

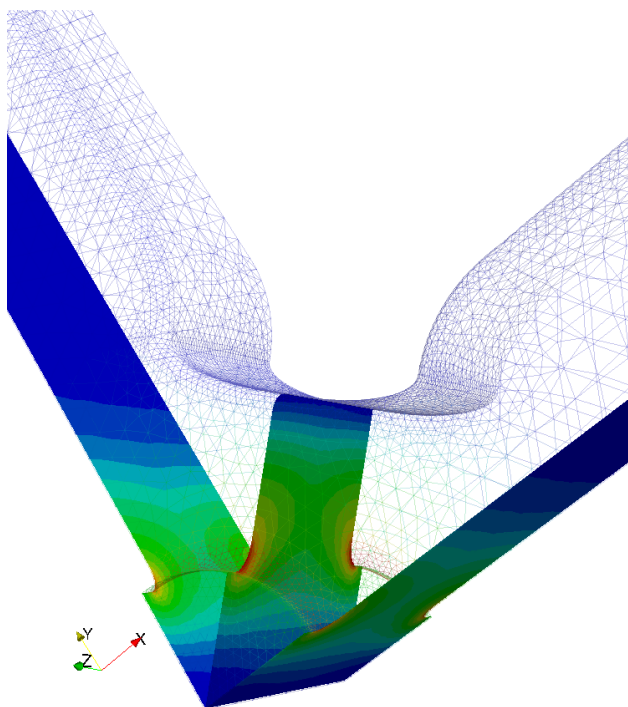
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PhD Thesis

**Avoiding vacuum arcs in high gradient  
normal conducting RF structures**

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# Abstract

In order to build the Compact Linear Collider (CLIC), accelerating structures reaching extremely high accelerating gradients are needed. Such structures have been built and tested using normal-conducting copper, powered by X-band RF power and reaching gradients of 100 MV/m and above. One phenomenon that must be avoided in order to reliably reach such gradients, is vacuum arcs or “breakdowns”. This can be accomplished by carefully designing the structure geometry such that high surface fields and large local power flows are avoided.

The research presented in this thesis presents a method for optimizing the geometry of accelerating structures so that these breakdowns are made less likely, allowing the structure to operate reliably at high gradients. This was done primarily based on a phenomenological scaling model, which predicted the maximum gradient as a function of the break down rate, pulse length, and field distribution in the structure. The model is written in such a way that it allows direct comparison of different criteria, i.e. the peak electric field, the peak local power flow or “modified Poynting vector”  $S_c$ , and the global power flow per iris circumference. Using this method, a set of highly optimized accelerating cells were created, as was a C++ library capable of estimating the performance of an RF structure based on these accelerating cells. This library was used in the rebaselining of the CLIC machine.

In addition to this, the thesis also presents a particle in cell simulation of the initial stages of a vacuum arc. This model follows the development of the arc from a small field emitter into a multi-ampere discharge, tracking the evolution of the plasma and the circuit, as well as the interaction between the plasma and the surface. From this model, our understanding of the importance of the ion bombardment under the plasma sheath was improved, especially the ion energy distribution and its effect on sputtering vs. the effective sputtering yields required for the arc to sustain itself and grow.





# Acknowledgments

In the work leading up to this thesis I've had the good fortune of being a part of both the CERN CLIC RF group and the Oslo experimental particle physics group. This environment has enabled me to learn a lot about accelerator physics, vacuum arcs, RF optimization, electromagnetics, high-performance computing and programming, how to present my results, and many other things.

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# 1. Introduction

The goal of particle physics is to understand how nature works at its presumably most fundamental level. One of the most important experimental techniques used to achieve this goal is to collide beams of particles, such as electrons or protons, at high energies. We can use such collisions to study the possible interactions between particles, and as each colliding pair can carry a lot of energy, it is even possible to produce short-lived types of particles not normally found in nature. Observing how often and under what conditions each type of interaction happens and how they unfold, it is possible to understand more about how the fundamental components of nature relate to each other. From this knowledge, we can create accurate models predicting how particles – and thus radiation – interacts with materials they are passing through. These models can be used for design of devices operating in radiation-heavy environments such as in space or near nuclear reactors, and also makes it possible to invent and improve technology such as X-rays machines for medicine and industry, positron emission tomography (PET) scanners and radiation treatment machines for medicine. But finally, and maybe most important, is that the knowledge about how particles interact allows us to propose and test hypotheses in order to explain puzzles about the world around us, increasing our understanding of it at its most fundamental level.

Historically, as shown in Figure 1.1, particle collisions have been done at ever increasing energies, which has made it possible to discover new and increasingly heavy particles. These discoveries have in turn driven the development of theories describing the behavior of the newly discovered particles, and sometimes also predicting the existence of particles and interactions which were later found when accelerators reaching even higher energies became available. One prominent example of this was the discovery of the weak neutral current and later the force-carrying Z and W bosons, as predicted by the theory of electroweak interactions [1]. Another example is the bottom and top quark, which were postulated by Kobayashi and Maskawa in 1974 [2, 3]. The bottom quark was discovered in 1977 [4], and the much heavier top was discovered in 1995 [5, 6]. The most recent example is the prediction of the Higgs boson, postulated in 1964 as part of an explanation for why the Z and W bosons have mass [7, 8], and later discovered in 2012 [9, 10, 11].

After the discovery of the Higgs boson, all of the particles predicted by the Standard Model of particle physics have been confirmed. However, there are still multiple physical phenomena which cannot be explained within the framework of the Standard Model, such as dark matter, dark energy, neutrino masses, gravity and matter-antimatter symmetry. One candidate theory – or really a family of multiple theories – which may solve these problems are called the SUPERSymmetric theories (SUSY) [15]. These theories predicts an approximate doubling of the number of different particle types. It is expected that some of these particles have masses in the TeV range, and should thus be reachable with the Large Hadron Collider (LHC) at CERN in Geneva.

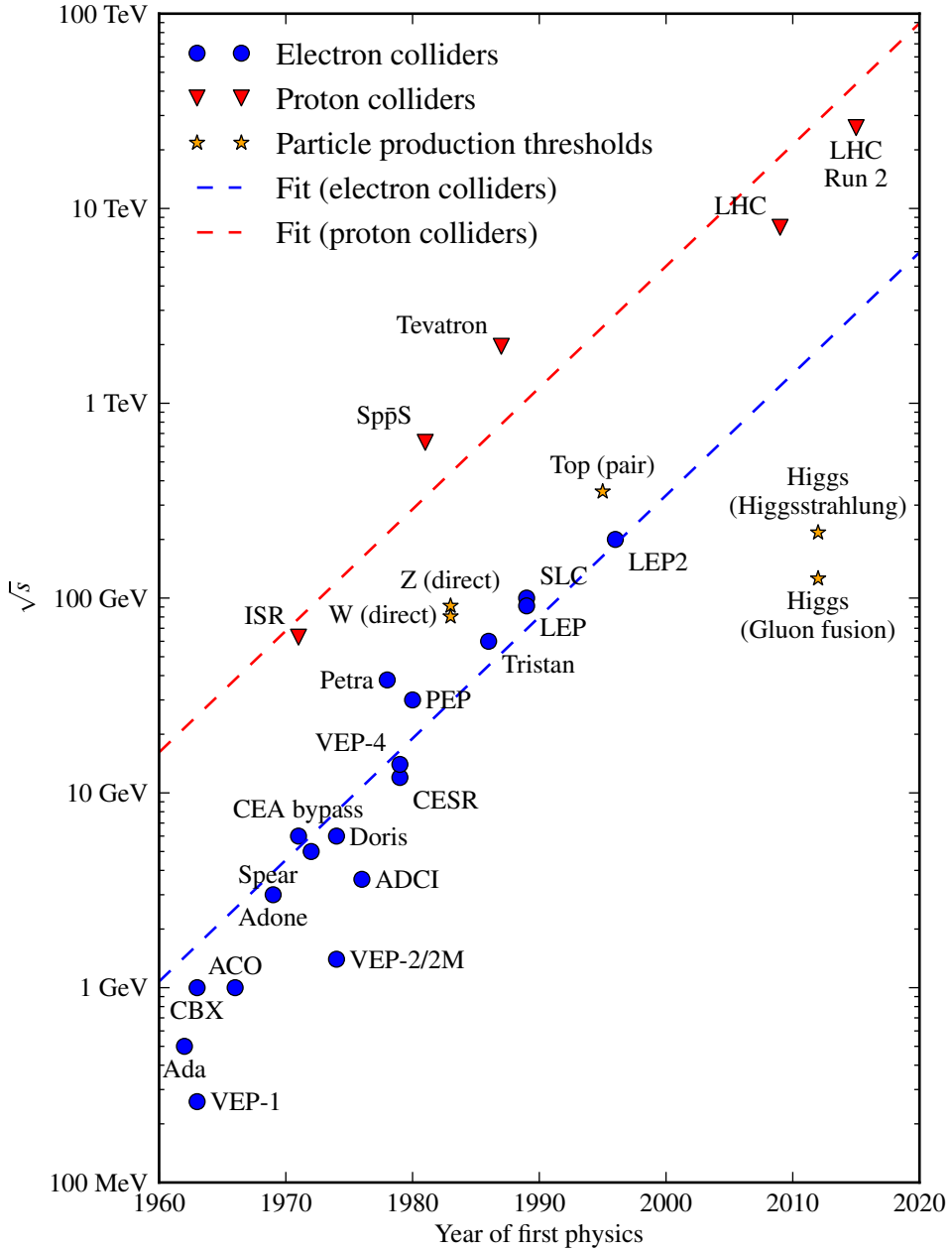


Figure 1.1.: Collision center of mass energy for a range of high-energy particle colliders as function of when they were constructed, together with production thresholds and year of discovery for important particles. Dashed parallel lines are exponential functions fitted to the record-setting machines. Particle accelerator data from [12, 13, 14].



