The gradient and curl operators are then
\[
\text{grad}_\rho f(r_\rho) = B^{-T} \text{grad}_\rho f^\Delta(\rho),
\]
\[
\text{curl}_\rho f(r_\rho) = (1,0) \cdot B^{-T} \text{grad}_\rho (f_2^\Delta)(\rho) - (0,1) \cdot B^{-T} \text{grad}_\rho (f_1^\Delta)(\rho).
\]
Since it can happen that two adjacent restricted Nédélec basis functions point in opposite directions, a global edge direction is defined. For the edge \((i,j) \in E\) (note that \(i,j \in \{1,\ldots,|V|\}\) and \(i \neq j\)),
\[
dir(i,j) = \begin{cases} 
1, & \text{if } i < j, \\
-1, & \text{if } i > j.
\end{cases}
\] (2.19)

**Remark 5.** Unrestricted linear Lagrange basis functions have the shape of a pyramid. The apex of \(N_j\) is located at the vertex \(V_j\) [cf. Fig. 2.5, right], and its height is one. Consequently, the total number of unrestricted linear Lagrange basis functions is \(|V|\). The base of the pyramid is comprised of all the triangles adjacent to \(V_j\). Therefore, the support of \(N_j\) is the union of these triangles. A linear combination of unrestricted linear Lagrange basis functions is a continuous piecewise linear function.

**Remark 6.** Unrestricted linear Nédélec basis functions are associated with edges in the mesh [cf. Fig. 2.5, right]. The support of \(N_i\) is the union of the triangles adjacent to the edge \(E_i\). A linear combination of unrestricted linear
\[
N_i = (N_i^{(r)}, N_i^{(z)})^T, \quad i = 1, \ldots, |E|,
\]
and the unrestricted linear Lagrange basis function corresponding to \( V_j \) by
\[
N_j, \quad j = 1, \ldots, |V|,
\]
the function spaces \( \hat{H}_0(\text{curl}; \Omega_p) \) and \( \hat{H}_1(\Omega_p) \) can be discretized as follows.

\[
D_0(\text{curl}; \Omega_p) = \left\{ w = \left( \sum_{i=1}^{|E|} q_i^{(p)} N_i^{(r)}, \sum_{j=1}^{|V|} q_j^{(\theta)} \frac{1}{r} N_j, \sum_{i=1}^{|E|} q_i^{(p)} N_i^{(z)} \right)^T : w \in \hat{H}_0(\text{curl}; \Omega_p) \right\}
\]
\[
D_0^1(\Omega_p) = \left\{ \varphi = \sum_{j=1}^{|V|} z_j N_j : \varphi \in \hat{H}_1(\Omega_p) \right\}
\]

**Remark 7.** Unrestricted Lagrange basis functions \( N_j \) [cf. (2.22)] are multiplied by \( r^{-1} \) in order to prevent the emergence of spurious modes [45, 104].

In order for \( w \) from (2.22) to belong to \( \hat{H}_0(\text{curl}; \Omega_p) \), and \( \varphi \) from (2.23) to belong to \( \hat{H}_1(\Omega_p) \), the following needs to be satisfied [23, §4.4.1].

For all indices \( i \in V_{\Gamma_p} \),
\[
z_i, q_i^{(\theta)} := 0.
\]
If \( m = 0 \), \( \forall i \in T_{\Gamma_0} \),
\[
q_{T_i}^{(\theta)}, q_{T_i}^{(\theta)} : z_{T_i}^{(\theta)}, q_{T_i}^{(\theta)} : 0.
\]
If \( m > 0 \), \( \forall i \in T_{\Gamma_0} \),
\[
z_{T_i}^{(\theta)}, q_{T_i}^{(\theta)}, q_{T_i}^{(\theta)}, q_{T_i}^{(p)} : 0,
\]
\[
q_{T_i}^{(p)} := -\frac{1}{m} q_{T_i}^{(\theta)},
\]
\[
q_{T_i}^{(p)} := \frac{1}{m} q_{T_i}^{(\theta)}.
\]
We now define the vector of all degrees of freedom (DoFs), i.e., of all coefficients from (2.22)
\[ \tilde{\mathbf{q}} = (q_1^{(p)}, \ldots, q_{|E|}^{(p)}, q_1^{(\theta)}, \ldots, q_{|V|}^{(\theta)})^T, \] (2.27)
and the following bilinear forms, which are the building blocks of (2.10) in Problem 3 \((a, b)^*\) again denotes \(a^T b\),
\[ \hat{a}_{cc}(\mathbf{g}, \mathbf{f}) = \int_{\Omega_p} r \langle \text{curl}_p(\mathbf{g}), \text{curl}_p(\mathbf{f}) \rangle \, d\Omega_p, \]
\[ \hat{a}_{pp}(\mathbf{g}, \mathbf{f}) = \int_{\Omega_p} \frac{1}{r} \langle \mathbf{g}, \mathbf{f} \rangle \, d\Omega_p, \]
\[ \hat{a}_{p\theta}(\mathbf{g}, \mathbf{f}) = \int_{\Omega_p} \frac{1}{r} \langle \mathbf{g}, \text{grad}_p(\mathbf{f}) \rangle \, d\Omega_p, \]
\[ \hat{a}_{\theta p}(\mathbf{g}, \mathbf{f}) = \int_{\Omega_p} \frac{1}{r} \langle \text{grad}_p(\mathbf{g}), \mathbf{f} \rangle \, d\Omega_p, \]
\[ \hat{a}_{\theta\theta}(\mathbf{g}, \mathbf{f}) = \int_{\Omega_p} \frac{1}{r} \langle \text{grad}_p(\mathbf{g}), \text{grad}_p(\mathbf{f}) \rangle \, d\Omega_p, \]
\[ \hat{b}_{pp}(\mathbf{g}, \mathbf{f}) = \int_{\Omega_p} r \langle \mathbf{g}, \mathbf{f} \rangle \, d\Omega_p, \]
\[ \hat{b}_{\theta\theta}(\mathbf{g}, \mathbf{f}) = \int_{\Omega_p} \frac{1}{r} \langle \mathbf{g}, \mathbf{f} \rangle \, d\Omega_p. \]

We also define the following matrices
\[ [\tilde{A}_{cc}]_{i,j} = \tilde{a}_{cc}(N_i, N_j), \quad i, j = 1, \ldots, |E|, \]
\[ [\tilde{A}_{pp}]_{i,j} = \tilde{a}_{pp}(N_i, N_j), \quad i, j = 1, \ldots, |E|, \]
\[ [\tilde{A}_{p\theta}]_{i,j} = \tilde{a}_{p\theta}(N_i, N_j), \quad i = 1, \ldots, |E|, \quad j = 1, \ldots, |V|, \]
\[ [\tilde{A}_{\theta p}]_{i,j} = \tilde{a}_{\theta p}(N_i, N_j), \quad i = 1, \ldots, |V|, \quad j = 1, \ldots, |E|, \]
\[ [\tilde{A}_{\theta\theta}]_{i,j} = \tilde{a}_{\theta\theta}(N_i, N_j), \quad i, j = 1, \ldots, |V|, \]
\[ [\tilde{M}_{pp}]_{i,j} = \tilde{b}_{pp}(N_i, N_j), \quad i, j = 1, \ldots, |E|, \]
\[ [\tilde{M}_{\theta\theta}]_{i,j} = \tilde{b}_{\theta\theta}(N_i, N_j), \quad i, j = 1, \ldots, |V|, \]

where \(\tilde{a}_*\) and \(\tilde{b}_*\) indicates that \(\hat{a}_*\) and \(\hat{b}_*\), respectively, from (2.28) are computed numerically on a given mesh \([\text{cf. (2.16)}]\). Since most of the basis function supports are disjoint, the integrals over most triangles are zero. In the case of
2.3 Mixed finite element method

the bilinear forms $\tilde{a}_{cc}$ and $\tilde{b}_{pp}$, the functions that need to be integrated over a triangle are polynomials. All other bilinear forms contain the factor $r^{-1}$ which requires a more careful approach, especially near the rotation axis. In this case the integrals over triangles are transformed into sums of one-dimensional integrals over triangle boundaries, and these line integrals are computed using an appropriate Gauss quadrature rule [24]. A detailed explanation is given in [23, pp.75-95].

Remark 8. It is clear from (2.28) that $\tilde{a}_{p\theta}(g, f) = \tilde{a}_{\theta p}(f, g)$, so $\tilde{A}_{p\theta} = \tilde{A}_{\theta p}^T$.

Using (2.29) we now also define the following matrices of dimension $|V| + |E|$, 

$$
\tilde{A} = \begin{bmatrix}
\tilde{A}_{cc} + m^2 \tilde{A}_{pp} & m\tilde{A}_{p\theta} \\
m\tilde{A}_{\theta p} & \tilde{A}_{\theta\theta}
\end{bmatrix}
\quad \text{and} \quad
\tilde{M} = \begin{bmatrix}
\tilde{M}_{pp} & 0 \\
0 & \tilde{M}_{\theta\theta}
\end{bmatrix}.
$$

Remark 9. We can see from (2.28) and Remark 8 that 

$$
\tilde{A} = \tilde{A}^T \quad \text{and} \quad \tilde{M} = \tilde{M}^T.
$$

Furthermore, for 

$$
u = \left(u_1^{(1)}, \ldots, u_1^{(|E|)}, u_1^{(2)}, \ldots, u_2^{(2)}\right)^T,$$

$u^T \tilde{M} u$ and $u^T \tilde{A} u$ are 

$$
\int_{\Omega_p} r\langle u_p, u_p \rangle \, d\Omega_p + \int_{\Omega_p} r\langle u_\theta, u_\theta \rangle \, d\Omega_p
$$

(2.30)

and

$$
\int_{\Omega_p} r\langle \text{curl}_p(u_p), \text{curl}_p(u_p) \rangle \, d\Omega_p \\
+ \int_{\Omega_p} \frac{1}{r} \langle m u_p + \text{grad}_p(ru_\theta), m u_p + \text{grad}_p(ru_\theta) \rangle \, d\Omega_p,
$$

(2.31)

respectively, where $u_p = \sum_{i=1}^{|E|} u_i^{(1)} N_i$ and $u_\theta = \frac{1}{r} \sum_{i=1}^{|V|} u_i^{(2)} N_i$. Therefore, $\tilde{M}$ is positive definite and $\tilde{A}$ is positive semi-definite, with (2.31) being equal to zero if and only if 

$$
u_p = -\frac{1}{m} \text{grad}_p(ru_\theta).
$$

(2.32)
2 Forward solver

In order to take the conditions in (2.24), (2.25) and (2.26) into account, we first define two matrices, \( L \) and \( Z \). The matrix \( L \) corresponds to the last two equations in (2.26). It is initialized as the identity matrix of dimension \(|E| + |V|\), denoted \( I_{|E|+|V|} \). For every DoF \( \widetilde{[q]}_i \) [cf. (2.27)] that is expressed using another DoF \( \widetilde{[q]}_j \) (we can see from (2.27) that \( i \in \{1, \ldots, |E|\} \) and \( j \in \{|E| + 1, \ldots, |E| + |V|\} \)) as \( \widetilde{[q]}_i := \alpha \widetilde{[q]}_j \) in (2.26) \( (\alpha \in \{-1/m, 1/m\}) \), \( [L]_{i,j} := \alpha \). Every DoF that is set to zero or expressed using another DoF \( i \) is removed if the corresponding DoF \( \widetilde{[q]}_i \) in (2.27) should be eliminated. This is accomplished using the matrix \( Z \), which is defined as the identity matrix \( I_{|E|+|V|} \) whose column \( i \) is removed if the corresponding DoF \( \widetilde{[q]}_i \) in (2.27) should be eliminated. Finally, applying these two matrices leads to the definition of the finite element matrices

\[
A = Z^T L^T \tilde{A} L Z \quad \text{and} \quad M = Z^T L^T \tilde{M} L Z. \tag{2.33}
\]

**Remark 10.** It is clear from Remark 9 and (2.33) that

\[
A = A^T \quad \text{and} \quad M = M^T.
\]

Furthermore, \( M \) is positive definite and \( A \) positive semi-definite since [cf. Remark 9]

\[
u^T M u = (LZu)^T \tilde{M}(LZu) \geq 0,
\]

and

\[
LZu = 0 \Rightarrow u = 0 \quad \tag{2.34}
\]

(2.34) can easily be seen using the definitions of \( L \) and \( Z \).

Similarly, in order to arrive at the discrete divergence freeness condition, we first define a matrix \( \tilde{C} \) of dimension \(|E| \times |V|\) in the following way. We set \( \tilde{C} \) to \( 0_{|E| \times |V|} \), and then for every \( i \in \{1, \ldots, |T|\} \) set [cf. (2.19)]

\[
\begin{align*}
[\tilde{C}]_{T_{i,1}^e, T_{i,1}^v} &:= -\text{dir}(T_{i,1}^v, T_{i,2}^v), \quad [\tilde{C}]_{T_{i,2}^e, T_{i,1}^v} := -\text{dir}(T_{i,1}^v, T_{i,3}^v), \\
[\tilde{C}]_{T_{i,1}^e, T_{i,2}^v} &:= \text{dir}(T_{i,1}^v, T_{i,2}^v), \quad [\tilde{C}]_{T_{i,3}^e, T_{i,2}^v} := -\text{dir}(T_{i,2}^v, T_{i,3}^v), \\
[\tilde{C}]_{T_{i,2}^e, T_{i,3}^v} &:= \text{dir}(T_{i,1}^v, T_{i,3}^v), \quad [\tilde{C}]_{T_{i,3}^e, T_{i,3}^v} := \text{dir}(T_{i,2}^v, T_{i,3}^v).
\end{align*}
\]

**Remark 11.** The \( j \)-th column of \( \tilde{C} \) stores the information on the Nédélec functions that need to be combined to obtain \( \text{grad}_p(N_j) \) [23, §4.3.3]. It is easy to show using (2.17) and (2.18) that

\[
\begin{align*}
\text{grad}_p(N_1^\triangle) & = -N_1^\triangle - N_2^\triangle, \\
\text{grad}_p(N_2^\triangle) & = N_1^\triangle - N_3^\triangle, \\
\text{grad}_p(N_3^\triangle) & = N_2^\triangle + N_3^\triangle.
\end{align*}
\]
that such relations also hold for arbitrary triangles, and that the contribution of the Nédélec function $N_i$ to the gradient of $N_j$ is positive if and only if $N_i$ points towards the vertex $V_j$. Since it is sometimes necessary to change the sign due to the direction of the edge [cf. (2.19)], this corresponds to (2.35).

Furthermore, we define a matrix $\tilde{Y}$ of dimension $(|E| + |V|) \times |V|$ as

$$\tilde{Y} = \begin{bmatrix} \tilde{C} \\ -mI_{|V|} \end{bmatrix}. \quad (2.36)$$

As in the case of $A$ and $M$, we need to take into account the conditions in (2.24), (2.25) and (2.26). Defining also a matrix $Z_Y$ as the identity matrix $I_{|V|}$ whose column $i$ is removed if $z_i$ is set to zero either in (2.24) or (2.26), we can finally define

$$Y = Z^T L \tilde{Y} Z_Y. \quad (2.37)$$

Remark 12. It can easily be seen that $Z^T L = Z^T$. Therefore [cf. (2.37)],

$$Y = Z^T \tilde{Y} Z_Y.$$

We now state the first order approximation of Problem 3 from section 2.1.

Problem 4. Let the geometry $\Omega$ be defined as in Problem 3, and let $V, E, T$ be the components of a mesh that approximates $\Omega_p$, and $m \in \mathbb{N}_0$ a fixed azimuthal mode number. Find a (non-zero) vector $q$ and $\lambda \in \mathbb{R}$ such that

$$Aq = \lambda Mq \quad (2.38)$$

and

$$Y^T M q = 0, \quad (2.39)$$

where $A$ and $M$ are defined in (2.33), and $Y$ is defined in (2.37).

Remark 13. The eigenvector $q$ contains the DoFs from (2.27) that do not get eliminated by applying (2.24), (2.25) and (2.26).

Remark 14. We know from Remark 10 that $M$ is symmetric positive definite and $A$ symmetric positive semi-definite. Since both matrices are symmetric and $M$ is positive definite, $\lambda \in \mathbb{R}$ [73, p.345]. Since $A$ is also positive semi-definite,

$$\lambda = \frac{q^* Aq}{q^* M q} \geq 0.$$

Furthermore, since most of the basis function supports are disjoint [cf. Remarks 5 and 6, (2.28) and (2.29)], $A$ and $M$ are sparse.
Remark 15. $(2.39)$ is the discrete divergence freeness condition which corresponds to $(2.11)$, $(2.4)$ and $(2.1)$. The matrix $Y$ is defined such that its columns form the basis for the null space of $A$ [cf. (2.32), Remark 11], i.e., the space of all eigenvectors that correspond to $\lambda = 0$. Therefore, $(2.39)$ ensures that we are only searching for the non-zero eigenvalues of $(2.38)$.

We use the implementation of the numerical computation of the integrals in $(2.28)$, and the resulting triangle contributions for $(2.29)$ from [23, 24]. We then construct the matrices $A$, $M$ and $Y$ [cf. (2.33), (2.37)] in parallel using the class `Epetra_FECrsMatrix` from Trilinos [49].

Furthermore, if the cavity cross section $\Omega_p$ is symmetric, as is often the case in practice, it is enough to solve time-harmonic Maxwell’s equations in only half of the cross section, once with PEC and once with PMC BC on the symmetry plane (BCSP) [56]. For example, pillbox cavities have a symmetric cross section. Half of the cross section of the pillbox cavity in Fig. 2.3 would have radius $R$ and length $L/2$. When dealing with PEC BCSP, the symmetry plane can simply be treated as part of the boundary $\Gamma_p$ [cf. (2.24)]. When dealing with PMC BCSP, the DoFs that correspond to the vertices located on the symmetry plane are not eliminated [cf. (2.24)], except for the DoF that corresponds to the one vertex that is also located on the boundary $\Gamma_p$. The first advantage of using the symmetry of $\Omega_p$ is that often only some of the smaller GEVPs need to be solved. For example, sometimes we are only interested in the properties of the FM, which is typically the TM$_{010}$ mode [103, p.615], i.e., the mode that corresponds to the smallest non-zero eigenvalue of the GEVP for $m = 0$ and PEC BCSP [cf. section 3.4]. Another example is in chapter 4, where we are only interested in the GEVPs corresponding to $m = 0$ with PEC BCSP and $m = 1$ with both PEC and PMC BCSP. In case both of the smaller GEVPs need to be solved, as is the case in section 3.4, it is still advantageous to use the symmetry of $\Omega_p$. One reason is that the two resulting GEVPs are much smaller [cf. Fig. 2.13]. The other is that they are better conditioned because their eigenvalues are better separated. Lastly, they can clearly be solved in parallel. Therefore, in the rest of the thesis, whenever the cross section $\Omega_p$ is symmetric, we will exploit this symmetry.

To sum up, the mixed FEM leads to a sequence of decoupled GEVPs [cf. Problem 4]. In practice, we need to consider only the GEVPs corresponding to a few of the smallest azimuthal mode numbers $m$, and one or both of the BCSP if the cross section is symmetric. Moreover, for each of these GEVPs, only the eigenpairs corresponding to some of the smallest non-zero eigenvalues need to be found. In the optimizations in chapters 3 and 4 we will search for the eigenpairs corresponding to at most 20 smallest non-zero eigenvalues. Moreover, in
most cases we will need to find only the eigenpair corresponding to the smallest non-zero eigenvalue. Therefore, we use an iterative eigensolver to find the necessary eigenpairs of the GEVP in Problem 4. Different iterative eigensolvers for the GEVPs that arise from the discretization of time-harmonic Maxwell’s equations in (not necessarily axisymmetric) 3D domains have been compared in [9, 10, 42]. Since these GEVPs have the same properties as the GEVP in Problem 4, and since the performance of the symmetric Jacobi–Davidson (JDSYM) algorithm in [9, 10, 42] was really good, we opt for the JDSYM algorithm. We will describe the JDSYM algorithm, as well as the very good parallel implementation from [8] that makes use of the Trilinos package, in the next section.

2.4 Generalized eigenvalue problem

In this section we will describe the solution of the GEVP from Problem 4 in section 2.3, using the Jacobi–Davidson algorithm [90] for symmetric GEVPs [8].

2.4.1 Symmetric Jacobi–Davidson algorithm

We will now give a sketch of the algorithm. Details can be found in [42, §5.1.2].

Assume that \( q \) eigenpairs have already been found and that the eigenvectors are the columns of the matrix \( Q \) \( (Y^T M Q = 0, Q^T M Q = I_q) \). Additionally, assume that the available search space is \( \mathcal{R}(V_k), V_k = [v_1, \ldots, v_k] \), with

\[
Y^T M V_k = 0, Q^T M V_k = 0, \quad \text{and} \quad V_k^T M V_k = I_k. \tag{2.40}
\]

The search space is expanded in the following way.

- **Extraction.** The spectral decomposition of \( V_k^T A V_k \) is computed and the Ritz pair \((\tilde{\lambda}, \tilde{x})\), such that \( \tilde{\lambda} \) is closest to some given target value \( \tau \), is chosen (\( \tilde{\lambda} \) is the Rayleigh quotient of \( \tilde{x} \)). In our case, \( \tau = 0 \) works well (in general, a value that is close to, but smaller than the smallest non-zero eigenvalue should be chosen).

- **Correction.** Setting \( \tilde{Q} = [Q, \tilde{x}] \),

\[
(I - M\tilde{Q}\tilde{Q}^T)(A - \tilde{\lambda}M)(I - \tilde{Q}\tilde{Q}^T) t = -(I - M\tilde{Q}\tilde{Q}^T)r, \tag{2.41}
\]

where \( r = A\tilde{x} - \tilde{\lambda}M\tilde{x} \), is solved approximately, using a Krylov subspace method [98, §7], namely Quasi Minimal Residual Simplified [42, §6.3]. The shift in (2.41) is initially set to \( \tau \), and then set to \( \tilde{\lambda} \) once the norm of the residual is small enough, i.e., once \( \|r\|_2 < \varepsilon_{tr} \).
Forward solver

- **Extension.** The solution $t$ of (2.41) is $M$-orthogonalized with respect to $V_k$ and $Y$,

$$
\tilde{t} = (I - V_k V_k^T M)(I - Y H^{-1} Y^T M)t,
$$

(2.42)

where $H = Y^T M Y$, and $V_{k+1} := [V_k, \tilde{t}]$. **Restart.** In order to limit the memory consumption and the computational cost of the iteration step, when the maximal dimension of the search space, $j_{\text{max}}$, is reached, the search space is set to $j_{\text{min}}$ best Ritz vectors in $V_{j_{\text{max}}}$.