## 1.1. Particle colliders

As the beams of the LHC are proton beams, and protons are not fundamental particles but composed of tightly bound quarks and gluons, the energy of each colliding pair is less than the full beam center of mass energy  $\sqrt{s}$ . This causes the collision energies to be distributed over a wide range, varying from collision to collision, with only the tail of the distribution reaching the full beam center of mass energy [15]. This impedes the precision of the measurements that are possible when using such a proton machine, but at the same time makes it easier to explore a larger parameter space.

Alternatively to colliding protons, it is possible to use elementary particles such as electrons and positrons. This can be used for more precise measurements. Such machines have been built before, with the highest energy per beam reached to date being 104.6 GeV at the Large Electron-Positron collider (LEP) at CERN [16]. The experiments at this machine measured the interactions of the standard model at high precision, one of the largest triumphs being the precise measurement of the width of the Z resonance. This measurement confirmed that there are only three species of light “invisible” particles coupling to the Z boson, generally assumed to be the three known neutrino flavors [17].

One important difference between electron and proton accelerators is how much synchrotron radiation is emitted. Synchrotron radiation is X-rays emitted from charged particles when they are traveling on a curved path. The amount of synchrotron radiation depends on the velocity of the accelerated particles. The emitted power per particle is given as

$$P = \frac{e^2 c}{6\pi\epsilon_0 r^2} \left( \frac{E}{m_0 c^2} \right)^4 \propto \frac{E^4}{m_0^4 r^2}, \quad (1.1)$$

where  $m_0$  is the rest mass of the particle,  $E$  is the total relativistic energy per particle,  $r$  the bending radius of the accelerator,  $e$  the particle charge,  $c$  the speed of light, and  $\epsilon_0$  the vacuum permittivity. As a proton weighs approximately 1836 times more than an electron [13], this shows that for the same energy and in the same machine, an electron would have a radiated power more than  $10^{13}$  times larger. It also shows that it is very hard to scale the machine in energy by increasing its radius, as doubling the machine energy would require quadrupling of the machine radius to keep the emitted power the same. For LEP2, the total loss from the beam was 18 MW when operating at a beam energy of 100 GeV and 6 mA beam current [12]. This means that building a circular electron/positron collider with a much higher collision energy than LEP is very demanding due to the size and power requirements.

The problem of synchrotron radiation can be avoided if the beam is traveling on a straight line. Such a machine is called a linear accelerator, and two linear accelerators pointing toward each other with the beams intersecting at an interaction point inside a detector is called a linear collider. However, in a linear accelerator the beam has to gain all its energy in one single pass, as it cannot swing around and reuse the same accelerating elements multiple times. It also means that the beam will only pass through the experiment once, making it more challenging to rapidly collect large amounts of data (achieving high luminosity).

There are currently two proposals for building a linear electron-positron collider at high energy: The Compact Linear Collider (CLIC) and the International Linear Collider (ILC). These have similar physics goals and share much of the detector technology, however the accelerator part of the projects are based on different technologies; ILC uses superconducting RF cavities, while CLIC is based around high gradient normal conducting cavities and a new method for RF pulse compression and power distribution.

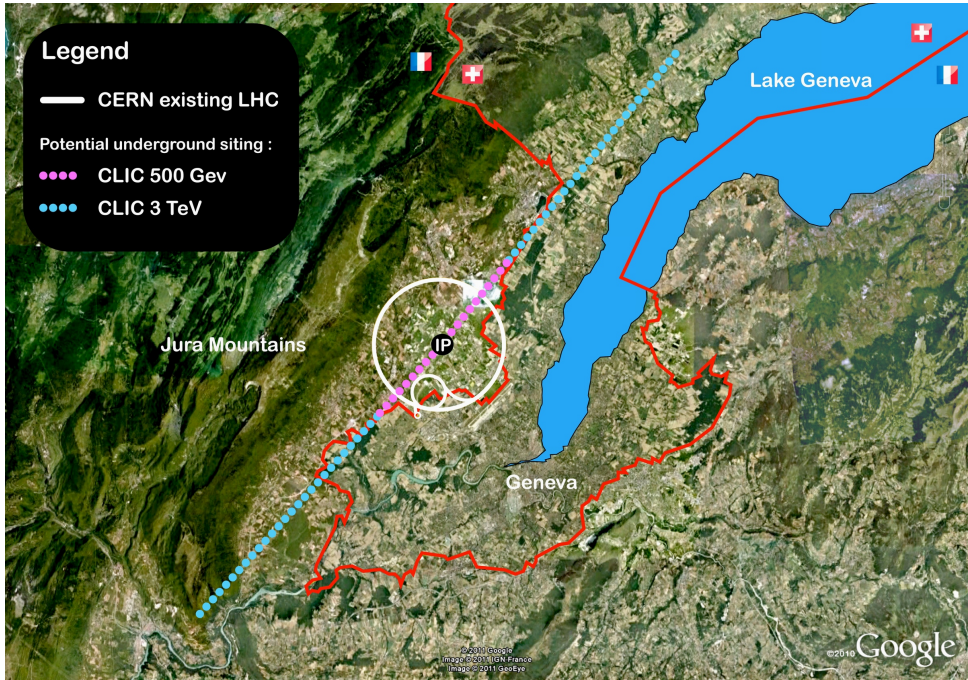
### 1.2. The Compact Llinear Collider (CLIC)

The Compact Llinear Collider (CLIC) is a project for constructing a linear electron-positron collider, as described above. It is based on high-gradient normal-conducting accelerating structures, targeting an accelerating gradient of 100 MV/m. Using such a high gradient makes it possible to reach very high energies with a reasonable machine length. The total length of the whole machine reaches 18 to 49 km, for a center of mass collision energy of 500 GeV to 3 TeV [18], as illustrated in Figure 1.2.

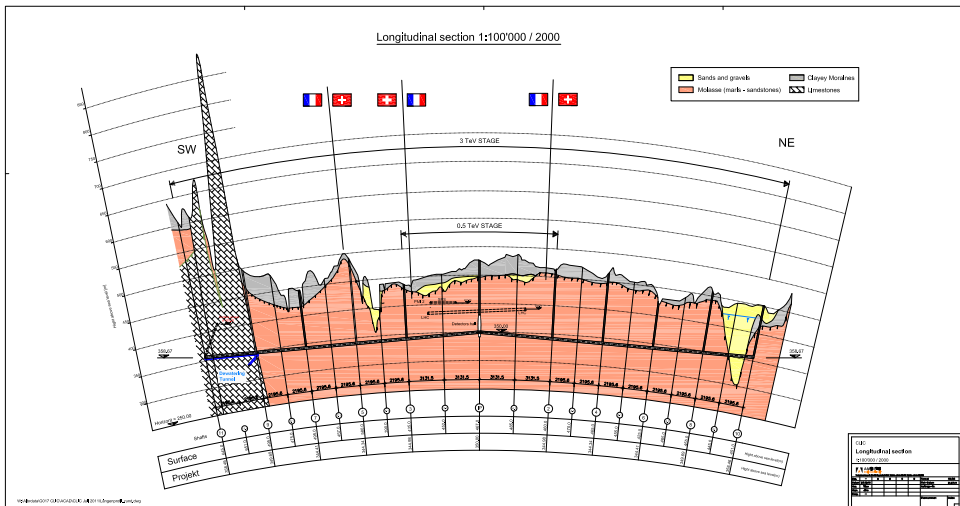
In order to reach the very high requirements for the accelerating gradient, each accelerating structure must be provided with a short (250 ns), high power (60 MW) and high-frequency (12 GHz) microwave pulse [18]. Providing this to all the structures along a 3 TeV CLIC using conventional klystron microwave amplifiers would be very challenging, requiring a large number of high-performance klystrons, RF pulse compressors, and other equipment. These klystrons would need to be placed relatively close to the accelerating structures they are powering, likely making it necessary to build a second parallel tunnel to house them and the necessary services. On top of this, klystrons have a non-negligible failure rate and a limited life-time, making a klystron-based full-energy CLIC very hard to run reliably.

A solution to this problem is the two-beam acceleration scheme, which is illustrated in Figure 1.3. In this scheme, a second beam line runs along the main beam accelerator in the same tunnel, carrying a second electron beam. This low energy but high intensity “drive beam” is generated in an efficient manner at a centralized drive beam generation complex on the surface, and is then transported to the accelerator tunnel. Here it is decelerated using Power Extraction and Transfer Structures (PETS), generating the microwaves pulse needed to power the main beam accelerating structures. This scheme reduces the amount and complexity of the equipment which needs to be located underground in the tunnel. It also makes upgrading the final energy of the main beam much easier, primarily requiring the production of more drive beam pulses to drive more decelerator sectors, in turn powering more accelerator structures. An accelerator based on CLIC technology is therefore much easier to scale to higher collision energies than a klystron-based accelerator such as the International Linear Collider (ILC). However, a low-energy version of CLIC may still be cheaper to build using klystrons, saving the expense and complexity of the drive beam system while requiring a relatively small number of klystrons and associated equipment [19, 20].

As mentioned above, in a linear collider the beams can only make a single pass through the interaction point, which makes collecting data more difficult than in a circular machine. In order to cope with this, a higher fraction of the accelerated particles must be brought to collision from each bunch, which requires much smaller beam spots at the interaction point. As a comparison, the beam spot at LEP was  $200 \times 2.5 \mu\text{m}$  [16], while CLIC is aiming at  $40 \times 1 \text{ nm}$  at 3 TeV. This is challenging, as the beams must first be generated with a very good quality, and then this quality must also be preserved through the machine. Another possible method of increasing the amount of data collected in a given time is to increase the pulse rate. However this quickly becomes unfeasible due to increased electrical power requirements, which is both a problem in itself and also requires more cooling equipment and other services.



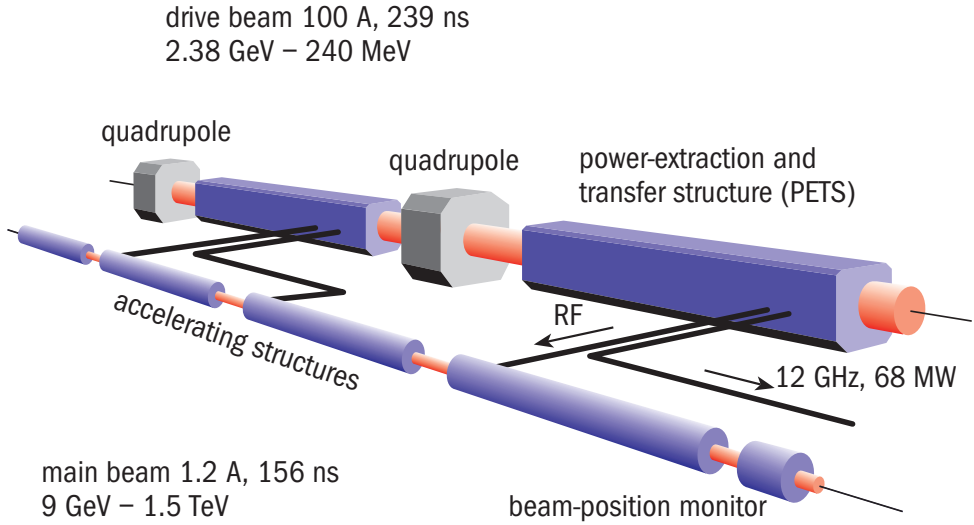
(a) Map of possible location of a CLIC accelerator complex near Geneva, Switzerland.



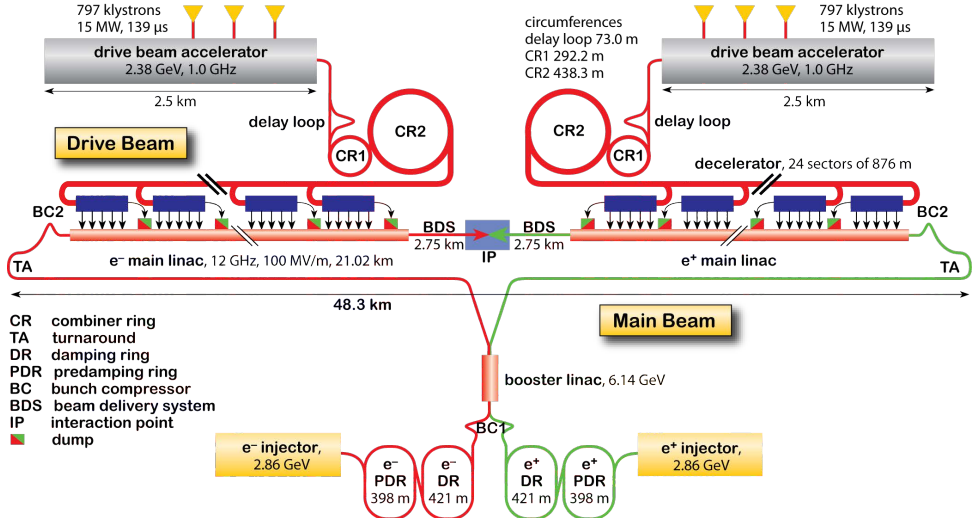
(b) Simplified geological profile, showing how the CLIC tunnels are bored “laser straight” approximately 100-150 meter below the surface, not following the curvature of the earth.

Figure 1.2.: Proposed location for the CLIC complex at CERN in Geneva, Switzerland. Also shown is the locations of the LHC and SPS tunnels. Both figures are from [18].

## 1. Introduction



(a) The CLIC two beam acceleration scheme, with the drive beam decelerator structures (PETS), microwave distribution network, and main beam accelerating structures.



(b) Layout of the CLIC accelerator complex, including the accelerator tunnel containing the main beam accelerator and drive beam decelerators (middle), the drive beam generation complex (above) and the main beam generation (below).

Figure 1.3.: The CLIC two-beam acceleration scheme. Both figures are from [18].

## 1.3. Accelerating structures

An accelerating structure is a device for accelerating charged particles using an electric field. This field is generated by a microwave source (typically a klystron or PETS), which drives an oscillating electromagnetic field inside the structure. The walls inside the structure are shaped such that when a driving wave with the correct frequency is applied, it is transmitted through the structure. Inside the structure, the field is reflected by the structure's conducting walls, focusing a strong electric field on and parallel to the structure's axis. This field can be used for acceleration of charged particles.

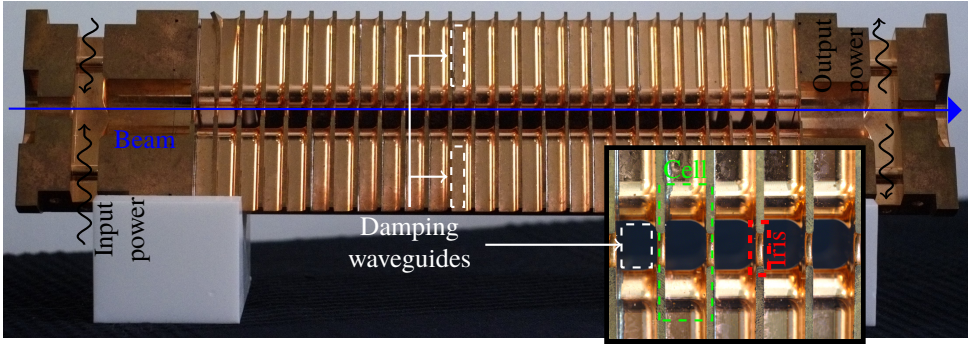


Figure 1.4.: A traveling wave accelerating structure, cut in half along the beam axis. The structure is a TD24, a tapered CLIC structure with 24 normal accelerating cells and waveguide wakefield damping. A closeup of five accelerating cells is shown in the insert. The main components are pointed out in annotations.

One example of an accelerating structure is shown in Figure 1.4. The picture shows where the beam passes through the structure. Also shown is the input coupler through which the microwave radiation powering the structure enters. This wave is then passed through a series of cells, which shapes the field of the wave such that it interacts with and accelerates the beam. At the end of the structure, the power in the wave has dropped to such a level that it is no longer usable for accelerating the beam. It is therefore here taken out of the structure through the output coupler and dumped in a load, which converts the remaining energy to heat.

Also visible in the picture are the damping waveguides. The purpose of these is to quickly drain the energy of unwanted field components out of the cells and away from the beam. These unwanted field components are created by the beam's wakefield, which is the field generated by the beam as it passes through the structure. The main unwanted field component is the geometric transverse wakefield, which can kick the beam the sideways. If this kick is too strong, it can result in parts of the beam not being able to pass through the accelerator, but instead being lost on the walls of the machine. Less dramatically, it can also lower the beam quality such that the size of the beam spot increases, reducing the rate of which collisions can be produced and data collected [18, 21].

One of the primary challenges which must be overcome for CLIC, is the design and production of accelerating structures which can reach very high accelerating gradients. This means minimizing the probability of vacuum arc “breakdowns” during the operation of the



## 1. Introduction

structures. This is important to minimize the size of the machine, and thus the construction costs.