Initially, $Q$ is ‘empty’ and $V_1 = [v_1]$, where $v_1$ is obtained by making a vector of ones $M$-orthogonal to $Y$ and then normalized with respect to $M$ [cf. (2.40)]. The algorithm stops when $k_{\text{max}}$ eigenpair approximations that satisfy $\|r\|_2 \leq \varepsilon$ are found, or the maximal number of iterations, $it_{\text{max}}$, is reached. The value of $k_{\text{max}}$ depends on the number of sought after eigenpairs. In the rest of the thesis, we will use $k_{\text{max}} \in [1, 20] \cap \mathbb{N}$. For example, when optimizing the properties of the FM, we will usually set $k_{\text{max}} = 3$ [cf. chapter 3], or even $k_{\text{max}} = 5$ [cf. chapter 4], in order to make sure that the smallest non-zero eigenpair is amongst the $k_{\text{max}}$ eigenpairs that are found. We set $it_{\text{max}} = 200$, $\varepsilon_{\text{tr}} = 10^{-3}$, and (usually) $\varepsilon = 10^{-8}$. Furthermore, we set $j_{\text{min}} = 6$ and $j_{\text{max}} = 15$ [8], and use the preconditioned conjugate gradient method (PCG) [98, §5], together with a multi-level preconditioner, for the solve which corresponds to applying $H^{-1}$ in (2.42).

We will first show some results, and then discuss the solution of the correction equation (2.41) in section 2.4.3.

2.4.2 Results: pillbox and ELETTRA-type cavity

The non-zero eigenvalues of the pillbox cavity [cf. Figs. 2.1 and 2.3] are [55]

$$
\begin{align*}
\lambda_{TM,m,p,l} & = \frac{1}{R^2} b_{m,p}^2 + \frac{l^2 \pi^2}{L^2}, & m \in \mathbb{N}_0, p \in \mathbb{N},
\end{align*}
$$

(2.43)

where $b_{m,p}$ and $b'_{m,p}$ are the $p$-th root of the $m$-th Bessel function of the first kind, $J_m$, and its derivative, $J'_m$, respectively [2]. For transverse magnetic (TM) modes, $l \in \mathbb{N}_0$, and for transverse electric (TE) modes, $l \in \mathbb{N}$. The first few roots of the Bessel functions $J_0$ and $J_1$, and the derivatives $J'_0$ and $J'_1$, are shown in Table 2.1.

Fig. 2.6 shows the relative error of the smallest non-zero eigenvalue of the pillbox cavity with $R = 2 \text{ m}$ and $L = 1 \text{ m}$, $\lambda_{TM_{010}}$, depending on the maximal triangle size, in the case of linear (black) and quadratic (red) basis functions. The eigenvalue $\lambda_{TM_{010}}$ is the smallest non-zero eigenvalue of the GEVP for $m = 0$ [cf. (2.8)] and PEC BCSP [cf. p.26]. We can see that it is advantageous
2.4 Generalized eigenvalue problem

Figure 2.6: The relative error of the smallest non-zero eigenvalue of the pillbox cavity [cf. Fig. 2.3, (2.43)] with $R = 2\,\text{m}$ and $L = 1\,\text{m}$, depending on the maximal element (i.e., triangle) size, for the linear and quadratic basis functions. The corresponding values are shown in Table 2.2.

Figure 2.7: Left: a mesh of half of the ELETTRA-type cavity. Right: a mesh of half of the cross section of its axisymmetric approximation.
to use quadratic basis functions if the domain boundary is comprised of straight line segments. The corresponding values are given in Table 2.2.

The shape of the ELETTRA-type cavity [36] used in the storage ring of SLS at PSI [cf. p.1] is shown in Fig. 2.7, left. Since the cavity shape is close to axisymmetric, we approximate it with the axisymmetric shape whose cross section is shown in Fig. 2.7, right (we neglect the three ports).

The comparison of the eigenvalues of the ELETTRA-type cavity and its axisymmetric approximation is given in Fig. 2.3. The agreement of the eigenvalues is quite good (around 2 significant digits) even though the cavity shapes are different, since the axisymmetric shape is only an approximation. The corresponding frequencies are computed according to (2.52) in section 2.5.2. The eigenvalues of the GEVPs for \( m = 0 \) correspond to a single eigenvalue of the 3D problem, and the eigenvalues of the GEVPs for \( m \in \mathbb{N} \) correspond to a double eigenvalue, and the two eigenfields in (2.13) and (2.14).

Figs. 2.8 and 2.9 show the magnitude of the electric and magnetic field for the first and ‘third’ mode in Table 2.3, respectively, i.e., the modes corresponding to \( \approx 500 \text{ MHz} \) and \( \approx 749 \text{ MHz} \), respectively. The magnitude of all fields is scaled to \([0, 1]\) for easier comparison. The first mode in Table 2.3 corresponds to the smallest non-zero eigenvalue of the GEVP for \( m = 0 \) and PEC BCSP, so the fields in Figs. 2.8 are axisymmetric [cf. (2.8), (2.50)]. The third mode in Table 2.3 corresponds to the smallest non-zero eigenvalue of the GEVP for \( m = 1 \) and PEC BCSP, so the field is not axisymmetric. The angle between the ‘slices’ in the last two rows is \( \pi/2 \).

Fig. 2.10 shows the relative error of two eigenvalues of the ELETTRA-type cavity depending on the maximal triangle size. These two eigenvalues are the smallest non-zero eigenvalues of the GEVPs with PEC BCSP and either \( m = 0 \) or \( m = 1 \). They correspond to 500 MHz and 749 MHz in Table. 2.3, respectively, and to Figs. 2.8 and 2.9, respectively. The domain has a curved boundary, so the advantage of quadratic basis function [cf. Fig. 2.6] is lost.

Table 2.1: The first 10 significant digits of the first few roots of the Bessel functions \( J_0 \) and \( J_1 \), as well as the derivatives \( J'_0 \) and \( J'_1 \) [2]. The \( p \)-th root is given in the \( p \)-th column.

| \( p \) | 1           | 2           | 3           | 4           | 5           |
|------|-------------|-------------|-------------|-------------|-------------|
| \( J_0 \) | 2.404825558 | 5.520078110 | 8.653727913 | 11.79153444 | 14.93091771 |
| \( J_1 \) | 3.831705970 | 7.015586670 | 10.17346814 | 13.32369194 | 16.47063005 |
| \( J'_0 \) | 3.831705970 | 7.015586670 | 10.17346814 | 13.32369194 | 16.47063005 |
| \( J'_1 \) | 1.841183781 | 5.331442774 | 8.536316366 | 11.70600490 | 14.86358863 |
2.4 Generalized eigenvalue problem

Figure 2.8: The magnitude of the electric (left column) and the magnetic (right column) field, scaled to $[0, 1]$ for easier comparison, for the first mode in Table 2.3, i.e., the mode corresponding to $\approx 500$ MHz. This mode corresponds to the smallest non-zero eigenvalue of the GEVP for $m = 0$ and PEC BCSP, so the fields are axisymmetric [cf. (2.8), (2.50)], and the eigenvalue computed in the 2D case corresponds to a single eigenvalue in the 3D case. The legend for the magnetic field plot in the 2D case is scaled differently in order to visually better match the 3D case. The triangular dark blue areas that can be seen in the plots in the first row are an issue of our visualization tool, not a part of the results.
Figure 2.9: The magnitude of the electric (left column) and the magnetic (right column) field, scaled to $[0, 1]$, for the ‘third’ mode ($\approx 749$ MHz) in Table 2.3. The legend for the magnetic field plot in the 2D case is scaled differently to visually better match the 3D case. The angle between the ‘slices’ in the last two rows is $\pi/2$. The triangular dark blue areas (first row) are an issue of our visualization tool.
2.4 Generalized eigenvalue problem

2.4.3 Solving the correction equation

The correction equation (2.41) is preconditioned by \[ (I - M\tilde{Q}\tilde{Q}^T)K(I - \tilde{Q}\tilde{Q}^T M), \] (2.44)

where \( K \) is a symmetric preconditioner for \( A - \tilde{\lambda} M \), i.e., a symmetric matrix which approximates \( A - \tilde{\lambda} M \) and is cheap to ‘invert’. For efficiency, the shift is fixed, i.e., the preconditioner is computed (only once) for \( A - \sigma M \). In our

| max. elem. size | LINEAR \(|A|\) | rel. err | QUADRATIC \(|A|\) | rel. err |
|-----------------|--------------|---------|----------------|---------|
| 0.1             | 471          | 4.7 \(\times 10^{-4}\) | 1 721       | 2.9 \(\times 10^{-8}\) |
| 0.075           | 905          | 2.7 \(\times 10^{-4}\)  | 3 267       | 1.1 \(\times 10^{-8}\) |
| 0.05            | 1 997        | 1.2 \(\times 10^{-4}\)  | 7 137       | 2.1 \(\times 10^{-9}\)  |
| 0.04            | 3 159        | 7.8 \(\times 10^{-5}\)  | 11 243      | 9.7 \(\times 10^{-10}\) |
| 0.03            | 5 738        | 4.3 \(\times 10^{-5}\)  | 20 330      | 2.9 \(\times 10^{-10}\) |
| 0.02            | 12 961       | 1.9 \(\times 10^{-5}\)  | 45 731      | 6.0 \(\times 10^{-11}\) |
| 0.01            | 52 353       | 4.8 \(\times 10^{-6}\)  | \(\times\)   | \(\times\)          |
| 0.009           | 64 873       | 3.1 \(\times 10^{-6}\)  | \(\times\)   | \(\times\)          |
| 0.008           | 81 611       | 3.9 \(\times 10^{-6}\)  | \(\times\)   | \(\times\)          |
| 0.007           | 108 069      | 2.3 \(\times 10^{-6}\)  | \(\times\)   | \(\times\)          |
| 0.006           | 146 803      | 1.7 \(\times 10^{-6}\)  | \(\times\)   | \(\times\)          |
| 0.005           | 209 622      | 1.2 \(\times 10^{-6}\)  | \(\times\)   | \(\times\)          |
| 0.004           | 329 685      | 7.7 \(\times 10^{-7}\)  | \(\times\)   | \(\times\)          |
| 0.003           | 585 546      | 4.3 \(\times 10^{-7}\)  | \(\times\)   | \(\times\)          |
| 0.002           | 1 320 403    | 1.9 \(\times 10^{-7}\)  | \(\times\)   | \(\times\)          |
| 0.0015          | 2 349 619    | 1.0 \(\times 10^{-7}\)  | \(\times\)   | \(\times\)          |

Table 2.2: The maximal element (i.e., triangle) size, the corresponding size of the matrix \( A \) [cf. (2.33), Problem 4], and the relative error of the smallest non-zero eigenvalue for the pillbox cavity [cf. Figs. 2.1 and 2.3] with \( R = 2 \) m, \( L = 1 \) m, in case linear and quadratic basis functions are used. The convergence plot is shown in Fig. 2.6.
2 Forward solver calculations, a shift $\sigma$ that is close to, but smaller than the smallest non-zero eigenvalue worked very well.

We first follow the approach from [8], where an algebraic multigrid preconditioner [76] was used, namely the Multilevel (ML) Maxwell preconditioner implemented in the Multilevel Preconditioner Package [40] from Trilinos [49]. The ML Maxwell preconditioner’s coarsening scheme expects all non-zero ele-

| $\lambda$        | $f$ [MHz] | $m$ | BCSP | $\lambda$        | $f$ [MHz] |
|------------------|-----------|-----|------|------------------|-----------|
| $1.1002 \times 10^{-4}$ | 500.46    | 0   | PEC  | $1.0939 \times 10^{-4}$ | 499.02    |
| $2.4325 \times 10^{-4}$ | 744.16    | 1   | PMC  | $2.4316 \times 10^{-4}$ | 744.03    |
| $2.4642 \times 10^{-4}$ | 748.99    | 1   | PEC  | $2.4462 \times 10^{-4}$ | 746.25    |
| $3.8237 \times 10^{-4}$ | 933.00    | 2   | PMC  | $3.8189 \times 10^{-4}$ | 932.41    |
| $3.9349 \times 10^{-4}$ | 946.47    | 0   | PMC  | $3.9383 \times 10^{-4}$ | 946.88    |
| $4.3188 \times 10^{-4}$ | 991.57    | 2   | PEC  | $4.2786 \times 10^{-4}$ | 986.94    |
| $4.4052 \times 10^{-4}$ | 1001.4    | 0   | PMC  | $4.3955 \times 10^{-4}$ | 1000.3    |

Table 2.3: A comparison of the eigenvalues of the ELETTRA-type cavity (denoted 3D) and its axisymmetric approximation (denoted 2D). Half of the 3D cavity and half of the cross section of its approximation are shown left and right, respectively, in Fig. 2.7. $m$ is the azimuthal mode number [cf. (2.8), Problem 4], $\lambda$ the computed eigenvalue, and $f$ the corresponding frequency in MHz, computed according to (2.52) in section 2.5.2. BCSP denotes the symmetry plane boundary conditions. In the 2D case, the correctness of the shown significant digits is checked using a finer mesh (404'831 and 1'125'663 triangles). In the 3D case, the shown results are obtained using a mesh with 5'039'993 tetrahedrons, which agrees with a coarser mesh with 655'562 tetrahedrons on 3-4 significant digits. Therefore, the agreement between the 2D and 3D case, colored blue, would not be improved by further mesh refinement.
ments of $Y$ [cf. (2.37), (2.39)] to be in $\{-1, 1\}$ (as is the case when solving Maxwell’s equations using the mixed FEM in not necessarily axisymmetric 3D domains [42]). Denoting the number of edge (Nédélec) and nodal (Lagrange) DoFs that do not get eliminated by applying (2.24), (2.25) and (2.26) by $|E_1|$

![Graph](image)

Figure 2.10: The relative error of two eigenvalues of the ELETTRA-type cavity [cf. Fig. 2.7] with respect to the corresponding eigenvalues computed with a much finer mesh, depending on the maximal element (i.e., triangle) size, for the linear and quadratic basis functions. The computed eigenvalues are the smallest non-zero eigenvalues of the GEVPs with PEC BCSP and either $m = 0$ or $m = 1$. These two eigenvalues correspond to $\approx 500$ MHz and $\approx 749$ MHz in Table 2.3, respectively. For an easier comparison with Fig. 2.6, the maximal element size is divided by the total cavity length $L$ [cf. Fig. 2.7, right].
and $|V_1|$, respectively, the matrix $Y$ has the form

$$Y = \begin{bmatrix} C \\ -mI_{|V_1|} \end{bmatrix},$$

where $C$ is a matrix of dimension $|E_1| \times |V_1|$ that contains only elements in $\{-1, 0, 1\}$ [cf. Remark 12, (2.36)]. Therefore, whenever $m > 1$ we scale the matrices in Problem 4 according to

$$A_1 = DAD, \quad M_1 = DMD, \quad Y_1 = D^{-1}Y,$$

where $D = \begin{bmatrix} I_{|E_1|} & 0 \\ 0 & mI_{|V_1|} \end{bmatrix}$.

Fig. 2.11, top, shows the strong scaling of specific parts of the forward solver [cf. sections 2.3 and 2.4] on a problem of size $|A| = 488'400$, for $m = 0$ and PEC BCSP, on Intel Xeon E5-2680 V3 (48 processes corresponds to two nodes). The cavity shape is the axisymmetric approximation of the ELETTRA-type cavity in Fig. 2.7, right. The run times are the averages of five runs.

Furthermore, we compute eigenvector approximations by first solving the problem on a much coarser mesh, then choosing three points per triangle in which to sample the solutions from the coarse problem and, lastly, using the values in these three points to find the nodal DoFs by solving a $3 \times 3$ system, and the edge DoFs that best fit these values by solving a $6 \times 3$ least squares problem. Fig. 2.11, bottom, shows the strong scaling of specific parts of the forward solver in case the eigenvector approximation, obtained using a smaller problem with $|A_{\text{small}}| = 694$, is used to compute the initial vector in the search space, $v_1$ [cf. p.28]. The scaling is quite good in both cases, and the eigenvector approximation helps speed up the JDSYM algorithm.

Fig. 2.12 illustrates the behavior of the eigensolver on axisymmetric (2D) problems, with and without the use of eigenvector approximations, compared to two 3D problems, one of a similar size, the other with a similar number of non-zeros. In the 3D case, the cavity shape is the ELETTRA-type cavity from Fig. 2.7, left. We consider the cases for $m \in \{0, 1, 2\}$ [cf. (2.8)], and both the PEC and the PMC BCSP [cf. p.26]. The size of the coarse problem is always around 700 (it differs slightly for different $m$ and different BCSP), and its solution takes less than a second, so it is not included in the run times. The case where only one eigenpair is computed ($k_{\text{max}} = 1$) is shown in at the top of Fig. 2.12, and the case for $k_{\text{max}} = 3$ at the bottom. In the latter case, we compare three different ways of using the computed eigenvector approximations: initializing the search space to all computed approximations (all), their average (avg) or running the block version of the symmetric Jacobi–Davidson (JDBSYM) algorithm [42, §5.1.4], with block size $k_{\text{max}}$ and the computed approximations as the initial guesses. The last option gives especially interesting
2.4 Generalized eigenvalue problem

ELETTRA-type cavity, \( m = 0 \), PEC BCSP, \( |A| = 488'400 \), \( \varepsilon = 10^{-8} \), \( k_{\text{max}} = 1 \)

Figure 2.11: Scaling of the individual parts of the forward solver described in sections 2.3 and 2.4: creating the finite element matrices in Problem 4, constructing the preconditioner (2.44) for the correction equation (prec), and solving the GEVP using the JDSYM algorithm [cf. section 2.4.1]. The run times are the average of five runs. Top: no eigenvector approximation available. Bottom: eigenvector approximation used, ‘approx-vec gen’ is the time for computing the eigenvector approximation.
Figure 2.12: Top: $k_{\text{max}} = 1$. Bottom: $k_{\text{max}} = 3$. The left part shows the run
times for the preconditioner construction and the eigensolver in
the 3D case [8], for a matrix with approximately the same number
of non-zeros (nnz), and a matrix of approximately the same size.
The right part shows the run times for the 2D case, including
also the computation of eigenvector approximations. $\varepsilon$ is different
because the matrix elements (2D vs 3D) differ by a factor of $10^3$.
The run times are the average of five runs (all serial).
results, as it performs poorly on its own (rarely converges to an eigenpair with a non-zero eigenvalue), yet often outperforms the other two methods in cases where some type of eigenvector approximation is most needed, as is the case for $m = 0$. This has been published in [63].

However, in the optimizations in chapters 3 and 4, it will be enough to solve rather small problems, in which case the serial sparse direct solver KLU [28] is better. The run times for different parts of the forward solver (for the axisymmetric approximation of the ELETTRA-type cavity, with $m = 0$ and PEC BCSP), depending on the size of the matrix $A$, are shown in Fig. 2.13. The figures of merit are computed according to section 2.5 and Appendix A.2. Meshing was described in section 2.2, and ‘FEM’ includes sections 2.3 and 2.4.

Note that the differences compared to Fig. 2.11, top are $k_{\text{max}} = 3$ and $\varepsilon = 10^{-10}$, and the computations are now run on one core of Intel Xeon Gold 6150. We can see that the figures of merit, and therefore the objective functions in chapters 3 and 4, can be cheaply computed from the eigenpairs of Problem 4.

![Figure 2.13: Run times for different parts of the forward solver, depending on the size of the matrix $A$ [cf. Problem 4], on one core of Intel Xeon Gold 6150. The run times are the average of five runs, and the variance is low.](image-url)
2 Forward solver

2.5 Figures of merit

In this section we will describe the computation of some figures of merit from the eigenpairs [cf. Problem 4] computed in the previous section. We consider a fixed eigenpair \((\lambda, \mathbf{q})\), and denote the corresponding eigenfield [cf. section 2.3] in Cartesian and cylindrical coordinates by \(\mathbf{e}\) and \(\mathbf{\hat{e}}\), respectively. This is slightly different from the notation in section 2.1 [cf. (2.8)]. Similarly, we will denote the corresponding magnetic field in Cartesian and cylindrical coordinates by \(\mathbf{h}\) and \(\mathbf{\hat{h}}\), respectively. In order to evaluate the electric and magnetic field in a point \((r, p) \in \Omega_p\) more easily, we will first define the simplex coordinates in section 2.5.1. For readability, in sections 2.5.2 and 2.5.3 we will describe only some of the figures of merit needed to define the objective functions in chapters 3 and 4. We give the rest of the definitions in Appendix A.2.