Another important challenge is the design of energy-efficient RF structures, measured as how much of the energy in the driving microwaves is converted to kinetic energy in the beam. This is also very important, as more efficient structures means we are able to create more collisions and collect more data for a given amount of electrical power.

The design of accelerating structures that are less susceptible to vacuum arcs, are efficient, and also have adequate damping of the unwanted wake fields, is one of the main topics of this thesis. This is accomplished using computer simulation of the fields inside the structures, both the accelerating field and the beam-induced wake fields. The simulations of RF structures presented in this thesis were performed using the high-performance code ACE3P [22].

Furthermore, the designs [23] were described parametrically, making it possible to predict the maximum gradient, RF-to-beam efficiency, wakefields etc. as a function of “overall” structure parameters. These parameters are typically the structure length, aperture and iris thickness at each end of the structure, the RF phase advance per cell and the resonance frequency [24]. This was later used for re-optimizing the overall design of the CLIC machine, by scanning through different RF structure types, machine lengths, gradients and more, searching for the minimum in price which reached certain performance goals [25].

### 1.4. Vacuum arcs

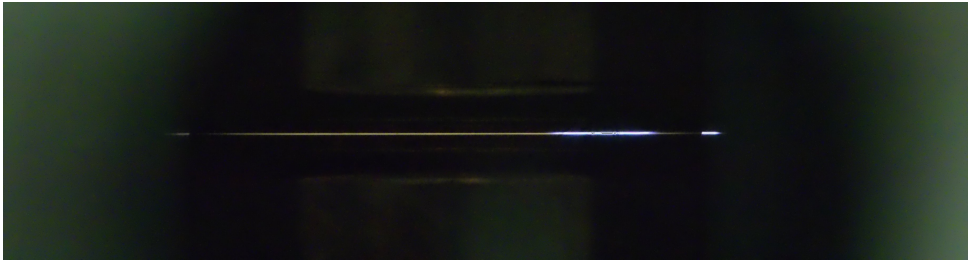


Figure 1.5.: Photograph of a vacuum arc in the DC spark fixed gap experiment.

One of the main challenges for reliably reaching the very high accelerating gradients required for CLIC is vacuum arcs. These arcs are plasmas, which sometimes spontaneously form under very high field conditions, such as inside an accelerating structure.

When these arcs appear, they reflect the wave in the accelerating structures. This causes a drop in the accelerating voltage seen by the beam, which can result in a spread in the beam energy along the bunch train. Furthermore, the arc plasma may cause the beam to be kicked transversely, which can result in the beams not colliding properly. Finally, the arcs can also damage the inside surfaces of the structures. It is therefore important to minimize the number of such breakdowns to below a maximum acceptable level.

Unfortunately, exactly how and under what conditions they arise are poorly understood, as will be discussed in Chapters 3 and 4. Therefore, in order to better understand the mechanisms of vacuum arcs, both experiments and simulations are used. The experiments directly related to the CLIC project are testing of prototype accelerating structures at klystron-

powered test stands such as XBox-1 [26] at CERN, and also experiments with high voltage pulsed DC spark gaps such as at the DC spark experiment at CERN [27]. The goal is to identify and understand the factors which increase the probability and severity of vacuum arcs in accelerating structures.

The testing of prototype structures are naturally the most direct experiments for understanding vacuum arcs in accelerating structures, but it has the downside that such testing is complicated, expensive and time-consuming. This makes it hard to obtain large amounts of data, and the need to directly test accelerating structures also makes it difficult to get time for experiments focusing on the basic physics. These experiments do however yield important data points on what are the acceptable field levels and the scaling behavior of the breakdown rate, as will be described in Section 3.3.

The DC spark experiment is based on the assumption that breakdown phenomena in DC and RF are fundamentally the same, and that what we learn by experimenting with vacuum breakdowns in the DC spark experiment can be transferred to RF. Observations of similar surface damage and breakdown rate scaling with gradient support this assumption. The benefit of doing experiments with pulsed DC voltage, such as in the DC spark experiment, is that the experiments are much simpler than the RF experiments, operating at higher repetition rates and allowing for quicker modification for testing different effects. The 2D ArcPIC simulation tool (described below) is primarily intended for simulating experimental setups similar to the DC spark experiment.

Using the information obtained through the experiments and vacuum arc theory, it is possible to set limits on acceptable surface fields in the accelerating structures. This leads to criteria which can be applied during the design of such structures, as will be discussed in Section 3.3.

## 1.5. Simulation tools

In order to increase the understanding vacuum arc initiation and designing accelerating structures capable of reaching very high accelerating fields, advanced computational techniques such as implemented in ACE3P and 2D ArcPIC are extremely useful. With these programs it is possible to quickly do large number of “experiments” on the computer, measuring properties which are very hard to access in a physical experiment. This allows for rapid testing of large numbers of structure designs, or gaining insight into the otherwise inaccessible conditions inside a vacuum arc.

### 1.5.1. ACE3P

The Advanced Computational Electromagnetics 3P (ACE3P) electromagnetics simulation suite [22] is a software package for solving the field patterns inside accelerating structures. It can work with both steady-state and transient fields, as well as calculating the motion of charged particles which are interacting with the electromagnetic fields. It is developed by the Advanced Computations Department (ACD) at SLAC, and is scaleable to a very large number of CPUs, making it possible to solve fields in very large and complicated geometries.

Comparing ACE3P to commonly used commercial tools such as Ansys HFSS, CST Microwave studio and GdFidL [28], ACE3P has the advantage of being massively parallel, and integrating all main types of RF simulations into a single framework, using the same tools for meshing, file formats etc. Further, it uses a conformal tetrahedral mesh not only for

## 1. Introduction

steady-state (frequency domain) simulations but also for time domain simulations, which means that complex geometries can be modeled to high precision while keeping the number of degrees of freedom moderate. On the other hand, it is not normally possible to run locally, but rather depending on a centrally managed cluster (making turn-around times sometimes unpredictable), and it also has a reputation for being harder to use. Still, the command line based running of the solvers and analysis tools combined with the excellent scriptability in Cubit allows rapid generation and running of large numbers of problems, quickly spanning large problem sets.

For the work presented in this thesis, the steady-state solver Omega3P in ACE3P was used for optimizing the geometry of accelerating cells. This was done by calculating the field distribution in a very large number of cell geometries, which allowed picking a good geometry for the cells. In order to help managing the very large number of computations required, the interface AcdOptiGui [29] was created. This interface allows semi-automatic running and analysis of thousands of ACE3P jobs. Once the wanted cell geometry was found, the transient solver T3P was used to calculate the long range geometric transverse wake fields in the cell.

### 1.5.2. 2D ArcPIC

The 2D ArcPIC code is used for simulating the plasma formation during the initial stages of vacuum arcs in spark gaps. This allows us to see how the arc evolves on shorter time-scales and finer length-scales than what we are able to observe in the laboratory, and to test models for how the surface and the external circuit interacts with the plasma. The code is a 2D3V electrostatic PIC-MCC code, which means that it simulates the dynamics of the plasma density in a 5-dimensional phase-space: 3 momentum directions and 2 positional degrees of freedom in a cylindrically symmetric geometry. The interactions between the charged plasma particles and the electric field are treated self-consistently, and collisions between plasma particles are also modeled. It is also capable of simulating plasma-surface interaction, i.e. injection and absorption of particles, and the effects of the external electrical circuit are also taken into account.

The code was originally written by Helga Timko at University of Helsinki and CERN [30] as an extension of a 1D code. The version used in the work presented in this thesis [31] has been extended to add a better circuit- and surface physics model, and also supports partial parallelization of some of the collisions using OpenMP [32]. Further, the code was refactored to support the improvements mentioned above. It is a straight-forward and flexible code, as the primary goal is to gain a better understanding of the mechanisms of vacuum arcs and testing of surface models.

The CERN DC spark experiment is a quite close analogue to the system we simulate. This interplay between experiment and simulation has lead to many useful discussions, furthering our understanding of the underlying physics. Further, the results from the simulations were compared to the experiment, showing close similarity.



## 1.6. Applications of high gradient acceleration outside high-energy physics

In addition to the high energy accelerators used for particle physics research, accelerators are used for many other purposes. It is estimated that there are around 26'000 accelerators in the world, and most of them are used for radiotherapy or technical applications [33]. While most of these machines are relatively simple and reaching relatively low beam energies, some applications require more powerful machines.

One example is hadron therapy [34], which exploits that hadrons (such as protons) traveling through matter deposit most of their energy in a small volume near the end of their trajectories, in the Bragg peak. This property enables precise irradiation of tumors, preserving surrounding tissues. In order to penetrate deep enough into tissues, the protons must have an energy in the order of a few hundred MeV. Furthermore, the energy must be adjustable in order to vary the penetration depth.

Most hadron therapy machines today [35] use either cyclotrons, which produce a beam of fixed energy and thus require the use of variable absorbers; or synchrotrons, which are large, complex and require relatively long time between each delivered pulse. High gradient RF acceleration technology, enables compact linear accelerators reaching the same energy, while being energy adjustable and having a high repetition rate. For this reason, the experience from design of CLIC high gradient structures has been applied to the design of RF structures for use in hadron therapy machines [36, 37], with the goal of creating relatively small, cheap, and performant hadron therapy centers [38].

Another application which are being studied for high gradient RF accelerators are X-ray free-electron-lasers (XFEL). These machines use linear accelerators to generate electron beams, which are then used to generate powerful coherent pulses of X-ray light, i.e. an X-ray laser. A few such machines are already in operation around the world [39], such as the SLAC Linac Coherent Lightsource (LCLS) [40], SACLA at Spring-8 [41], FERMI Elettra [42, 43], and FLASH at DESY [44]. Furthermore, several other machines are either in commissioning, being built, or in advanced stages of planning, such as the European XFEL at DESY [45], SwissFEL at PSI [46], PAL XFEL at PAL [47, 48], LCLS-II at SLAC [49], and SXFEL at SSRF [50]. This light can be used as a “super-microscope” in many different fields, including but not limited to studies of fundamental physics and chemistry, materials, and in the life sciences [51]. In the life sciences, reaching very good imaging resolutions for proteins that are difficult to crystallize such as membrane proteins, can unlock new understanding of how drugs interact with the human body. Also interesting is that XFELs can produce very short and intense pulses, and thus are able to image fragile structures before they are destroyed by the radiation. Another opportunity made possible by the short and intense pulses from XFELs is time-resolved imaging, which can show how the shape of a molecule such as a protein evolves as a function of time after some event such as excitation by optical laser. Using the LCLS, spatial resolutions down to 0.85 nm and time resolutions down to 30 ns has been demonstrated on membrane proteins [52]. (X)FELs may therefore also benefit from the high gradient technology originally developed for CLIC, by making it possible to build them more compact and cheaper [53, 54, 55]. Such a development would likely make the technology accessible to more users, boosting research in the mentioned fields.

While a free-electron laser produces coherent synchrotron light in the UV or X-ray spectrum by wiggling the electron beam, Compton sources can reach even higher photon energies. These machines work by inverse Compton scattering, shining a photon beam – typ-

## 1. Introduction

ically from an optical laser – on the electron beam. Some of the photons then scatter off the beam electrons, and this scattering can be viewed as Compton scattering taking place in the boosted reference frame of the beam. When observed in the lab frame, the result is a narrow beam of high-energy photons. Compton sources can be separate machine, or be an addition to synchrotron light source [56]. They are typically used for imaging in a similar way as X-rays, or to study nuclear structure, sometimes doing both at the same time. The resulting photon beam has a narrow energy spectrum determined by the initial beam energies and the crossing angle, meaning that the resulting photon energy can be tuned. It is therefore possible to make a photon beam that penetrates some materials while being absorbed by others [57]. This can be used to for example find pieces of nuclear materials mixed into shipments of other materials, which is useful for stopping smuggling of such materials. Since the energy levels of nuclei are isotope-specific, Compton sources can also be used to study the isotopic composition of e.g. nuclear waste or fuel in a clean and non-destructive manner. High-gradient X-band technology is currently being studied for use in Compton sources such as VELOCIRAPTOR [58], and high-gradient C-band in ELI-NP [59], due to the potential for producing very bright beams and smaller machines.

Another potential application of X-band technology is for use in industrial applications, such as non-radioactive sources for industrial radiography and non-destructive inspection food sterilization [60], cargo inspection systems etc. Here, high-gradient X-band technology may offer benefits in weight and size compared to lower frequencies [61].

### 1.7. Looking ahead

As discussed above, particle accelerators are important tools for both research and industry. The performance of these machines has been steadily increasing over time, reaching higher energies and enabling many discoveries. The LHC, which is now running, has already confirmed the existence of the Higgs boson, and might find other, undiscovered physics processes. It is planned to upgrade the LHC in order to reach higher luminosities [62], which will extend the its reach in the search for rare processes. As the LHC is a proton collider, it is well suited to explore new territory, however there are limitations to the precision of the results. The logical next step is therefore a collider using elementary particles. As the stable elementary particles that can be accelerated with electromagnetic devices (i.e. electrons and positrons) are much lighter than protons, they create synchrotron radiation if accelerated in a circular particle accelerator. This means that it would be very difficult to reach energies much higher than what was achieved in LEP (1989–2001) with a circular electron-positron collider.

One way to get around this limitation is to build a linear electron-positron collider. There are currently two projects aiming to construct such a machine, CLIC and ILC, which uses different technology (room temperature vs. superconducting RF and different energy distribution schemes) to achieve similar goals. This fundamental difference in technology results in different maximal performance, with the ILC maximal energy being lower than for CLIC. Which machine to build is therefore dependent of the physics results that are expected to come from the LHC; if the results show that very high energies are required to study a new set of particles, a CLIC-type design with compact, high gradient RF and a scaleable drive beam system would likely be required. However, if no such new physics is discovered, the next stepping stone for particle colliders would likely be a very detailed study of the Higgs

boson and the top quark, which could be accomplished using a ILC-type machine.

The technology needed for the ILC is relatively mature, having benefited from a long history of development and testing of superconducting accelerating cavities, initially for its predecessor project TESLA. Furthermore, the FLASH and European XFEL project at DESY is based on this type of cavities and cryomodules, which will give significant experience with production and initialization of these devices. For CLIC, the basic technology of high-gradient normal-conducting X-band accelerating structures is of a newer date, as is the commercial availability of high-power RF sources in this frequency range. However, the technology is maturing rapidly, and is starting to be picked up for many applications [63] such as the traveling wave accelerating structure with integrated alignment monitors that is being designed, built and tested at PSI in collaboration with CERN and Elettra [64]. Furthermore, high-gradient acceleration is also being tested for use in hadron therapy machines, as discussed in the section above.

Another possibility is the Future Circular Collider (FCC), which is a circular machine with a circumference of approximately 80–100 km [65]. This would first be an electron-positron collider at a energy slightly above that of LEP, and the tunnel then later used to house a proton collider at an energy of  $\approx 100$  TeV, in the same way as for LEP and LHC. Such machines would primarily be based on experience from the LHC and LEP. For the electron option, the primary technical challenge is to handle the very powerful and high-energy synchrotron radiation, which requires large ammounts of RF power for maintaining the beam energy, causes the beam energy to drop rapidly when not accelerated, and may create background problems in the experiments [66, 67]. Another challenge for this machine is the beam lifetime, which may neccessitate top-up injection. For the hadron option, the development and manufacturing of very strong superconducting bending is the main challenge, followed by the handling of heating from synchrotron radiation inside the bore of the superconducting magnets.

Looking even further into the future, plasma acceleration technology is expected to provide extreme accelerating gradients. This could be used as an “afterburner” stage for a linear accelerator like CLIC or ILC [68], significantly increasing the collision energies using relatively small devices placed between the end of the conventional RF acceleration section and the interaction point, although at the cost of some luminosity. However, while very interesting, this technology is still in the relatively early stages of development.

But whatever machine will be built as the successor to the LHC, which is expected to run at least until 2035, the research into the basic physics and technology necessary to build these machines is both enabling progress in particle accelerators for fundamental physics, and also opening new possibilities for other scientific disciplines such as material physics and biochemistry, and is paving the road for medical applications such as more precise radiotherapy for cancer.



## 2. RF structures for particle acceleration

As mentioned in Section 1.3, an accelerating structure is a device which accelerates electrically charged particles using a oscillating electric field created by microwaves (RF). Accelerating structures like the one shown in Figure 1.4 are the main component in a linear particle accelerator such as CLIC.

This chapter introduces basic definitions related to these devices, which are needed when discussing their design and optimization in the later chapters.

### 2.1. RF acceleration

The force used for accelerating electrically charged particles is the electric field. In machines reaching higher particle energies than a few tens of MeV [69], the electric field is varying with time and synchronized to the particle motion, using the principle of resonance or RF acceleration proposed by Ising [70] and first implemented by Widerøe [71].

Assuming that the particles are traveling in a straight line along the  $z$ -axis in the positive direction, the relevant field for acceleration is the  $z$ -component of the electric field  $E_z = \vec{E} \cdot \hat{z}$ . Further assuming the presence of a steady state field pattern, this field at position  $z$  and time  $t$  can in general be written as

$$E_z(z, t) = A(z) \cos(\omega t + \phi(z) + \theta_0) , \quad (2.1)$$

where  $A(z)$  is the local amplitude,  $\phi(z)$  is the local phase-offset,  $\theta_0$  is the global phase, and  $\omega$  the angular frequency of the oscillation.