2.5.1 Simplex coordinates

The simplex coordinates, also called barycentric coordinates, are linear functions in \(r\) and \(z\). We denote the simplex coordinates corresponding to a triangle \(T_i\) by \(L_{i,1}\), \(L_{i,2}\), and \(L_{i,3}\), where the order corresponds to the order of vertices in \(T_i^v\), i.e., \(L_{i,j}\) corresponds to the vertex \(V_{T_i^v,j}\). For a point \((r, z) \in \Omega_p\),

\[
L_{i,1}(r, z) = \frac{1}{2 \cdot \text{area}(T_i)} \begin{vmatrix}
1 & r & z \\
1 & r_{T_i^v,2} & z_{T_i^v,2} \\
1 & r_{T_i^v,3} & z_{T_i^v,3}
\end{vmatrix}
\]

\[
L_{i,2}(r, z) = \frac{1}{2 \cdot \text{area}(T_i)} \begin{vmatrix}
1 & r_{T_i^v,1} & z_{T_i^v,1} \\
1 & r & z \\
1 & r_{T_i^v,3} & z_{T_i^v,3}
\end{vmatrix}
\]

\[
L_{i,3}(r, z) = \frac{1}{2 \cdot \text{area}(T_i)} \begin{vmatrix}
1 & r_{T_i^v,1} & z_{T_i^v,1} \\
1 & r_{T_i^v,2} & z_{T_i^v,2} \\
1 & r & z
\end{vmatrix}
\]

The area of the triangle \(T_i\) is

\[
\text{area}(T_i) = \frac{1}{2} \begin{vmatrix}
1 & r_{T_i^v,1} & z_{T_i^v,1} \\
1 & r_{T_i^v,2} & z_{T_i^v,2} \\
1 & r_{T_i^v,3} & z_{T_i^v,3}
\end{vmatrix}
\]

where \((r_{T_i^v,j}, z_{T_i^v,j})\) are the coordinates of the vertex \(V_{T_i^v,j}\). We can see from (2.45) and (2.46) that for a point \(P\) inside \(T_i\), the simplex coordinates \(L_{i,1}\),

\[
\text{area}(T_i) = \frac{1}{2} \begin{vmatrix}
1 & r_{T_i^v,1} & z_{T_i^v,1} \\
1 & r_{T_i^v,2} & z_{T_i^v,2} \\
1 & r_{T_i^v,3} & z_{T_i^v,3}
\end{vmatrix}
\]

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2.5 Figures of merit

$L_{i,1}$, $L_{i,2}$, and $L_{i,3}$ are defined as the ratios of the (signed) areas of $PV_{T_{i,2}}^v V_{T_{i,3}}^v$, $PV_{T_{i,3}}^v V_{T_{i,1}}^v$ and $PV_{T_{i,1}}^v V_{T_{i,2}}^v$, respectively. Furthermore, it can easily be seen that

$$L_{i,1} + L_{i,2} + L_{i,3} = 1 \text{ and } L_{i,j}(r_{T_{i,k}}^v, z_{T_{i,k}}) = \delta_{jk}.$$  

We will now describe the way to compute $\hat{E}(r, z)$, where $\hat{E}$ is the approximation of $\hat{e}$ [cf. (2.6)] which corresponds to the eigenvector $q$, and $(r, z)$ is a point in $\Omega_p$. Let $(r, z)$ be located inside some triangle $T_i$. It is clear from Remarks 5 and 6 that only the unrestricted linear Lagrange basis functions that correspond to the vertices of $T_i$, and the unrestricted linear Nédélec basis functions that correspond to the edges of $T_i$ need to be considered, because the contribution of all other basis functions will be zero (this is true even if $(r, z)$ is located on a vertex or edge of $T_i$). Furthermore, $\hat{E}_\theta(r, z)$ can be computed as [cf. (2.22)]

$$\hat{E}_\theta(r, z) = \frac{1}{r} \sum_{j=1}^3 q_{T_{i,j}}^{(\theta)} L_{i,j}(r, z).$$

Using the gradient matrix

$$J_i = \begin{pmatrix}
\frac{\partial L_{i,1}}{\partial r} & \frac{\partial L_{i,2}}{\partial r} & \frac{\partial L_{i,3}}{\partial r} \\
\frac{\partial L_{i,1}}{\partial z} & \frac{\partial L_{i,2}}{\partial z} & \frac{\partial L_{i,3}}{\partial z}
\end{pmatrix},$$

$$\Rightarrow \frac{1}{2 \cdot \text{area}(T_i)} \begin{pmatrix}
z_{T_{i,2}}^v - z_{T_{i,3}}^v & z_{T_{i,3}}^v - z_{T_{i,1}}^v & z_{T_{i,1}}^v - z_{T_{i,2}}^v \\
r_{T_{i,2}}^v - r_{T_{i,3}}^v & r_{T_{i,3}}^v - r_{T_{i,1}}^v & r_{T_{i,1}}^v - r_{T_{i,2}}^v
\end{pmatrix},$$

$\hat{E}_p(r, z)$ can be computed as [cf. (2.18), (2.19)]

$$\hat{E}_p(r, z) = \begin{pmatrix}
\hat{E}_r(r, z) \\
\hat{E}_\theta(r, z)
\end{pmatrix},$$

\begin{align*}
= & \text{dir}(E_{T_{i,1}}^e) \cdot q_{T_{i,1}}^{(p)} (L_{i,1}(r, z) \cdot J_i(:, 2) - L_{i,2}(r, z) \cdot J_i(:, 1)) \\
+ & \text{dir}(E_{T_{i,2}}^e) \cdot q_{T_{i,2}}^{(p)} (L_{i,1}(r, z) \cdot J_i(:, 3) - L_{i,3}(r, z) \cdot J_i(:, 1)) \\
+ & \text{dir}(E_{T_{i,3}}^e) \cdot q_{T_{i,3}}^{(p)} (L_{i,2}(r, z) \cdot J_i(:, 3) - L_{i,3}(r, z) \cdot J_i(:, 2)),
\end{align*}

where $J_i(:, j)$ denotes the $j$-th column of $J_i$. The magnetic field is given by

$$h = \frac{\text{curl}(e)}{\mu_0 \omega},$$

(2.48)
where $\mu_0 = 4\pi \cdot 10^{-7} \text{ H/m}$ is the permeability of vacuum, and $\omega = c \cdot \sqrt{\lambda}$ [cf. Remark 1]. The magnetic field in cylindrical coordinates, $\hat{h}$, is given by

$$\hat{h} = \frac{1}{\mu_0\omega} \begin{pmatrix}
\frac{1}{r} \partial_\theta \hat{e}_z - \partial_z \hat{e}_\theta \\
\partial_z \hat{e}_r - \partial_r \hat{e}_z \\
\frac{1}{r} (\partial_r (r \hat{e}_\theta) - \partial_\theta \hat{e}_r)
\end{pmatrix}. \quad (2.49)$$

If $m = 0$, the eigenfield is $\hat{e} = (c_{e,r}^{(0)}, c_{e,\theta}^{(0)}, c_{e,z}^{(0)})^T$ [cf. (2.9)], so the corresponding magnetic field [cf. (2.49)] (denoting $\gamma = 1/\mu_0\omega$)

$$\hat{h} = \gamma \begin{pmatrix}
\frac{1}{r} \partial_\theta c_{e,z}^{(0)} - \partial_z c_{e,\theta}^{(0)} \\
\partial_z c_{e,r}^{(0)} - \partial_r c_{e,z}^{(0)} \\
\frac{1}{r} (\partial_r (r c_{e,\theta}^{(0)}) - \partial_\theta c_{e,r}^{(0)})
\end{pmatrix} =: \gamma \begin{pmatrix}
w_{h,r}(r,z) \\
w_{h,\theta}(r,z) \\
w_{h,z}(r,z)
\end{pmatrix} \quad (2.50)$$

is also axisymmetric. If $m \in \mathbb{N}$, the eigenfield is [cf. (2.9)]

$$\hat{e} = (c_{e,r}^{(m)} \cos(m\theta), s_{e,\theta}^{(m)} \sin(m\theta), c_{e,z}^{(m)} \cos(m\theta))^T,$$

and the corresponding magnetic field [cf. (2.49)]

$$\hat{h} = \gamma \begin{pmatrix}
-m c_{e,z}^{(m)} + \partial_z s_{e,\theta}^{(m)} \\
\partial_z c_{e,r}^{(m)} - \partial_r c_{e,z}^{(m)} \\
\frac{1}{r} (\partial_r (r s_{e,\theta}^{(m)}) + mc_{e,r}^{(m)})
\end{pmatrix} =: \gamma \begin{pmatrix}
w_{h,r}(r,z) \sin(m\theta) \\
w_{h,\theta}(r,z) \cos(m\theta) \\
w_{h,z}(r,z) \sin(m\theta)
\end{pmatrix}. \quad (2.51)$$

### 2.5.2 Resonant frequency

The resonant frequency (in Hz) is given by [cf. Remark 1]

$$f(d) = \frac{c \cdot \sqrt{\lambda(d)}}{2\pi}, \quad (2.52)$$

where $c = 299'792'458 \text{ m/s}$ is the speed of light in vacuum [96]. Furthermore, we will sometimes write $f(d)$ in order to emphasize that the value depends on the cavity shape determined by the design vector $d$.

### 2.5.3 Peak electric field on surface

In our application the operating mode and the FM [cf. p.1] both correspond to the TM$_{010}$ mode, so we do not make a distinction, but simply refer to it as the FM. An important figure of merit is the peak value of the electric field
of the FM on the surface of the cavity, $E_{pk}$, normalized by the accelerating voltage, $V_{acc}$ [cf. Problem 1]

$$
\frac{E_{pk}(d)}{V_{acc}(d)} = \frac{\max_{x \in \partial \Omega} \| e(x) \|_2}{V_{acc}(d)},
$$

(2.53)

where the accelerating voltage is the longitudinal voltage along the longitudinal axis, i.e., (assuming that the particles travel at the speed of light)

$$
V_{acc}(d) = \left| \int_0^L e_z(0, z) e^{i \sqrt{\lambda} z} dz \right| \overset{(2.6)}{=} \left| \int_0^L \hat{e}_z(0, z) e^{i \sqrt{\lambda} z} dz \right|,
$$

(2.54)

where $L$ is the length of the cavity (Figs. 2.1, 2.3, 1.1), $i$ the imaginary unit, $\lambda = \lambda(d)$ the computed eigenvalue, and $e_z$ the component of the electric field of the accelerating mode [cf. Problem 1] in the direction of the axis of rotation (the orientation of the axes is shown, e.g., in Fig. 2.1).

The electric field of the FM is axisymmetric [cf. (2.8) for $m = 0$], so

$$
\max\| e(x) \|_2 \overset{(2.8)}{=} \max_{r_p \in \partial \Omega_p} \| e(r_p) \|_2 \overset{(2.6)}{=} \max_{r_p \in \partial \Omega_p} \| \hat{e}(r_p) \|_2,
$$

which we approximate by the maximum value of $\hat{E}_p(r, z)$ in the vertices and on the edges on the boundary of $\Omega_{p,T}$ [cf. (2.15)] using (2.47).

The normalized peak electric field on the cavity surface is sometimes defined as

$$
\frac{E_{pk}}{E_{acc}} = \frac{E_{pk}}{V_{acc}/L},
$$

(2.55)

where $L$ is the characteristic cavity length [cf. Fig. 4.1, (4.2)]. We will use the definition (2.53) in chapter 3, where the characteristic length of the cavity will be fixed, and the definition (2.55) in chapter 4, where $L$ will be a parameter in the optimization. The units are: $E_{pk}/V_{acc}$ [1/m] and $E_{pk}/E_{acc}$ [-].
In this chapter we will use an EA [cf. p.4] to solve a real-world constrained multi-objective RF cavity shape optimization problem. In order to do this, we will first define the concept of dominance and describe an EA (section 3.1), as well as discuss different constraint handling methods that can be used with EAs (section 3.2). In sections 3.3 and 3.4 we will compare different problem formulations and constraint handling techniques on two simple problems. We will then use this information to solve the more complicated problem in the last section of this chapter, section 3.5.

3.1 Evolutionary multi-objective optimization

Having fixed a parameterizable geometry type [cf. section 1.2.3], e.g., the pillbox cavity (Fig. 2.3) with $d = (L, R)^T$ or the geometry type with a symmetric cross section from Fig. 3.1 with $d = (R, a, b)^T$, we consider the multi-objective optimization problem

$$\begin{align*}
\min F_i(d), & \quad i = 1, \ldots, n, \\
G_i(d) \leq 0, & \quad i = 1, \ldots, k, \\
H_i(d) = 0, & \quad i = 1, \ldots, l,
\end{align*}$$

(3.1)

where $d = (d_1, \ldots, d_N)^T \in X \subseteq \mathbb{R}^N$ is a design point, $F_1, \ldots, F_n : X \to \mathbb{R}$ are objective functions, and (3.1) and (3.2) are inequality and equality constraints, respectively, with

$$G_1, \ldots, G_k, H_1, \ldots, H_l : X \to \mathbb{R}.$$

The objective functions could be defined as properties of the FM [cf. pp.1,42], e.g., the normalized peak electric field on the cavity surface, $E_{pk}/V_{acc}$, or, since the shunt impedance $R_{sh}$ [cf. (A.8)] should be maximized, $-R_{sh}$. A possible equality constraint could be that the frequency of the FM, $f$, should match a given target frequency $f_{RF}$, i.e.,

$$H(d) = |f(d) - f_{RF}| = 0,$$

(3.3)
where \( f(d) \) indicates that \( f \) depends on the cavity shape determined by \( d \).

Since the minimizers of different objective functions are usually different points, we need a way to compare candidate solutions. For example, in the case of the geometry type from Fig. 3.1, RF cavity shapes, i.e., design points, with a low value of \( E_{pk}/V_{acc} \) often also have a low value of \( R_{sh} \) [cf. section 3.4.3] and vice versa. If the goal is to simultaneously minimize one and maximize the other, we need a way to compare the fitness of two design points. The concept of dominance can be used [89, p.519].

**Definition 1.** A point \( d_1 \) **Pareto dominates** \( d_2 \) (denoted \( d_1 \prec d_2 \)) if
\[
\forall i \in \{1, \ldots, n\}, \quad F_i(d_1) \leq F_i(d_2) \quad \text{and} \quad \\
\exists i \in \{1, \ldots, n\}, \quad F_i(d_1) < F_i(d_2).
\]

**Definition 2.** A point \( d \) is **Pareto optimal** if it is not Pareto dominated by any other point, i.e. \((X \subset \mathbb{R}^N \text{ is the design space})\)
\[
\{d' \in X : d' \prec d\} = \emptyset.
\]
3.1 Evolutionary multi-objective optimization

Definition 3. The set of all Pareto optimal points is called the Pareto optimal set, \( P_s \). The Pareto front, \( P_f \), is defined as

\[
P_f = \{ F(d) : d \in P_s \},
\]

where \( F = (F_1, \ldots, F_n)^T \).

Because of conflicting objectives, the ability of EAs to escape local optima and deal with possibly discontinuous objective functions, as well as their suitability for parallelization, we use a multi-objective EA to search for the Pareto optimal set. Due to the availability of the massively parallel implementation from [51, 52, 70], and the fact that it gave good results in the field of particle accelerators, we use this framework, called opt-pilot. In order to use it for RF cavity shape optimization, we combine it with the forward solver described in chapter 2 and, to enforce constraints such as, e.g., the one from (3.3), we also combine it with constraint handling techniques that will be described in section 3.2.

The main steps of an EA, as used in this thesis, are shown in Algorithm 1. The population of the first generation comprises \( M \in \mathbb{N} \) design points with randomly chosen design variable values (line 1). More precisely, for \( i = 1, \ldots, N \), the value of \( d_i \) is chosen uniformly at random from some given interval \([l_i, u_i]\).

In the context of an EA the design points are called individuals, and their design variables are called genes. In line 2 the individuals in the initial population are evaluated, i.e., the objective functions are evaluated in the corresponding design points [cf. chapter 2]. The algorithm then performs a number of cycles, each resulting in a new generation (lines 3–11). In every cycle, new individuals are created using two operators: crossover, which models the exchange of genetic material between homologous chromosomes, and mutation, which models accidental changes in the set of genes (lines 5–7). It should be noted here that we do not require the new value of \( d_i \) to be in \([l_i, u_i]\), since this interval is only used for generating a new random value for \( d_i \), and feasible points (in which the objective functions are defined) can have \( d_i \) outside of it.

The new individuals are evaluated (line 8) and, out of these new individuals and the individuals in the current generation, approximately \( M \) fittest ones are chosen to form a new generation (lines 10,11). This is repeated until a stopping criterion [51, 101] is satisfied or a predetermined number of generations reached.

In the rest of this section, we will explain the purpose of the variator and the selector, and briefly describe the parallelization of opt-pilot. Even though there are many possibilities for the variator and the selector, we will primar-
3 Evolutionary algorithm

Algorithm 1 Evolutionary algorithm

1: initialize a random population of individuals, $I_i, i = 1, \ldots, M$
2: EVALUATE($I_i$), $\forall i \in \{1, \ldots, M\}$
3: while stopping criterion not satisfied do
4:   // variator
5:   for pairs of individuals ($I_i, I_{i+1}$) do
6:       crossover($I_i, I_{i+1}$),
7:       mutate($I_i$) and mutate($I_{i+1}$) with some probability
8:   for each new individual $I_{new}$, EVALUATE($I_{new}$)
9:   // selector (NSGA-II)
10: sort individuals according to levels of dominance
11: choose $M$ fittest individuals to form the next generation

illy focus on those already available in opt-pilot and choose the ones most suitable for our problem.

3.1.1 Variator

The variator applies gene recombination operators and evaluates the fitness of newly created individuals. Recombination operators comprise crossover, which creates a new individual (child) from two individuals (parents), and mutation, which creates a new individual from a single individual in order to ensure diversity in the population.

Simple crossover operators generate individuals with each of the genes copied from one of the parents. For example, the one point crossover randomly chooses a crossover point $q \in \{0, \ldots, N\}$, and copies the genes $d_1, \ldots, d_q$ from the first parent, and $d_{q+1}, \ldots, d_N$ from the second parent, or vice versa. The multiple point crossover is similar, but it employs multiple crossover points and alternates between the parents, while the uniform crossover randomly chooses the parent to copy the value from with probability 0.5, for each of the genes. On the other hand, instead of copying the gene from one of the parents, blending crossover operators create completely new values for the offspring. One option is to randomly choose a value between the values of the parent genes. Another, called the $\alpha$-blend crossover, chooses the new value uniformly at random from a wider interval. For a specific gene $d_{i}, i \in \{1, \ldots, N\}$, denoting the parent genes by $d_{1,i}$ and $d_{2,i}$ (such that $d_{1,i} \leq d_{2,i}$), the interval is

$$[d_{1,i} - \alpha(d_{2,i} - d_{1,i}), d_{2,i} + \alpha(d_{2,i} - d_{1,i})],$$

for some $\alpha \in (0,1)$.

According to [30], $\alpha = 0.5$ performs the best. Another blending crossover is
3.1 Evolutionary multi-objective optimization

the simulated binary crossover, which creates two new gene values

\[ 0.5 \cdot ((1 + \beta_i)d_{1,i} + (1 - \beta_i)d_{2,i}) \quad \text{and} \quad 0.5 \cdot ((1 - \beta_i)d_{1,i} + (1 + \beta_i)d_{2,i}) , \]

with \( \beta_i \) chosen according to [31]. Since our genes are real-valued, we opt for a blending crossover. We will compare the \( \alpha \)-blend crossover and the simulated binary crossover, both available in opt-pilot, in section 3.4.1.

Common mutation operators are the independent bit mutation, where the value of each gene is changed with a given probability, and the one bit mutation, where one gene is chosen uniformly at random and its value changed. The new value can be chosen in different ways. In opt-pilot it is chosen uniformly at random from the same intervals as the initial values of the genes. Different design variables can have a lower or higher influence on each the objectives. For example, in the case of the geometry type from Fig. 3.1, the value of \( E_{pk}/V_{acc} \) mostly depends on the part of the boundary defined by \( a \) and \( b \). On the other hand, the frequency \( f \) is greatly influenced by \( R \) [cf. section 3.4.3]. With this in mind, we usually opt for the one bit mutation.

3.1.2 Selector

The purpose of the selector is to choose the individuals that will comprise the next generation. It needs to prevent fitness deterioration from one generation to the next and ensure the diversity of the individuals. State-of-the-art methods include PESA (Pareto Enveloped-based Selection Algorithm) [25], SPEA2 (Strength Pareto Evolutionary Algorithm 2) [112] and NSGA-II (Non-dominated Sorting Genetic Algorithm-II) [32]. It was shown in [59] that the performance of these three methods depends on the problem and the number of objectives, and that none of them can be said to be the best in all cases. We use the NSGA-II implementation from the PISA [15] library, because it was used in opt-pilot and it also gives good results on our problem.

In order to prevent fitness degeneration, NSGA-II sorts the set comprising the current generation and the new individuals by levels of dominance [cf. Definition 1]. It then creates the new generation, choosing first the non-dominated individuals, then the individuals dominated by one individual, etc. In order to improve diversity, when choosing between two equally fit individuals it uses a crowding distance measure to prevent niches.

3.1.3 Parallelization

The parallelization of opt-pilot employs a client/server mechanism, where the processes are assigned one of three roles: pilot, optimizer, or worker. A
worker is in charge of running a forward problem [cf. chapter 2], i.e., of evaluating a single individual. Alternatively, worker groups can be used to perform this evaluation in parallel. An optimizer runs the EA, requesting the function evaluations from a pilot process. Pilots correspond to servers, receiving the simulation requests from the optimizers and assigning them to workers. A job queue on the pilot is used to store the simulation requests, and the number of idle workers is reduced in the following way. Instead of waiting for all of the new individuals in a generation to be created and evaluated before starting the selection process [cf. Algorithm 1], ‘continuous’ generations are used. The selector is called whenever a predetermined number of new individuals, denoted num-ind-gen, is evaluated. A lower value reduces the number of idle workers, but it calls the selector, which is quite expensive, more often.

In the optimizations shown in this thesis it was enough to use one pilot and one optimizer, and have the rest of the processes perform the role of workers.

3.2 Handling constraints

Equality constraints (3.2) are difficult to satisfy, so they are often ‘relaxed’, i.e., converted it into inequality constraints [30, 89]. More precisely,

\[ H(d) = 0 \text{ is converted into } |H(d)| \leq \varepsilon, \]

for some small positive constant \( \varepsilon \). In the rest of this section we will therefore only deal with inequality constraints (3.1).

An overview of the most popular constraint handling methods for single-objective EAs [89], though not a comprehensive list of all possible methods, is given in Fig. 3.2. These methods can be broadly divided into penalty function approaches, the idea of which is quite similar for all problems though there are numerous parameters that might need to be tuned differently, and methods like special representation, special operators or repair methods which greatly depend on the specific problem. Additionally, features from more than one method can be used simultaneously, which results in a hybrid constraint handling method.

In the case of multi-objective EAs popular constraint handling methods are the following [30].

- **Ignoring infeasible individuals**, i.e., individuals that violate a constraint. As in the death-penalty-approach approach from Fig. 3.2, infeasible individuals can be created using crossover and mutation operators, but they are discarded once it is determined that they violate a constraint.
3.2 Handling constraints

- **Penalty function approach.** Objective function values of infeasible individuals are penalized. For example, according to [30, p.278], after the constraints are normalized, the objective function values are modified in the following way [cf. (3.1)]

\[
F_i(d) \mapsto F_i(d) + c_i \sum_{s=1}^{k} \max\{0, G_s(d)\}. \quad (3.5)
\]

This is similar to the static non-death-penalty approach from [89, p.486]. Additionally, there are more elaborate methods that change the way feasible-feasible, feasible-infeasible, and infeasible-infeasible comparisons are handled in the selection process, such as the constrained tournament method [30], or the Ray-Tai-Seow’s method [75].

In this chapter we will deal with ‘relaxed’ forms of constraints such as the one from (3.3), which we call the frequency constraint, i.e., [cf. (3.4)]

\[
|f(d) - f_{RF}| \leq \varepsilon, \quad (3.6)
\]

for a suitably chosen small positive constant \(\varepsilon\). We will first try to determine if there is a benefit to discarding infeasible individuals (section 3.3.3). Afterwards, in section 3.4.2, we will employ a penalty function approach. Since this approach works well enough on our problem (sections 3.4 and 3.5), we will not explore other constraint handling methods for multi-objective EAs. Instead, in section 4.3.1, due to the nature of the frequency constraint, we will formulate the problems such that the frequency constraint is automatically satisfied by all individuals. This bears some resemblance to special representation methods and, in a slightly different formulation, also to repair methods from Fig. 3.2.