For highly relativistic particles, such as the electrons in the CLIC main linac, it can be assumed that their velocity  $v$  is constant and equal the speed of light. This means that their position as a function of time may be written as

$$z(t) = v \cdot (t - t_0) , \quad (2.2)$$

when  $z(t_0) = 0$ . From this, the accelerating voltage seen by the particle is

$$V = \int_0^L E_z(z(t)) \, dz = \int_0^L A(z) \cos\left(\omega \frac{z}{v} + \phi(z) + \theta_0 + \omega t_0\right) \, dz , \quad (2.3)$$

and the average gradient in the structure is

$$G \equiv \langle E_z \rangle = \frac{V}{L} , \quad (2.4)$$

where  $L$  is the length of the structure.

## 2.2. Eigenmodes

Different cavity geometries implies different field patterns, which determines  $A(z)$  and  $\phi(z)$ . In a closed cavity, the field patterns are typically described as *eigenmodes*, which are solutions to Maxwell's equations obtained by factorizing out the time dependency, as will be discussed in Section 2.4. Such eigenmodes may be real, where the phase of the fields is not dependent on the position, as is the case for *standing wave* structures – or complex, where the fields must be described as complex vector fields, as will be discussed in Section 2.3. For a given geometry, an infinite spectrum of such eigenmodes exists, each of them having a corresponding eigenvalue. These eigenvalues represent the oscillation frequency  $\omega$  of the mode, and in the case of *degenerate modes* there may be more than one eigenmode per frequency.

While the modes are often calculated under the assumption of no energy loss, this is not exactly true for a real cavity. In actual cavities, the modes loses energy due to resistive losses from induced wall currents, radiation through openings in the cavities, and losses on RF-absorbing materials inside the cavity. This leads to a gradual damping of the amplitude and stored energy  $U$  of the mode. How quickly this damping happens is described by the Q-factor, which is defined as

$$Q = \frac{\omega U}{P}, \quad (2.5)$$

where  $P$  is the power loss from the mode.

Another important quantity is the effective shunt impedance

$$R = \frac{V^2}{P}, \quad (2.6)$$

which relates the accelerating voltage to the power loss. This is often normalized by the length of the structure as  $R' \equiv R/L$ . Another related and useful quantity is

$$R/Q = \frac{V^2/P}{\omega U/P} = \frac{V^2}{\omega U}, \quad (2.7)$$

which is independent of the power loss and thus independent of the cavity's material, determined only by the field pattern which is determined by the geometry.

### 2.2.1. The eigenmodes of pillbox cavities

One geometry commonly used when discussing accelerating cavities are cylindrical cavities, which are also often called *pillbox cavities*. The reason these are useful is that their geometry and field patterns closely resemble those found in most accelerating cavities of similar geometries, while the field pattern and frequencies are possible to find analytically [72, 73]. The modes in pillbox cavities thus provides a standard vocabulary for discussing the modes in other cavities.

There are two types of modes in cylindrical cavities – *Transverse Magnetic* (TM) with  $B_z = 0$  and *Transverse Electric* (TE) modes with  $E_z = 0$ . As will be discussed in Section 6.5, only the TM modes are interacting with the beam. Both TM- and TE-modes are typically named like  $TX_{m,n,p}$ . For a cavity with radius  $R$  in the  $r$ -direction and length  $L$  in the  $z$ -direction, the indices have the following meaning:

- 1<sup>st</sup> index  $m$ : Counts the number of full period oscillations in any field component (radial/azimuthal/longitudinal) when going once around in the azimuthal direction.
- 2<sup>nd</sup> index  $n$ : Counts the number of zeroes in the field's  $z$  component in the interval  $0 < r \leq R$ .
- 3<sup>rd</sup> index  $p$ : Counts the number of half-period oscillations in any field component between  $z = 0$  and  $z = L$ . This index is dropped when describing modes consisting of a mixture of multiple space harmonics, as in the case for cells for traveling wave structures (Section 2.3).

Examples of TE- and TM-modes in a pillbox cavity are shown in Figures 2.1, 2.2 and 2.6.

For particle acceleration, the most commonly used mode is  $\text{TM}_{0,1}$ , shown in Figure 2.1 for  $p = 0$ . In pillbox cavities, this is the mode with the slowest oscillation frequency. It also has the property of concentrating most of the electric field, which is parallel to  $\hat{z}$ , near  $r = 0$  where it can be used for accelerating the beam.

## 2.3. Traveling wave structures

The accelerating structures used for CLIC are *traveling wave* structures. These consist of several *accelerating cells*, which are coupled such that an oscillating field in one cell will drive an oscillation in the next cell etc. This generates an accelerating field  $E_z(z, t)$  where the position of  $E_z$ 's peak is moving with a phase velocity  $v_p$ , that by design is synchronous to the particle velocity  $v$ , as illustrated in Figure 2.3. This type of accelerating structures has the advantage of having a high power flow along the structure, making it possible to tolerate large beam loading, and allowing longer structures and shorter filling times compared to standing-wave structures.

Traveling wave structures are typically implemented as periodic (or almost-periodic) structures, meaning that the geometry repeats itself after a period  $h$  along the axis of the structure  $z$ . For infinitely long periodic structures, the Floquet theorem predicts [72] that the complex field<sup>1</sup>  $\tilde{E}_z$  repeats itself with the same period as the structure, up to a complex constant. For a lossless structure excited in a *passband*, which is a range of frequencies where the wave passes through the structure without attenuation, this constant is  $\exp(ik_0h)$ . The the accelerating field must then obey the condition:

$$\tilde{E}_z(z + h, t) = \tilde{E}_z(z, t) \exp(\pm ik_0h) . \quad (2.8)$$

This can be ensured if  $\tilde{E}_z$  is given as

$$\tilde{E}_z(z, t) = \tilde{a}(z) \exp(i\omega t \pm ik_0z) , \quad (2.9)$$

where the  $\exp(i\omega t)$  time dependence of the field is also included. This shows that the sign in front of the wavenumber  $k_0$  determines the sign of the phase velocity. Further, the complex and periodic function  $\tilde{a}(z)$  can be expanded as a Fourier series as

$$\tilde{a}(z) = \sum_{n=-\infty}^{\infty} \tilde{a}_n \exp\left(\frac{-i2\pi n z}{h}\right) . \quad (2.10)$$

---

<sup>1</sup>Where the physical field  $E_z = \Re(\tilde{E}_z)$ .

## 2. RF structures for particle acceleration

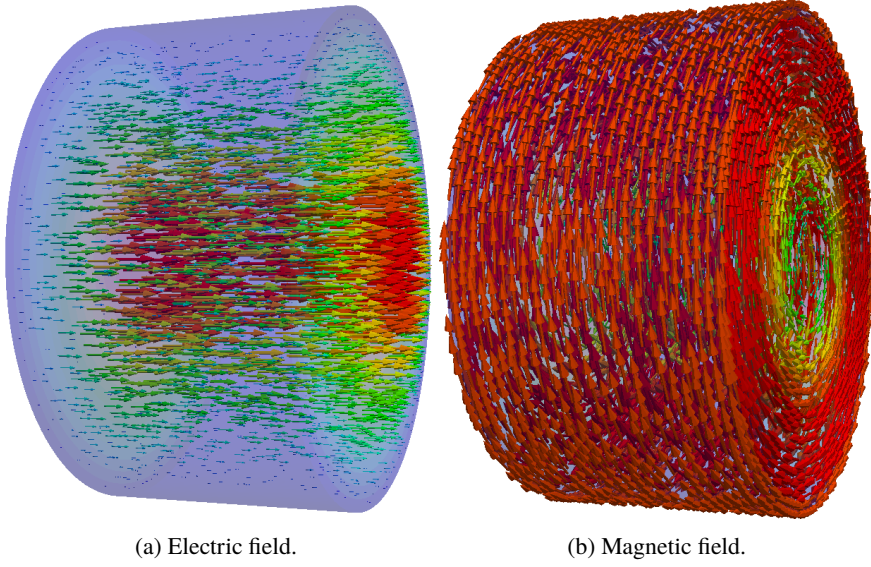


Figure 2.1.: The  $TM_{0,1,0}$  eigenmode in a pillbox cavity. This cavity has a length  $L = 10$  mm and radius  $R = 9.57$  mm, making the oscillation frequency  $f = 12$  GHz for this mode.

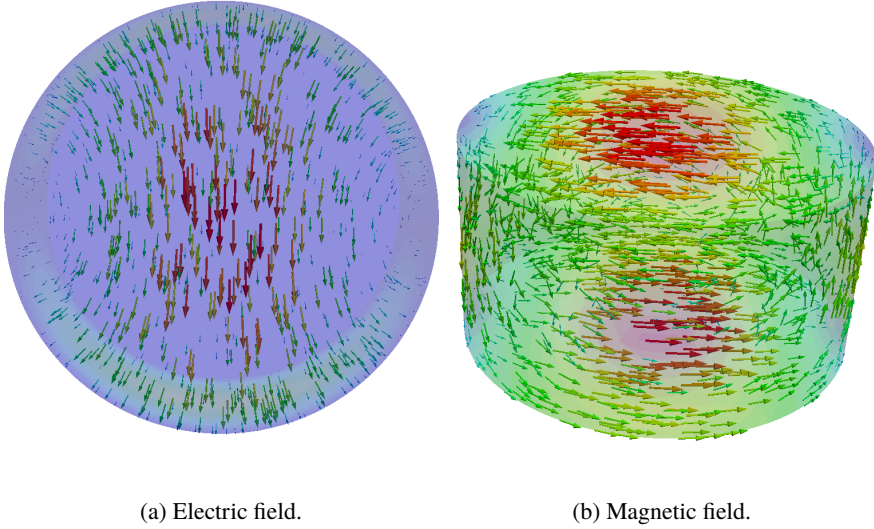


Figure 2.2.: The  $TE_{1,1,1}$  eigenmode in a pillbox cavity. This cavity has a length  $L = 10$  mm and radius  $R = 9.57$  mm, making the oscillation frequency  $f = 17.6$  GHz for this mode.