In the rest of this chapter we will solve a few RF cavity shape optimization problems in order to analyze the performance of the EA, find good parameters, and determine the benefit of applying some constraint handling methods. We will then use these conclusions to hypothetically optimize the RF cavity for SLS 2.0 [cf. p.8]. As explained in chapter 2, p.26, whenever the cavity cross section is symmetric it is sufficient to use only half of it. When referring to a property of the FM, we will either write the superscript ‘(0)’, e.g., \(f^{(0)}\), or omit it and write \(f\). When referring to a property of a HOM [cf. p.1], we will write the superscript ‘(i)’, e.g., \(f^{(i)}\), for the mode corresponding to the \(i\)-th smallest frequency, starting from 0 and considering all relevant azimuthal mode numbers (2.8) and BCSP [cf. p.26].
Figure 3.2: An overview of constraint handling methods for single-objective EAs [89]. Interior nodes in this classification are colored gray. Blue marks the methods which are similar in the multi-objective case and which we will use in this chapter. Red methods are loosely connected to our approach in chapter 4. The rest is colored orange.
3.3 Problem #1

We first consider an artificial problem with a known solution: finding the radius $R$ and length $L$ of a pillbox cavity [cf. Fig. 2.3] such that the smallest non-zero eigenvalue, $\lambda$, of the GEVP corresponding to $m = 0$ [cf. (2.8)] and PEC [cf. p. 12] BCSP [cf. p. 26] is as close as possible to $b_{0,1}^2/2^2 \approx 1.445796491$ (from (2.43): $\lambda = b_{0,1}^2/R^2$, from Table 2.1: $b_{0,1} \approx 2.404825558$), and that $L$ is as close as possible to 1. This leads to the multi-objective optimization problem (MOOP)

$$\min_{R,L} \left( \underbrace{|\lambda - 1.445796491|}_{F_1}, \underbrace{|L - 1|}_{F_2} \right), \quad (3.7)$$

with two design variables, $R$ and $L$, two objectives, and a known solution $(R, L) = (2, 1)$. The initial values of $R$ and $L$ are randomly chosen from the intervals (in meters) $[1, 5]$ and $[0.5, 1.5]$, respectively. The dependence of the first objective function, $F_1$, on the design variables is shown in Fig. 3.3. Note that $\lambda$, and therefore also $F_1$, depends only on $R$, not $L$. In this section we use the blend crossover and the one bit mutation.

Figure 3.3: The dependence of the objective function $F_1 = |b_{0,1}^2/R^2 - b_{0,1}^2/2^2|$ [cf. (3.7)] on the design variables $R$ and $L$ for the pillbox cavity type [cf. Fig. 2.3]. The function $F_1$ depends only on $R$, not $L$, and it attains the value 0 for $R = 2$. 

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Table 3.1: The required mesh and matrix sizes needed to achieve a desired number of correct significant digits for the smallest non-zero eigenvalue $\lambda$ of the pillbox cavity [cf. Fig. 2.3] with $R = 2$ m, $L = 1$ m using quadratic elements [cf. Fig. 2.6, Table 2.2]. The run times are the average of 5 runs on one core of Intel Xeon Gold 6150. The variance is small.

| # triangles | $|A|$ | # correct significant digits | time [s] |
|-------------|------|------------------------------|---------|
| COARSE      | 34   | 203                          | 6       | 0.74    |
| FINE        | 6 604| 45 731                       | 10      | 8.422   |

### 3.3.1 Using a coarser mesh

In order to compare the values of $F_1$ for two design points, $\lambda$ needs to be computed with a sufficient accuracy. Some information on the required mesh and matrix sizes to achieve a desired number of correct significant digits using quadratic elements is presented in Table 3.1 [cf. Fig. 2.6, Table 2.2]. Taking into account the fact that a good approximation of the smallest non-zero eigenvalue, $\lambda_{\text{approx}}$, is needed to compute the shift $\sigma$ [cf. 34], it can be seen that, in case a coarse mesh with around 30 triangles is used to compute $\lambda_{\text{approx}}$, this value can be considered to be ‘enough’ if

$$|\lambda_{\text{coarse}} - 1.445796491| > \beta,$$

with, e.g., $\beta = 0.1$ or $\beta = 0.01$. Our reasoning is as follows. If the values of $F_1$ for two design points are both smaller than $\beta$, they will be computed and compared accurately. If, on the other hand, one of the two points that are being compared has a value of $F_1$ above $\beta$ and the computed significant digits (in this example 6 instead of 10) are not enough to accurately compare them, these two individuals are both ‘quite bad’ and ‘quite close’, so even if the wrong one is chosen for the next generation it will likely bring similar information. Therefore, we trade the ability to accurately compare two such points for a significantly shorter computation time.

An illustration of strong scaling of opt-pilot on an optimization with 100 generations, $M = 40$ and $\text{num-ind-gen} = 20$ [cf. section 3.1.3], which comprises around 1’000 fine runs and 2’020 coarse ones ($40 + 99 \cdot 20 = 2020$), is shown in Fig. 3.4. Different design points are evaluated in parallel, but the evaluation of a single design point is executed by only one worker, i.e., each of the worker groups consists of only one worker. The $x$ and $y$ coordinates of a point represent the ‘expected’ time and the run time, respectively. The ‘expected’
Figure 3.4: An illustration of strong scaling of \texttt{opt-pilot} on an optimization with around 1'000 fine runs and 2'020 coarse runs. The $x$ coordinate of a point is the ‘expected’ run time for the corresponding number of workers [cf. (3.8), Table 3.1]. The $y$ coordinate represents the run time of the optimization. The optimizations were run on 3, 4, 6, 10, 18, and 36 processes of Intel Xeon Gold 6150. Different design points are evaluated in parallel, but the evaluation of a single design point is executed by only one worker [cf. section 3.1.3].
3 Evolutionary algorithm

time is computed as

\[
\frac{\# \text{coarse-runs} \cdot \text{time-coarse} + \# \text{fine-runs} \cdot \text{time-fine}}{\# \text{workers}},
\]

(3.8)

using the values in Table 3.1 as the run times for the coarse (time-coarse) and fine (time-fine) forward solve. Since the run times in Table 3.1 are close to, but not equal to the coarse and fine run times for an arbitrary point in the design space, depending on the actual problems that are run, the optimization can either take a shorter or longer amount of time (e.g., this can already be seen in the case of 1 worker). However, in all cases, the computed value is very close to the ‘expected’ one, i.e., the points lie close to the y = x line (dashed). We can conclude that the EA implementation from \([51, 52]\) scales really well.

3.3.2 Optimization with an evolutionary algorithm

The 200-th generation of an optimization with the population size \(M = 40\) and \(\text{num-ind-gen} = 20\) [cf. section 3.1.3], with coarse and fine simulation runs as described in Table 3.1 and \(\beta = 0.1\), is shown at the top of Fig. 3.5. We will refer to this approach as \text{use-coarse}. On 36 processes (18 cores) of Intel Xeon Gold 6150 (1 optimizer, 1 pilot, 34 workers) this took 901 s, i.e., almost exactly 15 min. The squares represent the individuals in the population, i.e., the RF cavity shapes, and their \(x\) and \(y\) coordinates show the values of \(F_1\) and \(F_2\), respectively. The orange line is the Pareto front approximation [cf. Definition 3]. As illustrated in Table 3.2, most individuals in the population have a value of \(F_1\) and \(F_2\) quite close to zero. Considering that in the first generation the values of \(F_1\) and \(F_2\) were in \([0.070, 3.65]\) and \([0.013, 0.480]\), respectively, this shows that the EA approaches the known solution.

Table 3.2: Additional information on the quality of the generations shown at the top (\text{use-coarse}) and bottom (\text{coarse-discard}) of Fig. 3.5. For each of these approaches, the value in a certain column shows the number of individuals with both \(F_1\) and \(F_2\) smaller than the corresponding \(\delta\).

| \(\delta\) | \(10^0\) | \(10^{-1}\) | \(10^{-2}\) | \(10^{-3}\) | \(10^{-4}\) | \(10^{-5}\) | \(10^{-6}\) |
|-----------|---------|---------|---------|---------|---------|---------|---------|
| \text{use-coarse} | 40 | 33 | 23 | 17 | 9 | 4 | 0 |
| \text{coarse-discard} | 40 | 33 | 29 | 14 | 0 | 0 | 0 |
3.3 Problem #1

Figure 3.5: Top: the 200-th generation of the use-coarse approach applied to the MOOP (3.7). The squares represent the individuals, and the orange line the Pareto front approximation. Bottom: the 46-th generation (chosen because it also took around 15 min) of the coarse-discard approach applied to the CMOOP (3.10).
3 Evolutionary algorithm

3.3.3 Discarding infeasible individuals

In addition to the objective functions from (3.7), the requirement that \( \lambda \) should match the target value 1.445796491 can be considered as the equality constraint [cf. (3.2)]

\[ |\lambda - 1.445796491| = 0, \]

or the ‘relaxed’ inequality constraint [cf. (3.4), (3.6)]

\[ |\lambda - 1.445796491| \leq \varepsilon, \quad (3.9) \]

where \( \varepsilon \) is a small positive constant. We set \( \varepsilon = 0.01 \) and enforce this constraint by ignoring individuals that violate it. This means a generation will take longer to form, since it often happens that the smallest non-zero eigenvalue of many of the randomly chosen individuals is further away from 1.445796491 than \( \varepsilon = 0.01 \). These individuals will simply get discarded and new ones with random values created until \( M \) of them satisfy (3.9). Using the same seed as in the use-coarse approach, and even setting \( \beta = 0.01 \) which means that, compared to use-coarse with \( \beta = 0.1 \), the results of the coarse simulation run will additionally be used if \( F_1 \) is between 0.1 and 0.01, in the process of finding \( M = 40 \) feasible individuals to form the first generation, 13'266 infeasible ones are discarded. This takes 1'342 s, i.e., around 22 min. Also, these individuals are just randomly chosen points for which the value of \( F_1 \) is smaller than \( \varepsilon = 0.01 \), which means that \( F_2 \) was not optimized in any way. For example, there are only two points with both the values of \( F_1 \) and \( F_2 \) smaller than 0.01, and no points with both of these values smaller than 0.001, which is not nearly as good as the results obtained with the use-coarse approach in a comparable amount of time using the same resources [cf. Table 3.2].

The chosen value of \( \varepsilon \) is clearly too small, so we try setting it to a higher value, \( \varepsilon = 0.1 \), which leads to the constrained multi-objective optimization problem (CMOOP) [cf. (3.7)]

\[
\min_{R,L} \left( |\lambda - 1.445796491|, |L - 1| \right),
\]

subject to \( |\lambda - 1.445796491| \leq 0.1. \quad (3.10) \)

In order to compare the quality of the solution with the results obtained with the use-coarse approach (Fig. 3.5, top), we show the results that are obtained using the same resources after a comparable time. Again using 36 processes of Intel Xeon Gold 6150, with \( M = 40 \), num-ind-gen= 20 [cf. section 3.1.3] and \( \beta = 0.1 \), the 46-th generation is formed in 902 s. This generation is shown at the bottom of Fig. 3.5 (we call this approach coarse-discard.). The squares again represent the individuals in the population, and their \( x \) and
3.4 Problem #2

$y$ coordinates show the values of $F_1$ and $F_2$, respectively. The Pareto front approximation in the use-coarse approach contains individuals that violate the constraint in (3.10), such as the individual with $(F_1, F_2) = (0.61, 8.1 \cdot 10^{-9})$. On the other hand, all individuals in the coarse-discard approach satisfy the constraint in (3.10), i.e., their value of $F_1$ is smaller than 0.1, which results in a different scale on the $x$ axis and makes it difficult to compare the quality of the results. However, the additional information given in Table 3.2 shows that better results are obtained when the individuals which are infeasible with respect to (3.10) are kept in the population (use-coarse), as opposed to being discarded (coarse-discard). If the number of infeasible individuals was much smaller, and if they brought little information on the location of good points, it might be wise to discard them in order to remove unwanted points which are technically good in the Pareto sense [cf. Definition 1], such as the one with $(F_1, F_2) = (0.61, 8.1 \cdot 10^{-9})$, from the population, especially if we could cheaply check whether a constraint is violated. This will be explored in chapter 4 when dealing with a constraint which is significantly different from the one in (3.10).

To summarize the results of this section, the EA found a good approximation of a known solution and it scales really well. When taking into account the scaling of the forward solver [cf. section 2.4.3], it can be seen that it is better to use the available workers to evaluate different design points than to have a few of them evaluate a single point in parallel. Furthermore, a coarse mesh can be used in some cases to significantly speed up the computations, and, in case it is difficult to obtain feasible individuals, keeping infeasible individuals in the population leads to better results than discarding them and losing the corresponding information.

3.4 Problem #2

In this section we solve a simple problem considering the geometry type from Fig. 3.1. This means that $N = 3$ and $d = (R, a, b)^T$. Setting $L = 500$ mm, $l = 125$ mm, and $r = 50$ mm, we try to find

$$R[\text{mm}] \in [200, 250] \text{ and } a, b[\text{mm}] \in [5, 100]$$ (3.11)

such that the frequency of the FM matches the accelerating frequency of SLS, i.e., that

$$f(d) = 499.636 \text{ MHz} \equiv f_{RF(SLS)}.$$ 

In order to avoid discharges and excessive dark current in the RF cavity, the normalized electric field of the FM on the surface of the cavity, $E_{pk}/V_{acc}$ [cf. (2.53)], should not be too high. Therefore, we aim to minimize $E_{pk}/V_{acc}$. 

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Additionally, in order to reduce the power load, we aim to maximize the shunt impedance of the FM, $R_{sh}$ [cf. (A.8)]. This can be written as the MOOP

$$\min_{d=(R,a,b)^T} \left( \begin{array}{c} f(d) - f_{RF(SLS)} \quad -R_{sh}(d) \quad E_{pk}(d)/V_{acc}(d) \end{array} \right),$$

with $f(d)$ in MHz. Since all three objective functions are defined as properties of the FM, only the eigenpair corresponding to the smallest non-zero eigenvalue of the GEVP corresponding to $m = 0$ [cf. (2.8)] and PEC BCSP [cf. p.26] needs to be found. However, in order to ensure that this eigenpair is found, we set $k_{max} = 3$ [cf. p.28]. Using linear elements [cf. Fig. 2.10], 6 significant digits of $f$ can be accurately computed in around 95 s (matrix size around 650’000), and 4 in a few seconds (matrix size around 10’000). Contrary to the situation in section 3.3.1, where only $F_1$ was influenced by the use of a different mesh size, now $F_2$ and $F_3$ are also affected. However, $F_2$ and $F_3$ do not have to be computed as accurately as $F_1$, especially in case $F_1$ is not close to zero. Therefore, we apply the approach from section 3.3.1 with $\beta = 1$ MHz (we again refer to this as use-coarse).

3.4.1 Crossover comparison

We first compare the two blending crossovers described in section 3.1.1: the $\alpha$-blend crossover with $\alpha = 0.5$, denoted by blend, and the simulated binary crossover, denoted by simulated-binary. The 80-th generation obtained with blend and the 65-th generation obtained with simulated-binary are shown at the top and bottom of Fig. 3.6, respectively. The specific generations were chosen such that the run times are approximately the same (around 3 h 30 min). Using 36 processes of Intel Xeon Gold 6150 (1 optimizer, 1 pilot, 34 workers), computing 80 generations with blend takes 12’544 s, and computing 65 generations with simulated-binary takes 12’705 s. In both plots, the $x$ and $y$ coordinates of a square, i.e., an individual, represent the values of the objective functions $F_3$ and $F_2$, respectively, and the color shows the value of $F_1$. The results in both cases are quite good and comparable, and the scale is the same for easier comparison. Since blend seems to find a ‘wider’ part of the Pareto front, we will use that in the rest of this chapter. An inverse correlation between $F_2$ and $F_3$ can be seen, but the values of $F_1$ can be very high. For example, there are even a few points with $F_1 \geq 200$ MHz, and we are interested in individuals with $f$ that matches $f_{RF(SLS)}$ to around 5 significant digits.
3.4 Problem #2

Figure 3.6: Top: the 80-th generation obtained with the use-coarse approach using the blend crossover, applied to the MOOP (3.12). Bottom: the 65-th generation of the use-coarse approach using the simulated-binary crossover, applied to the same problem. These two generations were chosen such that they both take approximately the same amount of time.
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3.4.2 Penalty function approach

Similarly to the approach in section 3.3.3, we formulate the requirement that \( f \) matches the target frequency \( f_{RF(SLS)} \) as both an objective and an inequality constraint with a suitably chosen \( \varepsilon \) [cf. (3.9)], which leads to the CMOOP

\[
\min_{d=(R,a,b)^T} \left( |f(d) - f_{RF(SLS)}|, -R_{sh}(d), E_{pk}(d)/V_{acc}(d) \right),
\]

subject to \( |f(d) - f_{RF(SLS)}| \leq \varepsilon \).  

(3.13)

Looking at the scale of \( F_1 \) in Fig. 3.6, we want to choose a value of \( \varepsilon \) that would help us get rid of individuals with ‘too high’ values of \( F_1 \). Together with the fact that \( \beta = 1 \text{ MHz} \), we set \( \varepsilon = 1 \text{ MHz} \).

Since we found out in section 3.3 that it is better to keep the individuals which violate the constraint in the population, we try the penalty function approach from (3.5). As we have only one inequality constraint, this becomes

\[
F_i(d) \mapsto F_i(d) + c_i \max\{0, |f(d) - f_{RF(SLS)}| - \varepsilon \}. 
\]

(3.14)

The penalty factors \( c_i \) need to be high enough for the constraint violation to have a sufficient influence on the corresponding objective functions, yet not so high that the objective function values become irrelevant. Different penalty factors are used for different objective functions in order to ensure that the summands in (3.14) have the same order of magnitude. If we first scale all objective functions such that they are of the same order of magnitude, we can use a single penalty factor, \( c \), for all \( i \in \{1, \ldots, n\} \). For the sake of simplicity, we also omit \( -\varepsilon \), which leads to the straightforward penalty method shown in Algorithm 2 (in this section, \( n = 3 \) and \( f_{RF} = f_{RF(SLS)} \)). We ran a few optimizations, with and without the \( \varepsilon \) term, and with \( c \) either equal to one or a bit larger and obtained comparable results.

**Algorithm 2** Penalization

1. if \( |f(d) - f_{RF}| > \varepsilon \) then
2. for \( i = 1, \ldots, n \) do
3. \( F_i(d) \mapsto F_i(d) + c \cdot |f(d) - f_{RF}| \)

The 97-th generation for \( c = 2 \), which takes around the same time (12’431 s, i.e., around 3 h 30 min) as the optimizations in Fig. 3.6 using the same resources, is shown in Fig. 3.7. As in Fig. 3.6, each square represents an individual in the generation, the \( x \) and \( y \) coordinates are again the values of the objective functions \( F_3 \) and \( F_2 \), respectively, and the color shows the value of
Figure 3.7: The 97-th generation of the penalize approach, using the blend crossover, applied to the CMOOP (3.13). This generation was chosen because it takes approximately the same amount of time as the ones shown in Fig. 3.6, using the same resources. Note that the scale for $F_1$ is significantly better than the one in Fig. 3.6 since now all individuals satisfy the constraint from (3.13). The arrows point to two individuals whose accelerating electric fields are shown is Fig. 3.8. Due to their positions in Fig. 3.8, we call these two individuals LEFT and RIGHT. Additional information is given in Table 3.3.

$F_1$. The scale of $F_2$ and $F_3$ is similar to the one in Fig. 3.6, but the scale of $F_1$ is significantly different. For all individuals, the fundamental frequency now differs from the target frequency by less than 1 MHz, i.e., all individuals in this generation satisfy the constraint from (3.13). The values of design variables and objective functions for two individuals marked in Fig. 3.7 are given in Table 3.3, and the cavities are shown in Fig. 3.8. Due to their positions in Fig. 3.8, we call these two individuals LEFT and RIGHT. LEFT has a better value of $F_1$ and $F_3$, while RIGHT has a better value of $F_2$, so these two individuals are equally good in the Pareto sense [cf. Definition 1].
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Figure 3.8: The magnitude of the axisymmetric electric field $E/V_{acc}$ in half of the cross section of the two good individuals, i.e., RF cavities with good objective function values, marked in Fig. 3.7. The values of design variables and objective functions are shown in Table 3.3.

Table 3.3: A description of individuals shown in Fig. 3.8. The objective function values for both individuals are very good. LEFT has a better value of $F_1$ and $F_3$, and RIGHT has a better value of $F_2$, so they are equally good in the Pareto sense [cf. Definition 1].

| In Fig. 3.8 | $R$ [mm] | $a$ [mm] | $b$ [mm] |
|-------------|----------|----------|----------|
| LEFT        | 236.588  | 23.4959  | 141.368  |
| RIGHT       | 232.616  | 14.7736  | 46.0276  |

| In Fig. 3.8 | $F_1$ [MHz] | $F_2$ [MΩ] | $F_3$ [1/m] |
|-------------|-------------|-------------|-------------|
| LEFT        | 0.002       | -3.2        | 5.7         |
| RIGHT       | 0.071       | -3.4        | 6.1         |

3.4.3 Checking results quality

In order to check the quality of these results, we evaluate a sample of 2'000 randomly chosen individuals in the design space (Fig. 3.9, blue and green points) and compare them with the points from Fig. 3.7 (Fig. 3.9, red points). The bottom plot shows a strong dependence of $F_1$ on $R$, and the values of $R$ for the found RF cavity shapes. The top plot shows the relationship between $F_2$ and $F_3$, and that the points found in Fig. 3.7 are very good. There are some randomly sampled points that have better values of both $F_2$ and $F_3$ than the points from Fig. 3.7, but none of these have $F_1 \leq 1$ MHz. Out of all the points
Figure 3.9: The points from Fig. 3.7 (red) compared with a random sample of 2’000 points (blue and green). The green point is the only point with $F_2 \leq -3 \, \text{M} \Omega$, $F_3 \leq 10 \, \text{1/m}$ and $F_1 \leq 1 \, \text{MHz}$. 
with $F_2 \leq -3 \, \text{M}\Omega$ and $F_3 \leq 10.1 \, \text{m}$, there is just one point, marked green, with $F_1 \leq 1 \, \text{MHz}$, with $(F_1, F_2, F_2) = (0.81 \, \text{MHz}, -3.5 \, \text{M}\Omega, 7.51 \, \text{m})$. Also, some of the red points, i.e., the points from Fig. 3.7, are outside of the bounds from (3.11). For example, all points with $E_{pk}/V_{acc} > 10.1 \, \text{m}$ have $a < 5 \, \text{mm}$.

We allow such behavior in the hope that, in case the initial intervals are not perfectly chosen, a good solution outside of them might still be found.

To summarize, the blend crossover and the simulated binary crossover both give quite good results, and the penalty function method brings a significant improvement to the values of $F_1$. The inverse correlation of $F_2$ and $F_3$ can be seen and, looking at a random sample, we can conclude that the found results are very good. One could put more effort into tuning the values of $\varepsilon$ and the penalty factor $c$, or consider different constraint handling methods for multi-objective problems. However, as we showed in this section, and as we will show in the next one, this approach works well enough in our case.