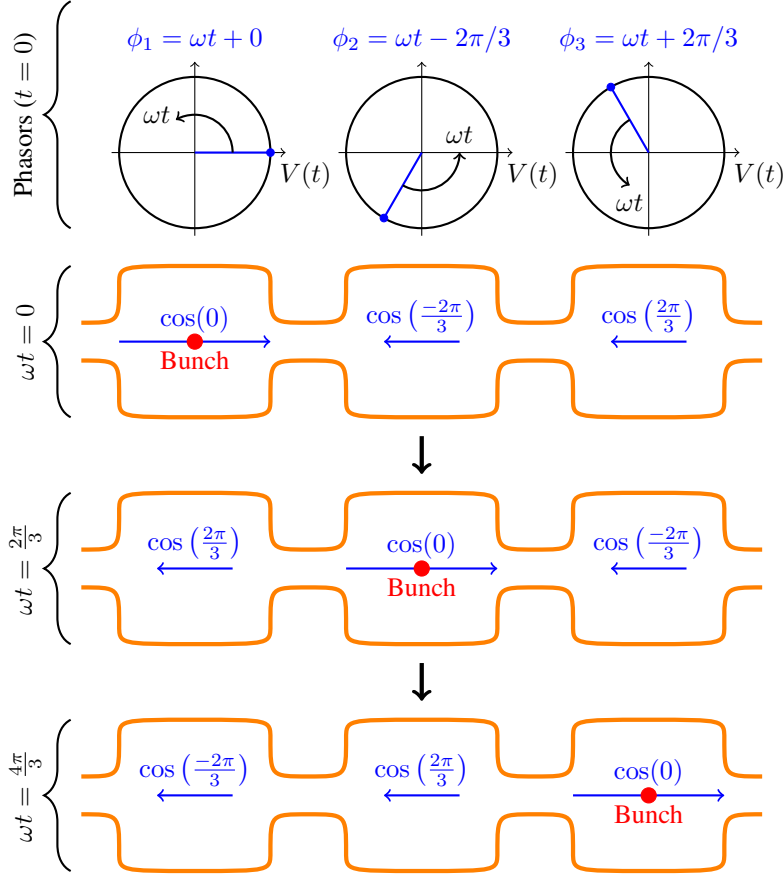


Figure 2.3.: Illustration of a 3-cell traveling wave accelerating structure with phase advance per cell  $\psi = 2\pi/3$  at three different points in time . The voltage in each cell is indicated with blue arrows, and is given as the real part of the phasors shown on the uppermost row of the figure.

Combining Equations (2.9) and (2.10), the accelerating field can be written as

$$\tilde{E}_z(z, t) = \sum_{n=-\infty}^{\infty} \tilde{a}_n \exp(i\omega t - ik_n z) , \quad (2.11)$$

where  $k_n = k_0 + 2\pi n/h$ , assuming that the negative sign in Equation (2.9) is chosen. This sum runs over multiple *space harmonics*, each of which have a phase velocity

$$v_p^{(n)} = \frac{\omega}{k_n} . \quad (2.12)$$

When designing accelerating structures, the geometry is made such that one of these waves are synchronous with the beam, usually the *principle wave*  $n = 0$ . In practice this is done by choosing the phase advance per cell  $\psi = hk_0$ , frequency  $f = \omega/2\pi$  and phase

## 2. RF structures for particle acceleration

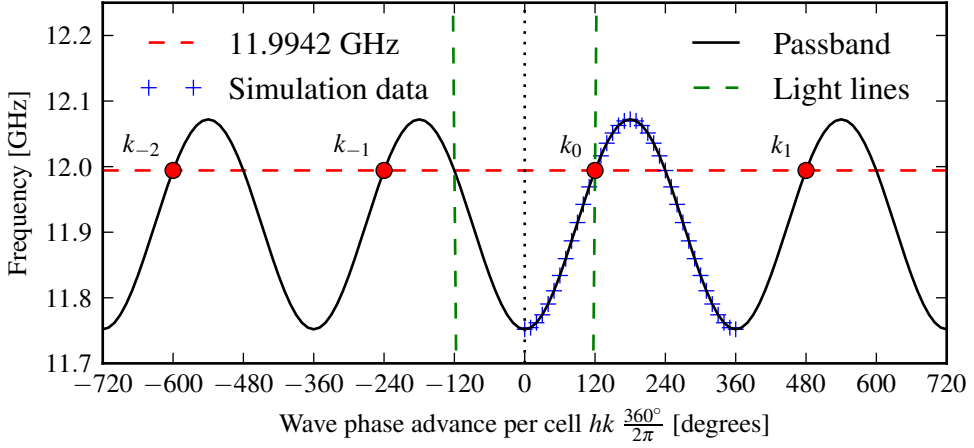


Figure 2.4.: Dispersion diagram for the  $\text{TM}_{0,1}$ -like mode of the accelerating cell described in in Section 5.6. Note that the light lines are not vertical.

velocity  $v_p$ , which determines the period  $h = \frac{v_p}{f} \cdot \frac{\psi}{2\pi}$ . The rest of the cell geometry is determined using simulations, as will be discussed in Chapter 5. This results in a mode where multiple space harmonics are usually present, but only one is actually interacting with the beam<sup>2</sup>. The general expression for the time harmonic field from Equation (2.1) may thus be taken as the real part of the complex accelerating field

$$\tilde{E}_z = A(z) \exp(i\omega t + i\phi(z) + i\theta_0) , \quad (2.13)$$

where the complex expression may then be written as a sum over the space harmonics as in Equation (2.11).

Traveling wave accelerating structures can be analyzed using a dispersion diagram, like the one shown in Figure 2.4. These diagrams shows the oscillation frequency as a function of the wavenumber  $k$ . This clearly shows the multiple space harmonics present for the same RF frequency. The figure also indicates the *light lines*, which is the dispersion relation  $\omega = k_z c$ , resulting from  $v_p = c$  for all  $\omega$ . Knowing the mode's dispersion relation, it is also possible to find the group velocity, which describes the velocity of the envelope of a wave packet traveling through the structure. The group velocity is given as

$$v_g = \frac{d\omega}{dk} , \quad (2.14)$$

and one should note that the group velocity  $v_g$  is in general different from the phase velocity  $v_p^{(n)}$ .

In practice, the group velocity is usually assumed to be equal<sup>3</sup> to the *energy velocity*  $v_E$ ,

<sup>2</sup>When integrating over a large number of accelerating cells, the energy gain and loss from a non-synchronous space harmonic sums up to zero.

<sup>3</sup>There exists a few systems where the group velocity is not equal to the energy velocity or signal velocity [74]. However, accelerating structures are normally not one of these cases. Finally, for the considerations in Chapter 7, the group velocity is anyway treated as the velocity of energy propagation through the structure.

which is easily calculated from the field pattern as

$$v_E = \frac{P_+}{U/h} . \quad (2.15)$$

Here  $P_+$  is the time-averaged electromagnetic energy passing through some plane that is perpendicular to the  $z$ -axis, and  $U/h$  is the stored electromagnetic energy per unit length. A non-zero energy velocity is necessary for a traveling wave structure, which operates with a continuous power flow through the structure, as will be discussed in Chapter 7.

## 2.4. Finite element calculation of RF modes

In order to calculate the Q-factor, the shunt impedance, the group velocity, and normalized peak fields as will be discussed in Section 2.4.3 and used in Chapter 5, the field pattern and frequency of the mode is needed. This is found by numerically solving Maxwell's equations, which in matter can be written as:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (2.16)$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}_f \quad (2.17)$$

$$\nabla \cdot \vec{D} = \rho_f \quad (2.18)$$

$$\nabla \cdot \vec{B} = 0 \quad (2.19)$$

Here  $\vec{E}$  is the electric field,  $\vec{B}$  the magnetic field,  $\vec{D}$  is the displacement field, and  $\vec{H}$  the magnetizing field. For linear media, the constitutive relations are

$$\vec{D} = \epsilon \vec{E} \quad (2.20)$$

$$\vec{B} = \mu \vec{H} , \quad (2.21)$$

where  $\epsilon = \epsilon_0 \epsilon_r$  is the permittivity of the material and  $\mu = \mu_0 \mu_r$  the permeability.