### 3.5 Problem #3

PSI is currently elaborating a proposal for the upgrade of SLS [cf. pp.1,8], called SLS 2.0 [93]. Even though it is planned to reuse the current RF cavity of SLS, the ELETTRA-type cavity from Fig. 2.7, in this section we focus on the hypothetical optimization of the RF cavity shape for SLS 2.0. This work was published in [62]. We consider different objective functions and two different geometry types with a symmetric cross section: an elliptical geometry type, illustrated in Fig. 3.10, and the geometry type where half of the cross section is defined as a complete cubic spline with horizontal end slopes, shown in Fig. 3.11. In both of these cases, in order to satisfy accelerator requirements we fix the value $r = 50 \, \text{mm}$, and, to have enough space for the modes to decay before the end of the beam pipe we set $l = 188.671 \, \text{mm}$ and $L = 680 \, \text{mm}$. We use the blend crossover, the independent bit mutation, and the penalty function approach [cf. section 3.4.2]. The number of individuals in a generation is around $M = 100$, and $\text{num-ind-gen}= 50$ [cf. section 3.1.3]. The description of interesting individuals is given in Table 3.5. We check the stability of the results by further mesh refinement and show the computed objective function values in Table 3.6. We compare these values with the corresponding values of an axisymmetric approximation of the current cavity of SLS, denoted ELETTRA 2D in Table 3.6.
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Figure 3.10: A geometry type with a symmetric cross section, defined by $L$, $l$, $R$, $r$, $A$, and $B$. We consider $L$, $l$, and $r$ to be fixed, and $R$, $A$, and $B$ to be design variables, i.e., $d = (R, A, B)^T$. Since this cross section is symmetric, it is sufficient to use only half of it.

3.5.1 Elliptical cavities

We first consider the elliptical geometry type from Fig. 3.10. Having fixed the variables $L$, $l$, and $r$, we are left with three design variables: $R$, the equator radius, and $A$ and $B$, the ellipse half axes. The initial values of these design variables are chosen randomly from the intervals given in Table 3.4. The accelerating frequency, i.e., the target frequency, usually defined by accelerator physics requirements such as longitudinal focusing, space limitations, and the availability of power sources, is in the case of SLS 2.0

$$f_{RF(SLS\ 2.0)} = 499.654\ MHz.$$  

As in section 3.4, the shunt impedance $R_{sh}$ [cf. (A.8)] has to be maximized and the normalized electric field on the surface of the cavity $E_{pk}/V_{acc}$ [cf. (2.53)] minimized. Therefore, we first consider the CMOOP [cf. (3.13)]

$$\min_{d=(R,A,B)^T} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = \begin{bmatrix} f(d) - f_{RF(SLS\ 2.0)} \\ -R_{sh}(d) \\ E_{pk}(d)/V_{acc}(d) \end{bmatrix},$$

subject to

$$|f(d) - f_{RF(SLS\ 2.0)}| \leq \varepsilon,$$

with $f(d)$ in MHz and $\varepsilon = 1$ MHz.

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Figure 3.11: A geometry type with a symmetric cross section whose boundary is a complete cubic spline with $s$ equidistant knots and horizontal end slopes. A geometry is defined by $L$, $l$, $r = y_1$, and $y_2, \ldots, y_s$. We set $s = 6$, fix the values of $L$, $l$, and $r$ and take $y_2, \ldots, y_6$ to be design variables, i.e., $d = (y_2, \ldots, y_6)^T$. Different values of design variables result in different instances of the same parameterization: the one at the top resembles the elliptical cavity from Fig. 3.10, while the one at the bottom has a more complicated shape. As in Fig. 3.10, it is enough to use half of the cross section.
Table 3.4: The initial intervals for the design variables in case of the elliptical and spline cavity, in mm. These geometry types are shown in Figs. 3.10 and 3.11, respectively.

| VARIABLE | ELLIPTICAL | SPLINE |
|----------|------------|--------|
|          | R  | A  | B | y_2 | y_3 | y_4 | y_5 | y_6 |
| LOWER BOUND | 200 | 50 | 50 | 100 | 150 | 200 | 250 | 250 |
| UPPER BOUND  | 350 | 150 | 150 | 200 | 250 | 250 | 275 | 275 |

Table 3.5: A description of chosen individuals.

| NAME     | GEOMETRY TYPE | FROM | SHOWN IN |
|----------|---------------|------|----------|
| CAVITY #1 | Fig. 3.10     | Fig. 3.12 | Fig. 3.13 |
| CAVITY #2 | Fig. 3.10     | Fig. 3.14 | Fig. 3.15 |
| CAVITY #3 | Fig. 3.11     | -     | Fig. 3.17 |

| NAME     | DESIGN VARIABLES |
|----------|------------------|
| CAVITY #1 | R = 249.901, A = 125.232, B = 70.2322 |
| CAVITY #2 | R = 251.972, B = 121.887, B = 78.5213 |
| CAVITY #3 | y_2 = 141.759, y_3 = 227.387, y_4 = 246.357, y_5 = 254.171, y_6 = 257.5 |

As in section 3.4, since we are only interested in the properties of the FM, only the eigenpair corresponding to the smallest non-zero eigenvalue of the GEVP corresponding to m = 0 [cf. (2.8)] and PEC BCSP [cf. p.26] needs to be found. We also apply the use-coarse approach with β = 1 MHz as in section 3.4, but the number of triangles in the fine mesh is now around 200’000. In order to ensure that the FM is found, k_{max} [cf. p.28] is again 3.

The 200-th generation is shown in Fig. 3.12. Each triangle again represents an individual in the generation, the x and y coordinates represent the values of the objective functions F_3 and F_2, respectively, and the color shows the value of F_1. For all individuals, the fundamental frequency differs from the target frequency by less than 1 MHz, and the inverse correlation of F_2 and F_3 can be observed. The marked individual possesses good objective function values. Its description is given in Table 3.5, where it is assigned the name CAVITY #1. The table contains the values of its design variables, as well as references to figures which contain additional information. The objective function values are listed in Table 3.6, where the shaded field indicates that the value was an
Figure 3.12: The 200-th generation in the optimization of $F_1$, $F_2$, and $F_3$ using the geometry type from Fig. 3.10. The arrow points to the individual whose accelerating electric field is shown in Fig. 3.13.

Figure 3.13: Top: the magnitude of the axisymmetric electric field $E/V_{acc}$ for the accelerating mode of the cavity corresponding to the individual pointed at in Fig. 3.12, called CAVITY #1 in Tables 3.5 and 3.6. Bottom: The magnitude of $E/V_{acc}$ on the cavity surface.
Table 3.6: A comparison of individuals described in Table 3.5. The values in the shaded fields were optimized for, and the other values are shown for a more thorough comparison.

| NAME           | $f$ [MHz] | $F_3$ [1/m] | $R_{sh}$ [MΩ] |
|----------------|-----------|-------------|---------------|
| ELETTRA 2D     | 500.461   | 5.65        | 3.56          |
| CAVITY #1      | 499.654   | 5.00        | 3.88          |
| CAVITY #2      | 499.654   | 4.98        | 3.83          |
| CAVITY #3      | 499.654   | 4.84        | 3.63          |

objective in the corresponding optimization. The fundamental frequency of CAVITY #1 matches the given target frequency $f_{RF(SLS \ 2.0)}$, and the values of $F_2$ and $F_3$ are better than the corresponding values for ELETTRA 2D, i.e., the shunt impedance is higher and the peak value of the electric field on the cavity surface lower. Since ELETTRA 2D is only an axisymmetric approximation of the cavity used at SLS, we avoid comparing the frequencies. The shape of CAVITY #1, as well as the electric field of the FM are shown in Fig. 3.13. Using two Intel Xeon E5-2680 V3 nodes (i.e., 48 processes), it takes 4 h 50 min to compute 200 generations.

### 3.5.2 Minimizing interaction with higher order modes

In addition to the three objectives in (3.15), the interaction of HOMs with the beam should be minimized. We now add another objective function, corresponding to the excitation of coupled beam modes, i.e., we next solve the CMOOP

$$
\min_{\mathbf{d}=(R,A,B)^T} \left( |f(\mathbf{d}) - f_{RF(SLS \ 2.0)}|, -R_{sh}(\mathbf{d}), E_{pk}(\mathbf{d})/V_{acc}(\mathbf{d}), F_4(\mathbf{d}) \right),
$$

subject to

$$
|f(\mathbf{d}) - f_{RF(SLS \ 2.0)}| \leq \varepsilon,
$$

(3.16)

where the new objective function, $F_4$, is defined in the following way.

For a cavity whose geometry is defined by the design point $\mathbf{d}$, with $p \in \mathbb{N}$,
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Figure 3.14: The 200-th generation in the optimization of $F_1$ (red), $F_2$, $F_3$ and $F_4$ (blue) using the geometry type from Fig. 3.10. The arrow points to the individual whose accelerating electric field is shown in Fig. 3.15.

Figure 3.15: Top: the magnitude of the axisymmetric electric field $E/V_{acc}$ for the accelerating mode of the cavity corresponding to the individual pointed at in Fig. 3.14, called CAVITY #2 in Tables 3.5 and 3.6. Bottom: The magnitude of $E/V_{acc}$ on the cavity surface.
3.5 Problem #3

$q \in \{0, 1, \ldots, 483\}$, and $f_{p,q} = p f_{RF(SLS \ 2.0)} \pm (q f_0 + f_s)$, where

\[ f_0 = f_{RF(SLS \ 2.0)}/484 \] is the rotation frequency, 
\[ f_s = 2.5 \text{ kHz} \] the synchrotron frequency without the harmonic cavity, and $i > 0$ the index of the longitudinal HOM, the longitudinal growth rate is given by [21]

\[
\frac{1}{\tau_{l,f_{p,q}}^{(i)}(d)} = \frac{|\alpha| f_0}{2 E/e f_s} I_b f^{(i)}(d) \frac{R_{sh}^{(i)}(d)}{1 + \left(2 Q^{(i)}(d) \frac{f^{(i)}(d) - f_{p,q}}{f^{(i)}(d)}\right)^2},
\]

where

\[
\alpha = -1.333 \cdot 10^{-4} \quad \text{is the momentum compaction factor,}
\]
\[ E/e = 2.4 \cdot 10^9 \text{ V} \quad \text{the beam energy divided by the electron charge,}
\]
\[ I_b = 400 \text{ mA} \quad \text{the beam current,}
\]
and $f^{(i)}(d)$, $R_{sh}^{(i)}(d)$ and $Q^{(i)}(d)$ are the frequency [cf. (2.52)], shunt impedance [cf. (A.8)] and quality factor [cf. (A.5)] of the $i$-th HOM of that cavity, respectively. Denoting by $f_c$ the cutoff frequency, we define

\[
F_4(d) = \sum_{\{i: f^{(i)}(d) < f_c\}} \sum_{\{f_{p,q} = pf_{RF(SLS \ 2.0)} \pm (q f_0 + f_s):}
\]
\[
p \in \{0, \ldots, p_{\text{max}}\},
\]
\[
q \in \{0, 1, \ldots, 483\}\}
\]

\[
a_{f_{p,q}}^{(i)}(d) = \begin{cases} 
\frac{1}{\tau_{l,f_{p,q}}^{(i)}(d)}, & \text{if } \frac{1}{\tau_{l,f_{p,q}}^{(i)}(d)} \geq b, \\
0, & \text{otherwise,}
\end{cases}
\]

\[
b = 0.5 \cdot \frac{1}{\tau_E},
\]

where 0.5 is a safety factor and $\tau_E = 6.5 \text{ ms}$ is the longitudinal damping time for SLS 2.0. With $r = 50 \text{ mm}$, $f_c = 2.29 \text{ GHz}$ and $p_{\text{max}} = 5$.

We consider only longitudinal modes, i.e., only the monopole case $m = 0$ [cf. (2.8)]. Since we are again using only half of the cross section, it is necessary to consider both the case with the PEC and the case with the PMC BCSP [cf. p.26]. In order to achieve the necessary accuracy for $F_4$, the number of triangles in the mesh is now around 400'000, and, in order for all the longitudinal
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modes with frequencies below $f_c$ to be computed, $k_{\text{max}} = 20$ [cf. p.28]. In this case it takes 2 days and 18 hours to compute 200 generations on two nodes, since the mesh size and the number of computed eigenpairs are larger, and we need to solve twice as many eigenproblems. Using eight nodes, however, brings the time down to 18 h 20 min, which amounts to the speedup of 3.6.

The 200-th generation is shown in Fig. 3.14. The red and blue triangles show the values of $F_1$ and $F_4$, respectively, and the $x$ and $y$ coordinates of the point where they meet represent the values of the objective functions $F_3$ and $F_2$, respectively. For all individuals, the fundamental frequency again differs from the target frequency by less than 1 MHz, and the inverse correlation of $F_2$ and $F_3$ can again be observed. An individual with good objective function values is chosen and marked, and its description and objective function values are given in Tables 3.5 and 3.6, respectively, where it is referred to as CAVITY #2. Its fundamental frequency matches the target frequency, the peak electric field on the cavity surface is slightly lower than for CAVITY #1,

Figure 3.16: A comparison of the values of $F_2$ and $F_3$ shown in Figs. 3.12 and 3.14. As one would expect, the values of these two objective functions are better when optimizing only 3 objectives (red) [cf. Eq. (3.15), Fig. 3.12] than when an additional, 4-th objective function is considered (blue) [cf. Eq. (3.16), Fig. 3.14].
i.e., \( F_3 \) is slightly better, but the shunt impedance is not as high, i.e., \( F_2 \) is not as good, though it is still better than the corresponding value for ELETTRA 2D. Since ELETTRA 2D is only an axisymmetric approximation, the longitudinal growth rate is above the threshold \( b \), defined in (3.17), for three of its HOMs. The value of \( F_4 \) is zero for CAVITY #2, and, coincidentally, also for CAVITY #1, even though it was not an objective in the optimization.

Since the scale in Figs. 3.12 and 3.14 is different, a comparison of the computed values of \( F_2 \) and \( F_3 \) in these two figures is shown in Fig. 3.16. The quality of these results is quite similar, yet, as one would expect, better in case the problem in (3.15) is being solved [cf. Fig. 3.12] than when an additional objective function, \( F_4 \), is also minimized, as is the case in the problem in (3.16) [cf. Fig. 3.14].

### 3.5.3 Spline cavities

We now consider the geometry type illustrated in Fig. 3.11. The symmetric cross section is defined as a complete cubic spline with equidistant knots and horizontal end slopes. We fix the number of knots to 6, and fix the values of \( L, l, \) and \( r = y_0 \). This leaves us with five design variables, \( y_1, \ldots, y_5 \).

Choosing the initial design variables in the ranges shown in Table 3.4 we find, for example, CAVITY #3, which is shown in Fig. 3.17, described in Table 3.5, and whose objective function values are given in Table 3.6. Its fundamental

![Figure 3.17: The magnitude of the axisymmetric electric field \( E/V_{acc} \) for the FM of the cavity referred to as CAVITY #3 in Tables 3.5 and 3.6. Bottom: The magnitude of \( E/V_{acc} \) on the cavity surface.](image)
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frequency matches the target frequency, $F_4 = 0$, the peak electric field on 
the cavity surface is slightly lower than for CAVITY #1 and CAVITY #2, 
i.e., $F_3$ is slightly better, but the shunt impedance is not as high, i.e., $F_2$ is 
not as good, though it is still slightly better than the corresponding value for 
ELETTRA 2D.
In this chapter we will solve two real-world constrained multi-objective RF cavity shape optimization problems for FCC-ee-Z [cf. p. 9] [14]. In this case, the frequency of the FM [cf. pp.1,42], \( f \), has to be tuned to

\[
f_{RF(\text{FCC-ee-Z})} = 400.79 \text{ MHz}. \tag{4.1}
\]

Additionally, it was suggested in [110] to use a single-cell elliptical cavity such as the one illustrated in Fig. 4.1. Setting the beam pipe length \( l \) to the value of the wave length, i.e., to \( \lambda = 748 \text{ mm} \), we are left with the geometric parameters \( R_{eq}, r, L, A, B, a, \) and \( b \).

![Figure 4.1: A symmetric elliptical geometry which generalizes the one from Fig. 3.10. The shape of the cross section is defined by \( R_{eq}, r, L, l, A, B, a, \) and \( b \). These eight variables also determine the wall slope angle \( \alpha \). Note that \( L \) is now defined differently than in Fig. 3.10. Also, the equator radius is now denoted \( R_{eq} \) as opposed to \( R \), in order to avoid a mix-up with shunt impedance (A.9).](image)
4 Sensitivity analysis

In section 4.2 we will perform a global SA [cf. p. 7] in order to analyze the influence of different geometric parameters. We will quantify the variability of the figures of merit, in this context called the quantities of interest (section 4.1), in the presence of uncertainty in the geometric parameters. We will then use this information to come up with a frequency tuning method for dealing with the frequency constraint (3.3) and find a good shape for the superconducting RF cavity for FCC-ee-Z, both with respect to the properties of the FM and the first dipole band, in section 4.3. This has been published in [64]. In section 4.4 we will search for cavities for FCC-ee-Z that are also robust with respect to geometric perturbations that can, e.g., arise from manufacturing inaccuracies. This is has been submitted to Phys. Rev. Accel. Beams [65].

4.1 Quantities of interest

Firstly, we are interested in some of the properties of the FM, which is typically the TM$_{010}$ mode, such as the frequency $f$ which needs to be tuned to (4.1) or $G \cdot R/Q$, which needs to be maximized because we want to minimize the surface losses of the FM [cf. (A.8)]

$$P_{\text{loss}} = \frac{(V_{\text{acc}})^2}{G \cdot R/Q} R_s,$$

where $G$, $V_{\text{acc}}$ and $R_s$ are the geometry factor, the accelerating voltage and the surface resistance, defined in (A.7), (2.54) and (A.3), respectively. $R$ is the shunt impedance and $Q$ the quality factor, defined in (A.9) and (A.5), respectively. Additionally, we also consider $R/Q$ to be a quantity of interest (QoI). Contrary to the CMOOP in section 3.5, in the case of FCC-ee-Z, we do not aim to minimize the normalized peak electric field on the surface of the cavity. Also, small values of the normalized peak magnetic field on the cavity surface usually go along with high values of $G \cdot R/Q$ [87]. Still, in the rest of this chapter, we consider both

$$E_{pk}/E_{acc} = L \cdot E_{pk}/V_{acc} \quad (4.2)$$

[cf. section 2.5.3, Fig. 4.1, (2.55)] and $B_{pk}/E_{acc}$ [cf. (A.1)] as QoIs.

Secondly, monopole and dipole modes are major sources of beam instability, but the dangerous higher order monopole modes can be untrapped by increasing the aperture radius $r$ [cf. Fig. 4.1] [65]. Therefore, we are interested in some of the properties of the first dipole band which stays trapped in the cavity, i.e., the TE$_{111}$ and the TM$_{110}$ mode. These trapped modes need to be damped, e.g., with coaxial or waveguide couplers. In order to facilitate this process, the frequencies of these two modes, $f_{\text{TE}_{111}}$ and $f_{\text{TM}_{110}}$, should be as
4.2 Global sensitivity analysis

close as possible, and far away from the frequency of the FM. Furthermore, the transverse impedances

\[ R/Q_{\perp,\text{TE}_{111}} \quad \text{and} \quad R/Q_{\perp,\text{TM}_{110}}, \]

defined in (A.10), should be minimized.

Lastly, we want to avoid re-entrant cavity shapes, so the wall slope angle \( \alpha \), defined in Fig. 4.1, should not be below 90°.

To sum up, the QoIs are

\[ f, f_{\text{TE}_{111}}, f_{\text{TM}_{110}}, R \cdot \frac{R}{Q}, R \cdot \frac{R}{Q_{\perp,\text{TE}_{111}}}, R \cdot \frac{R}{Q_{\perp,\text{TM}_{110}}}, G \cdot \frac{R}{Q}, \alpha, \frac{E_{pk}}{E_{\text{acc}}}, \frac{B_{pk}}{E_{\text{acc}}}. \]  

(4.4)

In order to compute the properties of the FM we need to find the eigenpair corresponding to the smallest non-zero eigenvalue of the GEVP corresponding to \( m = 0 \) and PEC BCSP [cf. 2.8, p.26]. In this chapter we will refer to this as ‘solving’ the GEVP corresponding to \( m = 0 \) and PEC BCSP. If the cavity shape is determined by the design point \( d \), we will denote this by

\[ \text{MAXWELL}_d(m,\text{BCSP}) = \text{MAXWELL}_d(0,\text{PEC}). \]  

(4.5)

In order to compute the properties of the TM\(_{110}\) and TE\(_{111}\) mode, we need to find the eigenpair corresponding to the smallest non-zero eigenvalue of the GEVPs corresponding to \( m = 1 \) and PEC and PMC BCSP, respectively. We will again refer to this as ‘solving’ the GEVPs, and denote it by

\[ \text{MAXWELL}_d(1,\text{PEC}) \quad \text{and} \quad \text{MAXWELL}_d(1,\text{PMC}). \]  

(4.6)

4.2 Global sensitivity analysis

In this section we will perform a global SA in order to get a better understanding of the problem so that we may devise a good optimization strategy in the following sections. In section 4.4 we will search for a cavity shape which is robust against geometric perturbations, i.e., a point in which the local sensitivities of the QoIs with respect to the design variables, defined as the partial derivatives of the QoIs with respect to the design variables, are small in magnitude. Calculating all the local sensitivities in a point is computationally expensive, so we want to determine the relative influence of each of the geometric parameters on a chosen QoI and then focus only on a few of the most influential ones. Additionally, we want to identify non-influential geometric parameters, as well as the geometric parameter which has the greatest influence on the frequency of the FM \( f \) in order to devise a frequency tuning method in section 4.3. We consider the geometric parameters [cf. Fig. 4.1] and
4 Sensitivity analysis

QoIs [cf. (4.4)] to be random variables, and we want to use the results of simulations [cf. chapter 2] to infer their statistical properties. In order to do this we perform a global SA, which quantifies the uncertainty of the output (QoIs) due to the uncertainties in the input (geometric parameters). Since it does not require linearity or monotonicity, we perform a variance-based global SA [91], and compute the Sobol’ indices [92] using a PC expansion [3,94] [cf. p.8]. In order to keep this section short and relevant to the specific problem tackled in this chapter, we give the auxiliary definitions in Appendix A.3.

Let the input uncertainties of the system be discretized and approximated by the random vector, i.e., a vector of random variables [cf. Definition 7] [91, §4.1.2]

\[ \boldsymbol{\xi} = (\xi_1, \ldots, \xi_N) : S \rightarrow \mathbb{R}^N. \]

A QoI \( u \in L_2(S, \mathcal{F}, P) \) [cf. Definition 10] can be written as

\[ u(\boldsymbol{\xi}) = \sum_{\|\boldsymbol{i}\|_1=0}^{\infty} \alpha_\boldsymbol{i} \Psi_\boldsymbol{i}(\boldsymbol{\xi}), \quad (4.7) \]

where

\[ \boldsymbol{i} = (i_1, \ldots, i_N) \in \mathbb{N}_0^N \text{ and } \|\boldsymbol{i}\|_1 = i_1 + \cdots + i_N, \]

the \( \alpha_{\boldsymbol{i}} \) are deterministic coefficients, and the \( \Psi_\boldsymbol{i} \) are multivariate PC basis functions [91, 10.1.1]. Let \( p \in \mathbb{N} \) and

\[ \mathcal{I}_{N,p} = \{ \boldsymbol{i} \in \mathbb{N}_0^N : \|\boldsymbol{i}\|_1 \leq p \}. \quad (4.8) \]

The PC expansion (4.7) truncated to polynomial degree \( p \) is

\[ \hat{u}(\boldsymbol{\xi}) = \sum_{\boldsymbol{i} \in \mathcal{I}_{N,p}} \alpha_\boldsymbol{i} \Psi_\boldsymbol{i}(\boldsymbol{\xi}). \quad (4.9) \]

The number of coefficients \( \alpha_{\boldsymbol{i}} \) that need to be computed is

\[ |\mathcal{I}_{N,p}| = \frac{(N + p)!}{N! \cdot p!}. \quad (4.10) \]

For \( \boldsymbol{i} = (i_1, \ldots, i_N) \in \mathcal{I}_{N,p} \), \( \Psi_\boldsymbol{i} \) is generated from

\[ \Psi_\boldsymbol{i}(\boldsymbol{\xi}) = \prod_{k=1}^{N} \Psi_{i_k}(\xi_k), \quad (4.11) \]

where the \( \Psi_{i_k} \) are univariate polynomials of degree \( i_k \) orthogonal with respect to the probability density function [cf. Definition 7] of \( \xi_k \).
4.2 Global sensitivity analysis

We consider the geometric parameters to be independent [67, §A.5.2], uniformly distributed [cf. Definition 8] random variables [cf. Definition 7], so the univariate polynomials in (4.11) are Legendre polynomials [107] [cf. Definition 11]. The truncated PC expansion (4.9) converges to \( u \) in the \( L_2 \)-norm [cf. (A.12)] if and only if \( u \) has a finite variance and [cf. Definition 12] [107]

\[
\alpha_i = \frac{\mathbb{E}[u(\xi) \cdot \Psi_i(\xi)]}{\mathbb{E}[\Psi_i^2(\xi)]}.
\]

We obtain the coefficients \( \alpha_i \) of the PC expansion (4.9) non-intrusively, because non-intrusive methods allow the use of an existing solver [cf. chapter 2] as a black box, requiring only an evaluation of the QoIs in a set of either deterministic or random points. Since some of the deterministic points may correspond to infeasible cavity shapes, we use a random sample, i.e., a set of random point, and compute the coefficients \( \alpha_i \) using regression [50, 94]. According to [94], it is enough to use a sample of size [cf. (4.10)]

\[
(N - 1)^{(N + p)!} \cdot N! \cdot p!
\]

(4.12)

where \( N \) is the number of parameters and \( p \) the polynomial degree [cf. (4.9)]. The values of (4.12), for a few relevant \( N \) and \( p \), are shown in Table 4.1.

![Table 4.1: The values of (4.12) for a few relevant values of \( N \), the number of parameters, and \( p \), the polynomial degree [cf. (4.9)].](image)

| \( N \) | \( p \) | 2 | 3 | 4 |
|-------|-------|---|---|---|
| 6     |       | 140| 420| 1050|
| 7     |       | 216| 720| 1980|

We use the Uncertainty Quantiﬁcation Toolkit (UQTk) [33,34], and evaluate the random sample in parallel, taking into account only feasible cavity shapes with \( \alpha \geq 90^\circ \).

In Fig. 4.2 we compare the polynomial surrogate (4.9) with the model, i.e., with the forward solver from chapter 2. We consider the parameterization from Fig. 4.1, so the number of parameters is \( N = 7 \), and the QoIs from (4.4). In the left column we use \( p = 2 \) and a random sample of size 216 [cf. Table 4.1], i.e., 216 training points, and in the right column \( p = 3 \) and 720 training points. In all cases we use 1000 new points, called validation points, to compare the polynomial surrogate with the model. We choose all training and validation points uniformly at random from the intervals in Table 4.2. Each point in
Figure 4.2: A comparison of the polynomial surrogate (y axis) with the model, i.e., the values computed with the forward solver (x axis) using 1'000 validation points (blue). Left column: $p = 2$, 216 training points. Right column: $p = 3$, 720 training points. We chose all the points uniformly at random from the intervals in Table 4.2.
4.2 Global sensitivity analysis

Table 4.2: Wide intervals for the geometric parameters in Fig. 4.1.

| VARIABLE [mm] | \( R_{eq} \) | \( r \) | \( L \) | \( A \) | \( B \) | \( a \) | \( b \) |
|----------------|---------|-----|-----|-----|-----|-----|-----|
| LOWER BOUND    | 325     | 145 | 240 | 65  | 65  | 10  | 10  |
| UPPER BOUND    | 375     | 160 | 380 | 140 | 140 | 60  | 60  |

The plot corresponds to a validation point, and its \( x \) and \( y \) coordinates show the values of the model and the polynomial surrogate, respectively, in that validation point. In each of the rows we show a representative case. In the case of

\[
f, f_{TE_{111}}, f_{TM_{110}}, R/Q, G \cdot \frac{R}{Q}, \text{ and even } \frac{B_{pk}}{E_{acc}},
\]

the agreement is already very good (i.e., the points are close to the \( y = x \) line) for \( p = 2 \). This is illustrated in the first row, where the agreement for \( f \) [MHz] is shown. The agreement in the case of \( R/Q, f_{TE_{111}} \) and \( R/Q, f_{TM_{110}} \) [Ω] is illustrated in the second row. For \( p = 2 \) there is a noticeable ‘tail’ which indicates that a higher polynomial degree should be used. The agreement in case \( p = 3 \) is much better. The third row shows the agreement for \( E_{pk}/E_{acc} \), which is the worst we observed. The agreement is also quite bad for \( \alpha \), though not as bad as for \( E_{pk}/E_{acc} \). The plots in the third row are the only case where the standard deviation (gray) [cf. Definition 12] is large enough to be seen.

The PC-based Sobol’ indices can be computed using the truncated PC expansion (4.9). First-order Sobol’ indices represent the individual influences of the parameters. For \( k \in \{1, \ldots, N\} \), the first-order Sobol’ index representing the influence of \( \xi_k \) (not including the effects between \( \xi_k \) and other parameters), denoted \( S_k \), is given by [94] [cf. Definitions 9 and 12]

\[
S_k = \frac{1}{\text{Var}(\hat{u}(\xi))} \sum_{\mathcal{I}_k} \alpha_i^2 \mathbb{E}[\Psi_i^2(\xi)],
\]

(4.13)

where [cf. (4.8)]

\[
\text{Var}(\hat{u}(\xi)) = \sum_{\mathcal{I}_{N,p}} \alpha_i^2 \mathbb{E}[\Psi_i^2(\xi)]
\]

(4.14)

and

\[
\mathcal{I}_k = \{ i = (i_1, \ldots, i_N) \in \mathcal{I}_{N,p} : i_k > 0, i_l = 0, \forall l \neq k \}.
\]

The relative contribution of \( \xi_k \) to the variance of \( u \) including the effects arising from interactions with other parameters is represented by [cf. (4.14)]

\[
S_{T,k} = \frac{1}{\text{Var}(\hat{u}(\xi))} \sum_{\mathcal{I}_{T,k}} \alpha_i^2 \mathbb{E}[\Psi_i^2(\xi)],
\]

(4.15)
4 Sensitivity analysis

where

\[ \mathcal{I}_{T,k} = \{ i = (i_1, \ldots, i_N) \in \mathcal{I}_{N,p} : i_k > 0 \} \]

We now show the results of the SA. The PC-based first-order Sobol’ indices (4.13), also called main sensitivities, are shown in Fig. 4.3. The polynomial degree is \( p = 2 \), and the intervals for the geometric parameters are given in Table 4.2. The value of the PC-based first-order Sobol’ index for a specific parameter (and QoI) is the height of the correspondingly colored part of the bar (for that QoI). For example, considering the QoI \( f \), the PC-based first-order Sobol’ index corresponding to \( R_{eq} \) is the height of the gray part of the bar for \( f \). Sobol’ indices are, by definition, normalized with respect to the total variance, so they (the first order and higher order indices) sum up to 1. Consequently, the sum of the first-order indices [cf. (4.13)], representing only the individual influences of the parameters, is at most 1. The higher-order indices represent mixed influences of the parameters [92], so the fact that the sum of the first-order indices, i.e., the height of the bars in the plots, is close to 1 indicates a low correlation between parameters [cf. Definition 12]. We can see this low correlation also in Fig. 4.4 where total sensitivities [cf. (4.15)] are shown. Looking at Fig. 4.5, which shows the main sensitivities considering the intervals from Table 4.2 and \( p = 3 \), we can see that the change from the results obtained with \( p = 2 \) is almost imperceptible. Looking also at Fig. 4.2, and having in mind that we are mostly interested in the sensitivities of \( f, f_{TE_{111}}, \) and \( f_{TM_{110}} \) [cf. section 4.4], that \( E_{pk}/E_{acc} \) is not an objective, and that \( \alpha \) can be computed from the geometric parameters, we decide to use \( p = 2 \) in the rest of the chapter. In addition to the intervals from Table 4.2, we also consider ‘narrower’ intervals. The main sensitivities with \( p = 2 \) and with geometric parameters in the intervals from Table 4.3 are shown in Fig. 4.6, where we can see that correlation between parameters is now virtually non-existent.

Table 4.3: Narrow intervals for the geometric parameters in Fig. 4.1.

| VARIABLE [mm] | \( R_{eq} \) | \( r \) | \( L \) | \( A \) | \( B \) | \( a \) | \( b \) |
|---------------|-------------|------|------|------|------|------|------|
| LOWER BOUND   | 345         | 145  | 280  | 70   | 70   | 45   | 45   |
| UPPER BOUND   | 355         | 155  | 300  | 80   | 80   | 55   | 55   |
4.2 Global sensitivity analysis

Figure 4.3: Main sensitivities using the intervals from Table 4.2 and $p = 2$.
The number of parameters is $N = 7$, so we use 216 training points.

Figure 4.4: Total sensitivities using the intervals from Table 4.2 and $p = 2$.
The number of parameters is $N = 7$, so we use 216 training points.
Figure 4.5: Main sensitivities using the intervals from Table 4.2 and $p = 3$. The number of parameters is $N = 7$, so we use 720 training points.

Figure 4.6: Main sensitivities using the intervals from Table 4.3 and $p = 2$. The number of parameters is $N = 7$, so we use 216 training points.
4.3 Problem #4

As stated in section 4.1, when optimizing the shape of the superconducting RF cavity for FCC-ee-Z, our goals are the following. First, we maximize the distance between the fundamental frequency $f$ and the frequencies of the dipole modes, $f_{TE_{111}}$ and $f_{TM_{110}}$. Denoting by $f_1$ the smaller of the two (in our application this is usually $f_{TE_{111}}$), and having in mind that $f_1 > f$, this means minimizing the negative value $f - f_1$. Second, denoting the larger of the two dipole mode frequencies by $f_2$, we minimize their distance $|f_1 - f_2|$. Third, we endeavor to minimize the transverse impedances of the dipole modes [cf. (4.3)] by minimizing their sum. Fourth, we maximize $G \cdot R/Q$, i.e., we minimize $-G \cdot R/Q$. We also add a constraint $\alpha \geq 90^\circ$ in order to avoid re-entrant cavity shapes. Together with the frequency constraint [cf. (3.3), (4.1)], this leads to the CMOOP

$$\min_{d=(R_{eq},r,L,A,B,a,b)^T} \left( f - f_1, |f_1 - f_2|, \frac{R}{Q_{\perp 1}} + \frac{R}{Q_{\perp 2}}, -G \cdot \frac{R}{Q} \right),$$
subject to

$$f = 400.79 \text{ MHz and } \alpha \geq 90^\circ.$$  \hspace{1cm} (4.16)

We again want to use the EA from chapter 3. Since we are not interested in re-entrant cavity shapes and we can compute the wall slope angle $\alpha$ quite cheaply, directly from the geometric parameters, we simply discard unwanted design points [cf. sections 3.2 and 3.3.3]. In order to deal with the constraint on the frequency of the FM [cf. pp.1,42], we use the information from the previous section in the following way.

### 4.3.1 Frequency tuning

We can see in Figs. 4.3, 4.4, 4.5, and 4.6 that the geometric parameter $R_{eq}$ has the greatest influence on the frequency of the FM, $f$, (closely followed by $A$), so we use it to tune $f$ to 400.79 MHz. Specifically, for a point

$$(d_2, \ldots, d_7) = (r, L, A, B, a, b)$$  \hspace{1cm} (4.17)

we use a root-finding method to find $d_1 = R_{eq} \in [l_1, u_1]$ such that

$$f(d = (R_{eq}, r, L, A, B, a, b)^T) = 400.79 \text{ MHz.}$$  \hspace{1cm} (4.18)

In this section and section 4.4 we will use the interval from Table 4.2, i.e., $l_1 = 325 \text{ mm, } u_1 = 375 \text{ mm}$. Even though in the CMOOP (4.16) we are also interested in the properties of the first dipole band, for the function evaluation in (4.18) we only need to compute $\text{MAXWELL}_d(0, \text{PEC})$ [cf. (4.5)]. Contrary to the approach in chapter 3, we now use $k_{\text{max}} = 5$ [cf. p.28] since the
4 Sensitivity analysis

consequences of the smallest non-zero eigenpair not being computed (which occasionally happens for \( k_{\text{max}} = 3 \)) are now more problematic.

We use the Boost\(^1\) C++ library for root-finding. In order to find a good method for our problem, we first compare three available methods: derivative-free bisection (which simply halves the interval) and the TOMS 748 [7] algorithm (which uses the interpolation to find the root), and the Newton–Raphson method which makes use of first-order derivatives. For a point (4.17) with values in the intervals in Table 4.2, we expect a single root in the given interval for \( R_{eq} \) [cf. Table 4.2]. If that is not the case, or if the method tries to evaluate an infeasible geometry, we stop the root-finding and discard the point. In order to avoid unnecessary computations in such cases, we keep the maximal number of steps a method is allowed to execute very low. If the root-finding method does find the root, as is usually the case, we stop it as soon as the first five significant digits of \( f \) match 400.79 MHz. As in chapter 3, we avoid the fine eigensolve if the difference between the approximate value of \( f \) obtained with a coarser mesh is further away from 400.79 MHz than 1 MHz. The coarse eigensolves use a mesh with around 20’000 triangles, and the fine ones around 500’000 triangles. On one core of Intel Xeon Gold 6150, solving just one coarse eigenproblem (meshing, computing 5 smallest eigenpairs and the objective function values) takes around 2 s, while solving a fine one takes around 95 s (18 s for meshing, 74 s for computing the eigenpairs, and 3 s for computing the objective function values). The number of fine eigensolves needed to find the root with each of these methods is given in Table 4.4. The number of fine eigensolves is computed as the average of the numbers obtained in 100 tests, each using a point (4.17) whose values are randomly chosen from the intervals in Table 4.2. We can see that bisection requires the largest average number of fine eigensolves. The Newton–Raphson method and the TOMS 748 algorithm are better, requiring 3 and 2.5 fine eigensolves on average, respectively. We also try to help these two methods by providing them with a better guess. In the case of the TOMS 748 algorithm, we first find a narrower interval for the root by evaluating \( f \) [cf. (4.18)] for \( R_{eq} \in \{325, 340, 360, 375\} \). This brings down the average number of fine eigensolves to 2.2. A similar approach, which starts the Newton–Raphson method from the middle of the corresponding narrower interval requires, on average, even fewer fine eigensolves. Since we avoid computing the derivative once a good enough cavity is found, often only one fine eigensolve is needed, so the average is 1.3. However, this method frequently encounters infeasible geometries and fails to find the root. The TOMS 748 algorithm on a narrower interval seldom encounters infeasible geometries, so we use this version in the rest of the chapter (and simply call it TOMS 748).

\(^1\)https://www.boost.org
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Table 4.4: A comparison of different root-finding methods. The number of fine eigensolves necessary to find the root is computed as the average of 100 tests on points (4.17) with values randomly chosen from the intervals in Table 4.2. The starting point for Newton–Raphson is 350 mm. The interval for bisection and the TOMS 748 algorithm is (in mm) [325,375]. Depending on the location of the root, the interval in the last column is (in mm) either [325,340], [340,360] or [360,375].

| METHOD        | Newton–Raphson | bisection | TOMS 748 | TOMS 748 (narrower) |
|---------------|----------------|-----------|----------|---------------------|
| # fine solves | 3.0            | 7.7       | 2.5      | 2.2                 |

The optimization method we use in this section is the following. We first reformulate the CMOOP (4.16) as

$$\min_{(r,L,A,B,a,b)^T} \begin{pmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \end{pmatrix} \begin{pmatrix} f - f_1, |f_1 - f_2|, R/Q_{\perp 1}, R/Q_{\perp 2}, -G \cdot R/Q \end{pmatrix},$$

subject to

$$f = 400.79 \, \text{MHz} \quad \text{and} \quad \alpha \geq 90^\circ, \quad (4.19)$$

and then use the EA (Algorithm 1) from chapter 3. The difference is that, compared to (4.16), in (4.19) we consider $I = (r,L,A,B,a,b)^T$ to be the design point, i.e., an individual. We evaluate the objective function values for this individual (lines 2 and 8 in Algorithm 1) as shown in Algorithm 3. We first find the value of the remaining geometric parameter, $R_{eq}$, using the frequency tuning method (line 1). We now have all the geometric parameters that define the cross section of an elliptical cavity [cf. Fig. 4.1, (4.16)]. Due to the way we found $R_{eq}$, this cavity satisfies the frequency constraint. We then compute the wall slope angle $\alpha$ [cf. Fig. 4.1]. In case it is below $90^\circ$, the found cavity is re-entrant, so we discard this individual (line 2). Otherwise, we found a feasible cavity, i.e., a cavity that satisfies both constraints from (4.19). Furthermore, during the frequency tuning in line 1 we already computed the necessary properties of the FM [cf. (4.19)], i.e., $f$ and $G \cdot R/Q$ for $F_1$ and $F_4$, respectively. It only remains to compute the necessary properties of the first dipole band (line 3) [cf. (4.6)].
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Algorithm 3 EVALUATE($I$), where $I = (d_2, \ldots, d_7)^T = (r, L, A, B, a, b)^T$

1: use MAXWELL$_d$(0,PEC) to compute $f(d)$ and TOMS 748 to find

$$d_1 = R_{eq} \in [l_1, u_1] \text{ s.t. } f(d)[\text{MHz}] - 400.79 = 0$$

2: if $\alpha(d) < 90^\circ$, return
3: compute the necessary properties of the dipole modes using

MAXWELL$_d$(1,PEC) and MAXWELL$_d$(1,PMC)

On three Intel Xeon Gold 6150 nodes (108 processes), computing 50 generations of the EA with $M = 100$ and num-ind-gen= 50 [cf. section 3.1.3] takes around 5 h 31 min. During an optimization, almost 30% of the evaluated individuals get discarded.

We will now show the results of an optimization that we presented in [64], even though this optimization used slightly different intervals for the initial guesses than those in Table 4.2, namely (in mm) [40, 140] for $A$ and $B$, and [10, 70] for $a$ and $b$. This is slightly inconsistent, but still quite reasonable since both versions are a decent guess and, if these intervals were used for the SA in section 4.2, the only significant difference would be a higher influence of $A$ on $f$, which indicates that $A$ would also be a good choice for tuning $f$. Therefore, and in order to be able to use them for comparison in the next section, we now show the results from [64].

The 50-th generation of an optimization with $M$ set to 100 and num-ind-gen to 50 is illustrated in Figs. 4.7 and 4.8, where each square represents an individual in the generation. For all of these individuals $f = 400.79\text{MHz}$ and $\alpha \geq 90^\circ$, i.e., both constraints from (4.19) are satisfied. In Fig. 4.7, the $x$ and $y$ coordinates represent the values of $F_1$ and $F_3$, respectively, and the color shows the value of $F_2$. The functions $F_1$ and $F_3$ are inversely correlated, and $F_1$ and $F_2$ do not seem to be conflicting, i.e., for lower values of $F_1$, the values of $F_2$ are usually also lower. In Fig. 4.8, the $x$ and $y$ coordinates represent the values of $F_2$ and $F_3$, respectively, and the value of $F_4$ is indicated by the color. The functions $F_2$ and $F_3$ are also inversely correlated.

We compare the individuals in this generation with three good single-cell cavities, called HL-LHC [78], CESR-B [71] and FCC$_{HO18}$ [80], whose dimensions are scaled such that $f = 400.79\text{MHz}$, in Table 4.5. The value in a certain row and $q$-th column is the number of distinct points in the generation that have at least $q$ objectives better than the cavity which corresponds to that row. We can see that all of these individuals are equally good in the Pareto
sense [cf. Definition 1]. We can also see, for example, that out of the 99 distinct individuals in this generation, 79 have at least two objectives better than CESR-B (second row and column). We show one such individual, with an extremely low value of $F_2$, in Fig. 4.9. We call this individual FCC#1 and compare its objective function values with the three good single-cell cavities in Table 4.6. The values of $F_1$ and $F_2$ are better than the corresponding values for the three cavities we are comparing with, but $F_3$ is worse. The value of $F_4$ is better than the one for FCC$\text{HO18}$, worse than the one for CESR-B and similar to the value for HL-LHC. We give additional information for all of these cavities, such as the values of geometric parameters and QoIs, in the following section, in Table 4.8.

Table 4.5: A comparison of the individuals shown in Figs. 4.7 and 4.8 with three good single-cell cavities. The value in a certain row and $q$-th column is the number of distinct points in the generation from Figs. 4.7 and 4.8 that have at least $q$ objectives better than the cavity which corresponds to that row. The generation contains 99 distinct individuals.

| $q$ | 1 | 2 | 3 | 4 |
|-----|---|---|---|---|
| HL-LHC | 99 | 77 | 15 | 0 |
| CESR-B | 99 | 79 | 23 | 0 |
| FCC$\text{HO18}$ | 99 | 89 | 2 | 0 |

Table 4.6: A comparison of FCC#1, shown in Fig. 4.9, with three good single-cell cavities. The values of geometric parameters and QoIs, both for these cavities and the cavities found in section 4.4 are given in Table 4.8 in section 4.4. Red indicates that the value is better than the corresponding value of our cavity. The color is otherwise blue (even when the values are ‘close’).

| OBJECTIVE | FCC#1 | HL-LHC | CESR-B | FCC$\text{HO18}$ |
|-----------|-------|--------|--------|-----------------|
| $F_1$ [MHz] | -147.03 | -122.74 | -112.42 | -127.97 |
| $F_2$ [MHz] | 0.40 | 19.83 | 29.44 | 0.85 |
| $F_3$ [Ω] | 36.3 | 31.3 | 29.6 | 30.1 |
| $F_4$ [kΩ$^2$] | -21.3 | -21.3 | -21.8 | -15.5 |
Figure 4.7: The relationship between $F_1$, $F_2$ and $F_3$ for the individuals in the 50-th generation of the EA. The marked individual, called FCC#1, is shown in Fig. 4.9. Its objective function values are given in Table 4.6 and additional information in Table 4.8.

Figure 4.8: The relationship between $F_2$, $F_3$ and $F_4$ for the individuals in the generation shown in Fig. 4.7. The same individual is marked.
Figure 4.9: The axisymmetric electric field of the FM in half of the RF cavity marked in Figs. 4.7 and 4.8. We call it FCC#1.

4.4 Problem #5

Manufacturing inaccuracies or perturbations during operation change the objective function values. If \( f \) is detuned from (4.1) additional power is needed for the same \( E_{\text{acc}} \) [cf. 4.2], so it is tuned to (4.1), usually by applying a longitudinal force to change the cell length. This force, however, should not be too large so as not to plastically deform the cavity. Furthermore, these inaccuracies and perturbations, as well as tuning \( f \), might detune \( f_{\text{TE}111} \) and \( f_{\text{TM}110} \), which would deteriorate their damping if coaxial couplers are used.

As illustrated in Fig. 4.10 using 1'000 random points in the intervals from Table 4.2, the local sensitivity of \( f \) (y axis) and \( f_{\text{TM}110} \) (color) with respect to \( R_{eq} \) (x axis) can be quite different in different points. We show the local sensitivities with respect to this design variable because, according to Fig. 4.3 it has the greatest influence on these frequencies.

Therefore, in addition to the goals in the previous section, we now want to find a cavity whose \( f \), \( f_{\text{TE}111} \) and \( f_{\text{TM}110} \) are robust with respect to geometric perturbations, i.e., denoting again [cf. (4.16)]

\[
\mathbf{d} = (d_1, \ldots, d_7) = (R_{eq}, r, L, A, B, a, b)^T,
\]

such that for \( j = 1, \ldots, 7 \),

\[
\begin{align*}
&\left| \frac{\partial f}{\partial d_j} \right|, \left| \frac{\partial f_{\text{TE}111}}{\partial d_j} \right|, \text{ and } \left| \frac{\partial f_{\text{TM}110}}{\partial d_j} \right|
\end{align*}
\]

are as small as possible. In order to avoid too many objectives that correspond to minimizing these local sensitivities, we sum up the sensitivities corresponding to the same frequency.
4 Sensitivity analysis

Figure 4.10: Local sensitivities of $f$ and $f_{TM_{110}}$ with respect to $R_{eq}$.

Furthermore, since a larger aperture radius $r$ is preferable [cf. section 4.1] and the cavity from Fig. 4.9, which has good objective function values considering the CMOOP (4.19), has $r = 141.614$ mm which is below the lower bound in Table 4.2, we now also try to maximize $r$.

To sum up, in this section we consider the CMOOP

$$\min_{(r,L,A,B,a,b)^T} \left( f - f_1, |f_1 - f_2|, \frac{R}{Q_{\perp_1}} + \frac{R}{Q_{\perp_2}}, -G \cdot \frac{R}{Q}, \right.$$ 

$$-r, \sum_{j=1}^7 \left| \frac{\partial f}{\partial d_j} \right|, \sum_{j=1}^7 \left| \frac{\partial f_{TE_{111}}}{\partial d_j} \right|, \sum_{j=1}^7 \left| \frac{\partial f_{TM_{110}}}{\partial d_j} \right| \bigg)$$

subject to $f = 400.79$ MHz and $\alpha \geq 90^\circ$.

As in section 4.3.1, we use the remaining geometric parameter, $R_{eq}$, [cf. Fig. 4.1] to tune $f$ to 400.79 MHz. However, computing all of the local sensitivities is very expensive, so we use the results of the global SA to determine the most influential geometric parameters and reformulate the CMOOP.
4.4.1 Sensitivity analysis in case of tuned frequency

We show the main sensitivities of the QoIs and $R_{eq}$ with respect to $d_2, \ldots, d_7$ [cf. (4.20)], considering the wide (Table 4.2) and narrow (Table 4.3) intervals in Figs. 4.11 and 4.12, respectively. The polynomial degree is again $p = 2$ [cf. section 4.2], but the number of variables is now 6, so, according to Table 4.1, we need only 140 training points.

First, we can see in Figs. 4.3-4.6 and 4.11-4.12 that the influence of $B$ on all of the QoIs is very low, and that $b$ significantly influences only $E_{pk}/E_{acc}$. Therefore, since $E_{pk}/E_{acc}$ is not part of any objective function in the CMOOP (4.21), these two geometric parameters can be omitted. We set $B = A$ and $b = a$, i.e., we consider circles instead of ellipses in the cross section parameterization in Fig. 4.1.

Second, based on the information from Figs. 4.3 and 4.6, we need to take into account

$$\frac{\partial f}{\partial R_{eq}}, \frac{\partial f}{\partial A}, \text{and} \frac{\partial f_{TM110}}{\partial R_{eq}}.$$ 

Similarly, from the information shown in Figs. 4.11 and 4.12, we also need to consider

$$\frac{\partial f_{TE111}}{\partial L}, \frac{\partial f_{TE111}}{\partial r}, \frac{\partial f_{TM110}}{\partial A}, \text{and} \frac{\partial f_{TM110}}{\partial r}.$$ 

However, due to the influence of $A$ on $R_{eq}$ (Figs. 4.11 and 4.12) and their geometric connection (Fig. 4.1), we omit the local sensitivities with respect to $A$ in order to decrease the computational cost.

Therefore, we reformulate (4.21) as

$$\min_{(r,L,A,a)^T} \left( \begin{array}{c} F_1 \\ F_2 \\ F_3 \\ F_4 \end{array} \right)$$

$$\begin{array}{c} f - f_1, |f_1 - f_2|, \frac{R}{Q_\perp_1} + \frac{R}{Q_\perp_2}, -G \cdot \frac{R}{Q} \\ \frac{\partial f}{\partial R_{eq}}, \frac{\partial f_{TE111}}{\partial L} + \frac{\partial f_{TE111}}{\partial r} \\ \frac{\partial f_{TM110}}{\partial R_{eq}} + \frac{\partial f_{TM110}}{\partial r} \end{array} \right),$$

subject to

$$f = 400.79 \text{ MHz and } \alpha \geq 90^\circ.$$ 

It is implied that for each design point $I = (r, L, A, a)^T$ we set the values of $B$ and $b$ [cf. Fig. 4.1] to $B = A$ and $b = a$, and then tune $f$ to 400.79 MHz using $R_{eq}$ [cf. 4.3.1].
4 Sensitivity analysis

Figure 4.11: Main sensitivities using the intervals from Table 4.2, $p = 2$, and with $f$ tuned to 400.79 MHz using $R_{eq}$ (140 training points).

Figure 4.12: Main sensitivities using the intervals from Table 4.3, $p = 2$, and with $f$ tuned to 400.79 MHz using $R_{eq}$ (140 training points).
4.4 Problem #5

4.4.2 Optimization method

The optimization method is similar to the method from section 4.3.1, and we again use the EA from Algorithm 1 in chapter 3. Taking \( \mathbf{I} = (r, L, A, a)^T \) to be a design point, we evaluate the objective functions as shown in Algorithm 4. After setting \( B = A \) and \( b = a \) (line 1), we perform the steps from Algorithm 3 (line 2): tuning the frequency \( f \), discarding the cavity if it is re-entrant, otherwise computing its dipole mode properties. We now have the values of \( F_1, \ldots, F_4 \) and, since \( r \) is a design variable, also \( F_5 \). It only remains to compute the local sensitivities for \( F_6, F_7 \) and \( F_8 \). We compute these numerically, using the forward difference method (line 3). In order to numerically compute the local sensitivity, i.e., the partial derivative \( \partial f_k / \partial d_l \) using the forward difference method, we need to evaluate \( f_k \) in the point \( d_{h,l} = (d_1, \ldots, d_l + h, \ldots, d_N) \), i.e., we need to solve another GEVP for the appropriate azimuthal mode number \( m_{f_k} \) and BC on the cross section symmetry plane \( BCSP_{f_k} \). In this section we use \( h = 1 \) mm.

Algorithm 4 EVALUATE-ROBUST(\( \mathbf{I} \)), where \( \mathbf{I} = (r, L, A, a)^T \)

1: set \( B = A \) and \( b = a \)
2: EVALUATE\(((r, L, A, B, a, b)^T)\) from Algorithm 3
3: for each partial derivative \( \partial f_k / \partial d_l \), with the corresponding \( BCSP_{f_k} \) and \( m_{f_k} \), and \( d_{h,l} = (d_1, \ldots, d_l + h, \ldots, d_N) \),

\[
\text{MAXWELL}_{d_{h,l}}(m_{f_k}, BCSP_{f_k})
\]

\( \text{to numerically compute } \partial f_k / \partial d_l \) using the forward difference method

On three Intel Xeon Gold 6150 nodes (108 processes), computing 50 generations of the EA with \( M = 100 \) and \texttt{num-ind-gen}= 50 [cf. section 3.1.3] using the mesh sizes as in section 4.3 now takes around 12 h 59 min.

The 60-th generation (because it already contains a very good RF cavity shape [cf. Fig. 4.16]) of an optimization with \( M = 100 \) and \texttt{num-ind-gen}= 50, and the initial values of design variables chosen from the intervals in Table 4.2, is illustrated in Figs. 4.13, 4.14 and 4.15, where each square represents an individual in the generation. For all of these individuals \( f = 400.79 \) MHz and \( \alpha \geq 90^\circ \), i.e., both constraints from (4.22) are satisfied. In Fig. 4.13, the \( x \) and \( y \) coordinates represent the values of \( F_1 \) and \( F_3 \), respectively, and the color shows the value of \( F_2 \). As in Fig. 4.7, the functions \( F_1 \) and \( F_3 \) are inversely correlated, and \( F_1 \) and \( F_2 \) again do not seem to be conflicting, though this is

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4 Sensitivity analysis

Figure 4.13: The relationship between $F_1$, $F_2$ and $F_3$ for the individuals in the 60-th generation of the EA. The marked individual, called FCC#2, is shown in Fig. 4.16. Its objective function values are given in Table 4.8.

Figure 4.14: The relationship between $F_2$, $F_3$ and $F_4$ for the individuals in the generation shown in Fig. 4.13. The same individual is marked.
Figure 4.15: The relationship between $F_6$, $F_7$ and $F_8$ for the individuals in Figs. 4.13 and 4.14. The same individual is marked.

Figure 4.16: The axisymmetric electric field of the FM in half of the RF cavity marked in Figs. 4.13, 4.14 and 4.15. We call this cavity FCC#2.
not as clear as in Fig. 4.7. In Fig. 4.14, the $x$ and $y$ coordinates represent the values of $F_2$ and $F_3$, respectively, and the value of $F_4$ is indicated by the color. Compared to Fig. 4.8, the relationship between $F_2$ and $F_3$ is more difficult to determine. It is also quite difficult to determine the relationship between $F_5$ ($x$ axis), $F_7$ ($y$ axis) and $F_8$ (color) from Fig. 4.15.

We again compare the individuals in the chosen generation with three good single-cell cavities [cf. section 4.3], called HL-LHC, CESR-B and FCC$_{HO18}$, as well as with the good cavity we found in section 4.3, called FCC#1 [cf. Fig. 4.9]. For all of these cavities, $f = 400.79$ MHz. In Table 4.7 the value in a certain row and $q$-th column is the number of distinct points in the generation from Figs. 4.13, 4.14 and 4.15 that have at least $q$ objectives better than the cavity which corresponds to that row. We can see, for example, that all of these cavities are equally good in the Pareto sense [cf. Definition 1]. Out of the individuals in shown in Figs. 4.13, 4.14 and 4.15, we choose and mark one which has very good objective function values. This individual, called FCC#2, is shown in Fig. 4.16. The comparison of its objective function values with the four good cavities, and the values of the geometric parameters and QoIs for all of these cavities are shown in Table 4.8. FCC#2 has the lowest value of $F_2$, $F_6$ and $F_8$, and other objective function values are quite good. The value of $F_7$ is higher than the corresponding values of HL-LHC and CESR-B. Cavities that outperform all four cavities we are comparing with, such as the circled individual in Fig. 4.15, usually have a higher value of $F_2$. Since $R/Q_{TE_{111}}$ is very small compared to $R/Q_{TM_{110}}$ and $R/Q$ (3.2 Ω compared to 26.8 Ω and 78.2 Ω, respectively), we consider $F_7$ to be less important.

The value of the geometric parameter $A$ for FCC#2 is outside of the intervals from Table 4.2 [cf. chapter 3]. Since we performed the SA in section 4.2 on these intervals, we show in Table 4.9 that the local sensitivities taken into account in (4.22) are also the largest in case of FCC#2.

| Table 4.7: The value in a certain row and $q$-th column is the number of distinct points in the generation from Figs. 4.13, 4.14 and 4.15 that have at least $q$ objectives better than the cavity which corresponds to that row. The generation contains 95 distinct individuals. |
|---|---|---|---|---|---|---|---|---|
| $q$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| HL-LHC | 95 | 95 | 92 | 79 | 47 | 10 | 0 | 0 |
| CESR-B | 95 | 95 | 92 | 68 | 40 | 9 | 0 | 0 |
| FCC$_{HO18}$ | 95 | 94 | 78 | 51 | 19 | 1 | 0 | 0 |
| FCC#1 | 95 | 95 | 93 | 86 | 35 | 5 | 0 | 0 |
Table 4.8: A comparison of the cavity from Fig. 4.16 with three good single-cell cavities and the cavity from Fig. 4.9. For all cavities $f$ is equal to 400.79 MHz. Red indicates that the value is better than the corresponding value of FCC#2 (otherwise, the color is blue).

| VARIABLE | FCC#2 | CESR-B | HL-LHC | FCCHO18 | FCC#1 |
|----------|-------|--------|--------|---------|-------|
| $r$ [mm] | 153.704 | 150.0 | 150.0 | 156.0 | 141.614 |
| $L$ [mm] | 274.199 | 300.0 | 280.0 | 240.0 | 292.54 |
| $A$ [mm] | 53.582 | 103.750 | 104.0 | 70.0 | 103.54 |
| $B$ [mm] | 53.582 | 103.750 | 104.0 | 70.0 | 127.521 |
| $a$ [mm] | 36.6831 | 25.0 | 25.0 | 25.0 | 41.921 |
| $b$ [mm] | 36.6831 | 25.0 | 25.0 | 25.0 | 45.812 |
| $R_{eq}$ [mm] | 363.346 | 341.856 | 338.512 | 350.574 | 339.166 |

| QOI | FCC#2 | CESR-B | HL-LHC | FCCHO18 | FCC#1 |
|-----|-------|--------|--------|---------|-------|
| $f_{TE_{111}}$ [MHz] | 526.80 | 513.20 | 523.53 | 529.61 | 547.82 |
| $f_{TM_{110}}$ [MHz] | 526.94 | 542.65 | 543.36 | 528.76 | 548.22 |
| $R/Q$ [$\Omega$] | 78.2 | 89.5 | 90.6 | 79.0 | 94.9 |
| $R/Q_{\perp TE_{111}}$ [$\Omega$] | 3.2 | 5.5 | 4.6 | 2.3 | 5.1 |
| $R/Q_{\perp TM_{110}}$ [$\Omega$] | 26.8 | 24.1 | 26.7 | 27.8 | 31.2 |
| $\alpha$ [°] | 109.2 | 104.9 | 99.0 | 102.8 | 91.7 |
| $\frac{E_{pk}}{E_{acc}}$ [-] | 1.8 | 2.0 | 2.0 | 1.9 | 1.9 |
| $\frac{B_{pk}}{E_{acc}}$ [mT/MV/m] | 4.7 | 4.2 | 4.0 | 4.1 | 4.2 |

| OBJECTIVE | FCC#2 | CESR-B | HL-LHC | FCCHO18 | FCC#1 |
|-----------|-------|--------|--------|---------|-------|
| $F_1$ [MHz] | -126.01 | -112.42 | -122.74 | -127.97 | -147.03 |
| $F_2$ [MHz] | 0.15 | 29.44 | 19.83 | 0.85 | 0.40 |
| $F_3$ [$\Omega$] | 30.0 | 29.6 | 31.2 | 30.1 | 36.3 |
| $F_4$ [k$\Omega$$^2$] | -15.0 | -21.8 | -21.3 | -15.5 | -21.3 |
| $F_5$ [mm] | -153.704 | -150.0 | -150.0 | -156.0 | -141.614 |
| $F_6$ [MHz/mm] | 1.21 | 1.32 | 1.36 | 1.31 | 1.39 |
| $F_7$ [MHz/mm] | 3.08 | 2.71 | 2.90 | 3.16 | 3.20 |
| $F_8$ [MHz/mm] | 1.68 | 1.98 | 1.99 | 1.79 | 1.92 |
Table 4.9: Some of the local sensitivities for FCC#2 [cf. Fig. 4.16, section 4.2]. The magnitude of other sensitivities is below 0.7 MHz/mm.

| SENSITIVITY | $\partial f / \partial R_{eq}$ | $\partial f / \partial A$ | $\partial f_{TE_{111}} / \partial r$ |
|-------------|-------------------------------|--------------------------|----------------------------------|
| VALUE [MHz/mm] | -1.21 | -1.15 | -2.62 |

| SENSITIVITY | $\partial f_{TM_{110}} / \partial R_{eq}$ | $\partial f_{TM_{110}} / \partial A$ |
|-------------|------------------------------------------|----------------------------------|
| VALUE [MHz/mm] | -1.34 | -1.00 |

4.5 Problem #6

In this section we will generalize the approach described in section 4.4 and apply it to a single-cell cavity with a symmetric cross section and half of its boundary defined as a complete cubic spline with horizontal end slopes. Such a geometry type, or parameterization, is shown in Fig. 3.11, and we refer to it as ‘the spline cavity’ or ‘the single-cell spline cavity’. A summary is in Fig. 4.17.

4.5.1 Sensitivity analysis for spline cavities

We only consider the local sensitivities of $f$ and $f_{TM_{110}}$, not $f_{TE_{111}}$, since, as discussed in the previous sections, the transverse impedance [cf. (4.3)] of the $TE_{111}$ mode is usually quite low. The main sensitivities, with the geometric parameters chosen uniformly at random from the intervals in Table 4.10, are shown in Fig. 4.18. We can see that the geometric parameter with the greatest influence of the frequency of the FM $f$ is $y_4$. The main sensitivities in the case where, analogously to the use of $R_{eq}$ in section 4.3.1, $y_4$ is used to tune $f$ to 400.79 MHz are shown in Fig. 4.19. Based on the information from Figs. 4.18 and 4.19, we need to take into account

$$\frac{\partial f}{\partial y_4}, \frac{\partial f_{TM_{110}}}{\partial y_4} \text{ and } \frac{\partial f_{TM_{110}}}{\partial y_1},$$

respectively. Additionally, the influence of $y_6$ is small, so we omit it by setting $y_6 = 350$ [cf. Table 4.10].

Table 4.10: Intervals for the parameters for the spline cavity (Fig. 3.11 with the change that, as in Fig. 4.1, $L$ does not include the beam pipe).

| VARIABLE [mm] | $L$ | $y_1$ | $y_2$ | $y_3$ | $y_4$ | $y_5$ | $y_6$ |
|---------------|-----|------|------|------|------|------|------|
| LOWER BOUND   | 240 | 145  | 150  | 220  | 270  | 320  | 340  |
| UPPER BOUND   | 380 | 160  | 230  | 280  | 330  | 345  | 360  |
Figure 4.17: A summary of the approach from section 4.4, applied to a different parameterization. The methods are orange, and the conclusions and results red. The concrete information for the spline cavity (Fig. 3.11) is referenced in the corresponding step, in parenthesis.
4 Sensitivity analysis

Figure 4.18: Main sensitivities for the spline cavity using the intervals from Table 4.10 and \( p = 2 \). The number of parameters is \( N = 7 \), so we use 216 training points [cf. Table 4.1].

Figure 4.19: Main sensitivities for the spline cavity using the intervals from Table 4.10, \( p = 2 \), and with \( f \) tuned to 400.79 MHz using \( y_4 \). The number of training points is 140 [cf. Table 4.1].
This leads to the CMOOP ($y_1$ is now the aperture radius) [cf. (4.22)]

$$\min_{(L,y_1,y_2,y_3,y_5)^T} \left( \begin{array}{c} F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \\ F_7 \end{array} \right) = \left( \begin{array}{c} f - f_1, \abs{f_1 - f_2}, \frac{R}{Q_{\perp 1}} + \frac{R}{Q_{\perp 2}}, -G \cdot \frac{R}{Q}, \frac{\partial f_{TM_{110}}}{\partial y_4}, \abs{\frac{\partial f_{TM_{110}}}{\partial y_1}} \end{array} \right),$$

(4.23)

subject to $f = 400.79$ MHz,

where it is implied that, for each point $(L,y_1,y_2,y_3,y_5)^T$, $y_6 = 350$ mm and that $f$ will be tuned to 400.79 MHz using $y_4$.

### 4.5.2 Generalized optimization method

The cavity shape is parameterized by $d = (d_1, \ldots, d_N)^T$. In the case of the spline cavity with $s = 6$ knots, once the beam pipe length is fixed to the value of the wave length, i.e., $l = 748$ mm, we are left with $d = (L, y_1, \ldots, y_6)^T$. Using the SA (Fig. 4.18) we then identify the geometric parameter $d_j$, where $j \in \{1, \ldots, N\}$, which has the highest influence on $f$. In the case of the spline cavity, $j = 5$, i.e., $d_j = d_5 = y_4$. We also identify and omit the parameters with a negligible influence. In the case of the spline cavity, we omit $y_6$. This leaves us with a subset of the geometric parameters, namely $d_{i_1}, \ldots, d_{i_k}$, where $\{i_1, \ldots, i_k\} \subset \{1, \ldots, N\} \setminus \{j\}$. We use the EA [cf. Algorithm 1], take $I = (d_{i_1}, \ldots, d_{i_k})^T$ to be an individual and compute the objective function values for $I$, i.e., evaluate this individual (lines 2 and 8 in Algorithm 1) according to Algorithm 5. In the case of the spline cavity, an individual is $I = (L, y_1, y_2, y_3, y_5)^T$.

When evaluating an individual (Algorithm 5), we first set the values of the omitted geometric parameters in line 1 ($y_6 = 350$ mm) [cf. Algorithm 4 : line 1]. We then use a root-finding method to tune $f$ to the desired value using $d_j$ in line 2 ($d_j = d_5 = y_4$ and, from Table 4.10, $l_5 = 270$ mm and $u_5 = 330$ mm) [cf. Algorithm 3 : line 1]. If there were additional constraints on the cavity shape [cf. Algorithm 3 : line 2], we would then have to check if the found cavity shape satisfies them (line 3). If the found cavity shape is feasible, we need to compute the necessary properties of the dipole modes (line 4) [cf. Algorithm 3 : line 3], and the necessary sensitivities (line 5) [cf. Algorithm 4 : line 3].
Algorithm 5 \textsc{evaluate-generalized}(I), with $j \in \{1, \ldots, N\}$ fixed and $I = (d_{i_1}, \ldots, d_{i_k})^T$, $\{i_1, \ldots, i_k\} \subset \{1, \ldots, N\} \setminus \{j\}$.

1. set the value of $d_i$, $\forall i \in \{1, \ldots, N\} \setminus \{i_1, \ldots, i_k, j\}$
2. use MAXWELL$_d(0,\text{PEC})$ to compute $f(d)$ and TOMS 748 to find

$$d_j \in [l_j, u_j] \text{ s.t. } f(d)[\text{MHz}] - 400.79 = 0$$

3. check if other constraints are satisfied (if any), otherwise return
4. compute the properties of the dipole modes using

MAXWELL$_d(1,\text{PEC})$ and MAXWELL$_d(1,\text{PMC})$

5. for each partial derivative $\partial f_k/\partial d_i$, with the corresponding BCSP$_{f_k}$ and $m_{f_k}$, and $d_{h,i} = (d_1, \ldots, d_i + h, \ldots, d_N)$,

$$\text{MAXWELL}_{d_{h,i}}(m_{f_k}, \text{BCSP}_{f_k})$$

to numerically compute $\partial f_k/\partial d_i$ using the forward difference method.

An interesting individual, chosen because its aperture radius $y_1$ is close to that of FCC#2 [cf. Table 4.8], is shown in Fig. 4.20. Its design variable and objective function values, as well as QoIs, are in Table 4.11. The values of $F_1, \ldots, F_5$ are very close to those for FCC#2, though the shape is quite unusual. The objective functions $F_6$ and $F_7$ are defined differently than the objective functions in section 4.4, so we have nothing to compare them with. The values of $F_1$, $F_2$ and $F_4$ are better than those for FCC#2, but the values of

Figure 4.20: The axisymmetric electric field of the FM in half of a chosen spline cavity, called FCC#3.
4.5 Problem #6

$F_3$ and $F_5$ are worse. The values of $F_5 = -y_1$ are quite close, but in the case of FCC#3 there is a ‘dip’, so the smallest aperture width is $r_{min} = 152.311$ mm, which is a bit lower, i.e., the value is a bit worse. In order to search for cavities without a ‘dip’, $F_5$ could be defined as $F_5 = -r_{min}$ [cf. (4.23)].

Table 4.11: Design variable and objective function values, as well as QoIs, for FCC#3 (Fig. 4.20). ‘OBJ.’ is short for ‘OBJECTIVE’, $F_5 = -y_1$, $y_6 = 350$ mm, the smallest aperture width is denoted by $r_{min}$, and the frequency of the FM is $f = 400.79$ MHz.

| VARIABLE | FCC#3 | QOI | FCC#3 | OBJ. | FCC#3 |
|----------|-------|-----|-------|------|-------|
| $L$ [mm] | 282.183 | $f_{TE111}$ [MHz] | 530.13 | $F_1$ [MHz] | -129.34 |
| $y_1$ [mm] | 153.796 | $f_{TM110}$ [MHz] | 530.21 | $F_2$ [MHz] | 0.08 |
| $y_2$ [mm] | 158.552 | $R/Q$ [Ω] | 80.5 | $F_3$ [Ω] | 30.8 |
| $y_3$ [mm] | 230.247 | $R/Q_{\perp TE_{111}}$ [Ω] | 3.0 | $F_4$ [kΩ$^2$] | -15.8 |
| $y_4$ [mm] | 329.518 | $R/Q_{\perp TM_{110}}$ [Ω] | 27.8 | $F_5$ [MHz/mm] | -153.796 |
| $y_5$ [mm] | 343.655 | $E_{pk}/E_{acc}$ [-] | 1.9 | $F_6$ [MHz/mm] | 0.49 |
| $r_{min}$ [mm] | 152.311 | $B_{pk}/E_{acc}$ [mT/MV/m] | 4.8 | $F_7$ [MHz/mm] | 1.08 |
In this chapter we will first present a summary of chapters 2-4 and then give some ideas about possible future work.

5.1 Chapter 2 - summary

In chapter 2 we described the forward solver. To sum up, for a design point \( d = (d_1, \ldots, d_N)^T \) that determines the axisymmetric RF cavity shape [cf. 1.2.3] by determining its cross section, we compute the objective function values in the following way.

1. We create and mesh (if the cross section is symmetric, half of) the resulting cross section using Gmsh C++ API (serial).

2. We then create the finite element matrices in Problem 4 in parallel, using Trilinos [49], and the serial implementation from [23, 24] for computing the triangle contributions for (2.29).

3. We solve the resulting GEVP using the parallel implementation of the JDSYM algorithm from [8] which is based on Trilinos, together with the good parameters that we found for our problem.

4. Finally, we cheaply compute the necessary figures of merit (in parallel) [cf. Fig. 2.13].

This results in a fast and stable forward solver for axisymmetric cavity shapes. For a single design point \( d \), step (1) needs to be performed only once, while steps (2)-(4) have to be computed for all relevant azimuthal mode numbers [cf. (2.8)] and BCSP [cf. p.26].

5.2 Chapter 3 - summary

In chapter 3 we combined a massively parallel implementation of a multi-objective EA [51, 52, 70] with the forward solver from chapter 2. Furthermore,
we combined this with a constraint handling method, and determined good options and parameters on a few simple problems.

We then hypothetically optimized the shape of the main RF cavity of the proposed SLS upgrade, for which it is planned to reuse the existing close-to-axisymmetric ELETTRA-type cavity, extended by a new type of absorber for the most troubling beam excited HOMs [93]. We computed a Pareto front approximation and found a few axisymmetric RF cavity shapes that outperform the axisymmetric approximation of the ELETTRA-type cavity in all of the considered objective functions (Table 3.6).

The higher value of the shunt impedance ensures that the power load is reduced, and the lower value of the peak electric field on the cavity surface makes discharges less likely. Moreover, the new-found cavity shapes are already optimized with respect to an objective function which corresponds to the excitation of coupled beam modes, i.e., the interaction with HOMs is already minimized.

5.3 Chapter 4 - summary

In chapter 4 we first performed a global sensitivity analysis in order to determine the relative influence of different geometric parameters on the figures of merit. We used these results to devise a frequency tuning method for dealing with the frequency constraint (3.3), and then found a good shape for the superconducting RF cavity for the Z-pole operating mode of the lepton collider at the FCC, both with respect to the properties of the FM [cf. p.1] and the first dipole band.

We then focused on finding an RF cavity shape that is also robust with respect to geometric perturbations. In order to decrease the computational cost, we used the results of the the sensitivity analysis to reformulate the CMOOP and reduce the search space.

We found an RF cavity that outperforms three good single-cell cavities from the literature (HL-LHC [78], CESR-B [71] and FCC$\text{HO18}$ [80]) in either five or six out of the eight considered objectives (Table 4.8). For example, the fundamental frequency is more robust, and the frequencies of the trapped dipole modes are closer to each other which would simplify their damping using coaxial HOM couplers.

In the end we also illustrated how the proposed optimization method could be generalized to other types of geometries and similar RF cavity shape optimization problems [cf. Fig. 4.17].
Some ideas about possible future work are given below.

First, a second order approximation (quadratic basis functions with curvilinear elements) could be used to further speed up the solution of time-harmonic Maxwell’s equations [cf. chapter 2].

Second, the EA could be combined with a gradient-based optimization method [cf. section 1.2.1] into a hybrid optimization method, preferably also including the frequency tuning method from chapter 4. For instance, in order to speed up the computation of the gradients, meshing could be avoided whenever the changes in the design variable values are ‘sufficiently small’. Instead, an existing mesh of a similar shape could be modified.

Third, different parameterizations could be considered. In the case of the spline cavity in section 4.5, a different number of knots could be chosen or constraints added to the optimization problem in order to get rid of the ‘dips’ [cf. Fig. 4.20].

Fourth, at the expense of increased computational cost, the approach could be generalized to (not necessarily axisymmetric) 3D problems. Moreover, an optimized axisymmetric cavity shape could be used as the starting point in a 3D optimization of close-to-axisymmetric RF cavities.
A.1 Solving Maxwell’s equations in axisymmetric domains

In this section we will define the operators and function spaces used in section 2.1, based on [23].

Definition 4. Let $\Omega \subset \mathbb{R}^3$ be an open bounded domain with a Lipschitz continuous boundary $\Gamma$. Then, for $d \in \{1, 2, 3\}$,

$$L_2(\Omega)^d = \left\{ g : \Omega \to \mathbb{R}^d : \int_{\Omega} \| g(x) \|_2^2 \, d\Omega < \infty \right\},$$

where the integral is defined in the sense of Lebesgue. Furthermore, denoting the normal to $\Gamma$ by $n$,

$$H(\text{curl}; \Omega) = \left\{ g \in L_2(\Omega)^3 : \text{curl}(g) \in L_2(\Omega)^3 \right\},$$

$$H_0(\text{curl}; \Omega) = \left\{ g \in H(\text{curl}; \Omega) : \forall x \in \Gamma, \, g(x) \times n(x) = 0 \right\},$$

$$H^1_0(\Omega) = \left\{ g \in L_2(\Omega) : \text{grad}(g) \in L_2(\Omega)^3, \, \forall x \in \Gamma, \, g(x) = 0 \right\}.$$

Definition 5. Let $\Omega \subset \mathbb{R}^3$ be an open bounded domain with a Lipschitz continuous boundary, and with cross section $\Omega_p \subset [0, \infty) \times \mathbb{R}$. Also, let $\Gamma_p = \partial \Omega_p \setminus \{(r, z) \in \partial \Omega_p : r = 0\}$ and $r_p = (r, z)^T$. Then, for $d \in \{1, 2, 3\}$,

$$L_2(\Omega_p)^d = \left\{ g : \Omega_p \to \mathbb{R}^d : \int_{\Omega_p} r \| g(r_p) \|_2^2 \, d\Omega_p < \infty \right\}.$$

Furthermore, denoting the normal to $\Gamma_p$ by $n_p$, and denoting $g = (g_r, g_\theta, g_z)^T$
A Definitions and auxiliary statements

and \( \mathbf{g}_p = (g_r, g_z)^T \), for a fixed \( m \in \mathbb{N}_0 \),

\[
\hat{H} (\text{curl}; \Omega_p) = \left\{ g \in \hat{L}_2 (\Omega_p)^3 : \right. \\
\left. \text{curl}_p (g_p) \in \hat{L}_2 (\Omega_p), \frac{1}{r} (mg_p + \text{grad}_p (r g_\theta)) \in \hat{L}_2 (\Omega_p)^2 \right\}, \\
\hat{H}_0 (\text{curl}; \Omega_p) = \left\{ g \in \hat{H} (\text{curl}; \Omega_p) : \right. \\
\forall r_p \in \Gamma_p, g_p (r_p) \times n_p (r_p) = g_\theta (r_p) = 0 \}, \\
\hat{H}^1 (\Omega_p) = \left\{ g \in \hat{L}_2 (\Omega_p) : \text{grad}_p (g) \in \hat{L}_2 (\Omega_p)^2, \frac{m}{r} g \in \hat{L}_2 (\Omega_p) \right\}, \\
\hat{H}^1_0 (\Omega_p) = \left\{ g \in \hat{H}^1 (\Omega_p) : \forall r_p \in \Gamma_p, g (r_p) = 0 \right\}.
\]

The cross product of \( \mathbf{g}_p \) and \( \mathbf{n}_p = (n_r, n_z)^T \) is defined as [cf. (2.12)]

\[
\mathbf{g}_p \times \mathbf{n}_p = g_r n_z - g_z n_r.
\]

A.2 Additional figures of merit

In this section we will define the rest of the figures of merit [13, 103] [cf. section 2.5] needed to define the objective functions in chapters 3 and 4.

A.2.1 Peak magnetic field on surface

The normalized peak magnetic field on the surface of the cavity can be computed as [cf. (2.53), (2.54), (2.55)]

\[
\frac{B_{pk}}{E_{acc}} = \frac{\max_{x \in \partial \Omega} \| \mathbf{b}(x) \|_2}{V_{acc}/L}, 
\]

where \( \mathbf{b} = \mu_0 \mathbf{h} \) [cf. (2.48)].

A.2.2 Surface losses

The power loss, or the surface loss, is defined as

\[
P_{\text{loss}} = \frac{R_S (d)}{2} \int_{\partial \Omega} \| \mathbf{h} \|_2^2 \, dS, 
\]
where $h$ is the magnetic field [cf. (2.48)], and $R_S$ is the surface resistance defined as

$$ R_s(d) = \frac{1}{\sigma \cdot \delta(d)}, \quad (A.3) $$

where $\sigma$ is the electrical conductivity and $\delta$ the skin depth given by [cf. (2.52)]

$$ \delta = \left( \sqrt{\pi \cdot f(d) \cdot \mu_0 \cdot \sigma} \right)^{-1}, $$

assuming that the relative permeability of the wall is $\approx 1$. In chapter 3 we use

$$ \sigma_{\text{Cu-OFE}} = 58.58 \cdot 10^6 \text{ S/m} $$

for the electrical conductivity of Cu-OFE [1].

The integral in (A.2) can be computed as [cf. (2.50), (2.51)]

$$ \int_{\partial \Omega} \|h\|_2^2 dS = \alpha \int_{\partial \Omega_p} r \|w_h\|_2^2 ds, \text{ where } \alpha = \begin{cases} 2\pi & \text{if } m = 0, \\ \pi & \text{if } m \in \mathbb{N}. \end{cases} \quad (A.4) $$

### A.2.3 Quality factor

The quality factor can be defined as [cf. (A.3), section 2.5.2, Remark 1]

$$ Q = \frac{\omega \cdot U}{P_{\text{loss}}}, \quad (A.5) $$

with the stored energy ($\varepsilon_0$ is the permittivity of vacuum$^1$) [cf. (A.4), (2.9)]

$$ U = \frac{\varepsilon_0}{2} \int_{\Omega} \|e\|_2^2 d\Omega = \frac{\varepsilon_0}{2} \int_{\Omega_p} r \|w\|_2^2 d\Omega_p. \quad (A.6) $$

Since the eigenvectors are normalized with respect to the matrix $M$ [cf. (2.30)], the rightmost integral in (A.6) is 1, and the stored energy $\alpha \cdot \varepsilon_0/2$.

### A.2.4 Geometry factor

Additionally, we define the geometry factor as [cf. (A.3), (A.5)]

$$ G = R_s \cdot Q. \quad (A.7) $$

---

$^1\varepsilon_0 \approx 8.854187817 \cdot 10^{-12} \text{ F/m} \quad [96]$
A.2.5 Shunt impedance

The shunt impedance is defined as [cf. (2.54), (A.2)]

\[ R_{sh} = \frac{(V_{acc})^2}{2 \cdot P_{loss}}. \] (A.8)

The alternative definition for the shunt impedance is [103, p.621]

\[ R = 2 \cdot R_{sh}. \] (A.9)

Following the convention of different communities, we use the definition (A.8) with the symbol \( R_{sh} \) in chapter 3, and the definition (A.9) with the symbol \( R \) in chapter 4.

A.2.6 Transverse impedance

The transverse impedance can be computed as [105] [cf. (A.6)]

\[ \frac{R}{Q_\perp} = \frac{(V_{||(r=r_0)} - V_{||(r=0)})^2}{k^2 r_0^2 \omega U}, \] (A.10)

where \( k \) is the wave number \( (k = \omega/c = \sqrt{\lambda}) \), \( r_0 \) the offset from the axis (in chapter 4 we use \( r_0 = 10 \) mm), and

\[ V_{||(r=r_0)} = \left| \int_0^L e_z(r_0, z)e^{i\sqrt{\lambda}z}dz \right|. \]

Note that \( V_{||(r=0)} = V_{acc} \) [cf. (2.54)].

A.3 Sensitivity analysis using polynomial chaos expansion

In this section we will give some details for section 4.2, based on [67,91].

**Definition 6.** A *probability space* \((S, \mathcal{F}, P)\) is comprised of:

- \( S \), the *sample space*, i.e., the set of all possible outcomes,
- \( \mathcal{F} \subset \mathcal{P}(S) \), the *\( \sigma \)-field*, i.e.,
  - \( S \in \mathcal{F} \),
  - if \( A \in \mathcal{F} \), then \( S \setminus A \in \mathcal{F} \),
  - if \( A_i \in \mathcal{F}, \forall i \in I \), then \( \cup_{i \in I} A_i \in \mathcal{F} \), where \( I \) is a countable set.
A.3 Sensitivity analysis using polynomial chaos expansion

- \( P : \mathcal{F} \rightarrow [0,1] \), the probability measure, i.e.,
  - \( P(\emptyset) = 0 \),
  - \( P(S) = 1 \),
  - if \( \{A_i \in \mathcal{F} : i \in I \} \) is a countable collection of pairwise disjoint sets (i.e., \( A_i \cap A_j = \emptyset, \forall i,j \in I, i \neq j \)), then \( P(\bigcup_{i \in I} A_i) = \sum_{i \in I} P(A_i) \).

The probability space is complete if every subset of a set of measure zero is measurable, i.e., if \( P(A) = 0 \) and \( B \subseteq A \) implies \( B \in \mathcal{F} \).

A probability space can always be completed, so we will implicitly assume that the probability space is complete.

**Definition 7.** A random variable is a function \( X : S \rightarrow \mathbb{R} \) such that
\[
\forall x \in \mathbb{R}, \{\omega \in S : X(\omega) \leq x\} \in \mathcal{F}.
\]

A cumulative distribution function (CDF) associated with \( X \) is \( F_X : \mathbb{R} \rightarrow [0,1] \) given by
\[
F_X(x) = P(\{\omega \in S : X(\omega) \leq x\}).
\]

The random variable \( X \) is continuous if its CDF is absolutely continuous [11, Definition 4.4.1]. Its CDF can then be expressed as [11, p.128-129]
\[
F_X(x) = \int_{-\infty}^{x} f_X(s) \, ds, \quad x \in \mathbb{R},
\]
where \( f_X : \mathbb{R} \rightarrow [0,\infty) \) is called the probability density function (PDF) of \( X \).

**Definition 8.** A random variable \( X \) is uniformly distributed on the interval \([a,b] \subseteq \mathbb{R}\), denoted by \( X \sim \mathcal{U}(a,b) \), if every value in \([a,b]\) is achieved with equal probability. The PDF is then
\[
f_X(x) = \frac{1}{b-a} \chi_{[a,b]}(x),
\]
where
\[
\chi_{[a,b]}(x) = \begin{cases} 
1, & \text{for } x \in [a,b], \\
0, & \text{otherwise}.
\end{cases}
\]

**Definition 9.** The expected value of the random variable \( X \) is denoted by \( \mu_X \) or \( \mathbb{E}[X] \) and defined as
\[
\mathbb{E}[X] = \int_{\mathbb{R}} x f_X(x) \, dx.
\]
A Definitions and auxiliary statements

For a random variable $X$ and a measurable function $g : \mathbb{R} \to \mathbb{R}$, $Y = g \circ X$ is a random variable with

$$\mathbb{E}[Y] = \int_{\mathbb{R}} g(x) f_X(x) dx. \quad (A.11)$$

**Definition 10.** Considering the probability space $(S, \mathcal{F}, P)$, $L_2(S, \mathcal{F}, P)$ is defined as a collection of random variables on $(S, \mathcal{F}, P)$ such that

$$\mathbb{E}[|X|^2] < \infty.$$ 

Together with the inner product

$$\langle X, Y \rangle = \mathbb{E}[XY], \quad X, Y \in L_2(S, \mathcal{F}, P)$$

and the $L_2$-norm

$$\|X\|_2 = \sqrt{\mathbb{E}[X^2]}, \quad X \in L_2(S, \mathcal{F}, P), \quad (A.12)$$

$L_2(S, \mathcal{F}, P)$ is a Hilbert space [67, §A.3.3].

**Definition 11.** Legendre polynomial of degree $k \in \mathbb{N}_0$, denoted by $P_k$, is defined as the solution of the differential equation [102, p.302]

$$(1 - x^2) \frac{d^2 y}{dx^2} - 2x \frac{dy}{dx} + k(k + 1)y = 0.$$ 

Legendre polynomials can be computed using the following recurrence relation:

$$P_0(x) = 1, \quad P_1(x) = x,$$

$$(k + 1)P_{k+1}(x) = (2k + 1)xP_k(x) - kP_{k-1}(x), \quad k \in \mathbb{N}.$$ 

The next two are

$$P_2(x) = \frac{3x^2 - 1}{2} \quad \text{and} \quad P_3(x) = \frac{5x^3 - 3x}{2}.$$ 

They are orthogonal with respect to the inner product [67, §B.1.1]

$$\langle P_k, P_l \rangle = \frac{1}{2} \int_{-1}^{1} P_k(x) P_l(x) dx \overset{(A.11)}{=} \mathbb{E}[(P_k \circ X) \cdot (P_l \circ X)],$$

where $X \sim \mathcal{U}(-1, 1)$ [cf. Definition 8].
A.3 Sensitivity analysis using polynomial chaos expansion

Definition 12. The variance of the random variable $X$, denoted by $\text{Var}(X)$, is defined as
\[
\text{Var}(X) = \mathbb{E}[(X - \mu_X)^2],
\]
and the standard deviation, $\sigma_X$, as $\sigma_X = \sqrt{\text{Var}(X)}$. The covariance of random variables $X$ and $Y$ [cf. Definitions 7, 9] is denoted by $\text{cov}(X, Y)$ and defined as
\[
\text{cov}(X, Y) = \mathbb{E}[(X - \mu_X)(Y - \mu_Y)],
\]
and their correlation, $\rho_{XY}$, as
\[
\rho_{XY} = \frac{\text{cov}(X, Y)}{\sigma_X \sigma_Y}.
\]
List of abbreviations

BC boundary conditions
BCSP boundary conditions on the symmetry plane
CMOOP constrained multi-objective optimization problem
DoF degree of freedom
EA evolutionary algorithm
FCC Future Circular Collider
FCC-ee lepton collider at FCC
FCC-ee-Z Z-pole operating mode of FCC-ee
FEM finite element method
FM fundamental mode
GEVP generalized eigenvalue problem
HOM higher order mode
JDSYM symmetric Jacobi–Davidson
MOOP multi-objective optimization problem
PEC perfectly electrically conducting
PC polynomial chaos
PMC perfectly magnetically conducting
PSI Paul Scherrer Institut
QoI quantity of interest
RF radio frequency
SA sensitivity analysis
SLS Swiss Synchrotron Light Source
TE transverse electric
TM transverse magnetic
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