In order to calculate eigenmodes, the field of interest are time-harmonic, so the following ansatz is assumed:

$$\vec{E} = \Re(\mathbf{E} \exp(i\omega t)) \quad (2.22)$$

$$\vec{H} = \Re(\mathbf{H} \exp(i\omega t)) \quad (2.23)$$

Here  $\mathbf{E}$  and  $\mathbf{H}$  are complex-valued vector fields. Using this ansatz together with the constitutive relations and assuming  $J_f = 0$ , the Equations (2.16) and (2.17) can be written as

$$\nabla \times \mathbf{E} = -\mu i\omega \mathbf{H} \quad (2.24)$$

$$\nabla \times \mathbf{H} = +\epsilon i\omega \mathbf{E} , \quad (2.25)$$

which leads to two equivalent equations for the field:

$$\nabla \times (\epsilon_r^{-1} \nabla \times \mathbf{H}) = \mu_r k^2 \mathbf{H} \quad (2.26)$$

$$\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) = \epsilon_r k^2 \mathbf{E} \quad (2.27)$$

## 2. RF structures for particle acceleration

Here  $k = \omega/c$  is the free-space angular wavenumber, and  $\mu_r$  and  $\epsilon_r$  may in general be tensors. The formulation in Equation (2.27) is generally called the *E-formulation*, while the formulation in Equation (2.26) is called the *H-formulation*. A more detailed description of the use of the finite element method for solving Equation (2.27) is given in Appendix A.

### 2.4.1. Phase difference between $\vec{E}$ and $\vec{B}$

One useful relation between the electric- and magnetic fields is their phase difference in time. To find this, equation (2.24) can be rewritten as

$$\mathbf{E}_\nabla \equiv \frac{\nabla \times \mathbf{E}}{\mu\omega} = -i\mathbf{H}, \quad (2.28)$$

and assuming that  $\nabla \times \mathbf{E}$ ,  $\mu$  and  $\omega$  are real,  $\mathbf{E}_\nabla$  is everywhere in phase with  $\mathbf{E}$ . This is true for standing waves, but for traveling waves  $\Im(\nabla \times \mathbf{E}) \neq 0$  for all global phases, as seen from the discussion below. For standing waves, the harmonic ansatz of Equation (2.22) and (2.23) can then be written as

$$\vec{E} = \Re(\mathbf{E} \exp(i\omega t)) = \Re(\mathbf{E}) \cos(\omega t) \quad (2.29)$$

$$\vec{H} = \Re(\mathbf{H} \exp(i\omega t)) = \Re(\mathbf{E}_\nabla) \cos(\omega t + \pi/2) = \Im(\mathbf{H}) \cos(\omega t + \pi/2), \quad (2.30)$$

or after introducing a global phase shift  $\omega t \rightarrow \omega t - \pi/2$ , as

$$\vec{E} = \Re(\mathbf{E}) \sin(\omega t) \quad (2.31)$$

$$\vec{H} = \Im(\mathbf{H}) \cos(\omega t). \quad (2.32)$$

The electric- and magnetic fields are thus oscillating  $90^\circ$  out of phase at all points in  $\Omega$ .

For traveling waves, discussed in Section 2.3, some fraction of the electric- and magnetic field must be in phase with each other if a net flow of energy is present. As an example, if the field contains only the first space harmonic such that  $\mathbf{E} = \vec{a}_0 \exp(i\omega t - ik_0 z)$  where  $\vec{a}_0$  is a real vector field, dropping the time-harmonic factor  $\exp(i\omega t)$  and inserting this into Equation (2.24) yields

$$\begin{aligned} \nabla \times \mathbf{E} &= \nabla \times (\vec{a}_0 \exp(-ik_0 z)) = \exp(-ik_0 z) \nabla \times \vec{a}_0 - \vec{a}_0 \times \nabla(\exp(-ik_0 z)) \\ &= \exp(-ik_0 z) (\nabla \times \vec{a}_0 + ik_0 \vec{a}_0 \times \hat{z}) = -\mu i \omega \mathbf{H}. \end{aligned} \quad (2.33)$$

Since  $\nabla \times \vec{a}_0 \in \mathbb{R}^3$  and  $ik_0 z \nabla \times \vec{a}_0 \in \mathbb{I}^3$ , the magnetic field  $\mathbf{H}$  can be written as the sum of an in-phase component

$$\mathbf{H}_{\text{TW}} = \frac{-k_0}{\mu\omega} \exp(-ik_0 z) \vec{a}_0 \times \hat{z} \quad (2.34)$$

and a out-of-phase component

$$\mathbf{H}_{\text{SW}} = \frac{i}{\mu\omega} \exp(-ik_0 z) \nabla \times \vec{a}_0. \quad (2.35)$$

As seen from Equation (2.43) and the discussion around the group velocity, a fraction of the fields being in phase implies that there is a net flow of energy through the structure.

### 2.4.2. Calculation of field patterns using Omega3P

The method discussed above and in Appendix A is the one implemented in the ACE3P eigenmode solver Omega3P [75, 22] for simple boundary conditions, i.e. only perfect electric- and magnetic conductors, and also periodic boundary conditions (described below). In order to calculate a set of eigenmodes for some geometry using Omega3P, the first step is to make or load a 3D model of the geometry to simulate in CUBIT [76], which can then be used to generate a tetrahedral mesh. The next step is to setup the solver, i.e. specify a boundary conditions and frequency range of interest<sup>4</sup>. To run the solver, it is usually necessary to upload the files containing the mesh and solver settings to a remote high performance computing (HPC) cluster, submitting a job to the batch system there, and then retrieving the results once the calculations have finished. This can be done through a tool such as AcdOptiGUI, described in Section 5.5 and [29].

When designing accelerating cells for traveling wave structures, as will be described in Chapter 5, a third form of boundary condition known as a *periodic boundary condition* is needed. This means that two surfaces are considered to be connected, and the field on these surfaces should be identical up to a complex factor  $\exp(i\psi)$ , where  $\psi$  is the phase advance per cell. These two surfaces are selected to enclose one period of the structure, so the simulation describes an infinite periodic lossless structure. Typically, the surfaces are chosen so that they are normal to the beam axis, and splits the iris that separates two cells of the infinite periodic structure in half, as is shown in Figure 2.5. Each calculated mode then includes multiple space harmonics, and the field patterns are given as complex vector fields  $\mathbf{E}$  and  $\mathbf{H}$ , which can be interpreted through Equations (2.22) and (2.23).

When solving field patterns at high resolution, it is useful to exploit the symmetries in the geometry of the cavity and the mode of interest. This typically reduces the number of mesh cells needed to cover the simulation domain by a factor 2–8, saving significant factors of calculation time and memory by avoiding redundant degrees of freedom. These symmetries can be exploited by splitting the cavity geometry along the symmetry planes, and then assigning a magnetic- or electric wall boundary condition on the plane, depending on the symmetry of the mode of interest.

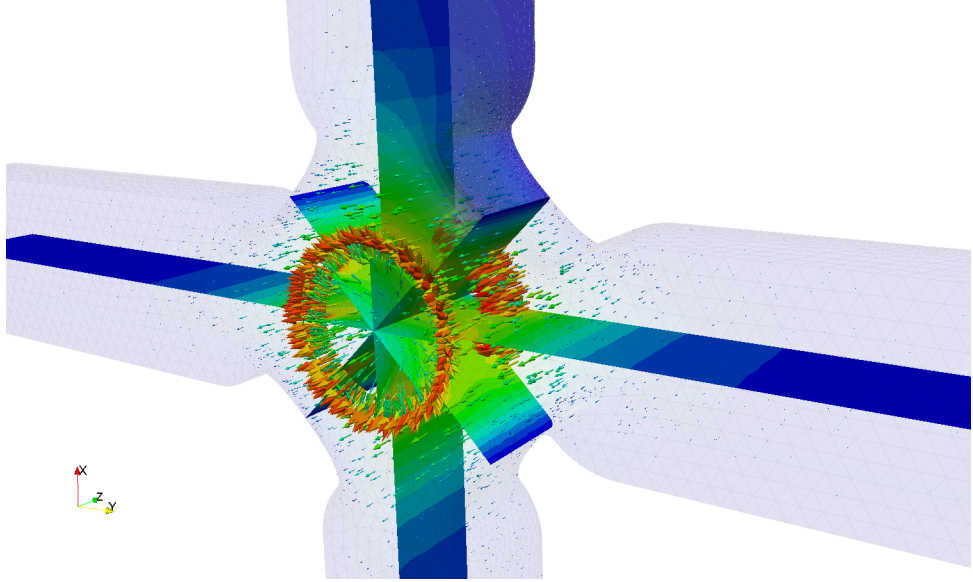
For  $\text{TM}_{0,1}$ -type modes, the magnetic field is perpendicular to the geometric mirror symmetry planes, as seen in Figure 2.5. These symmetry planes may be replaced by magnetic wall boundary conditions. A waveguide damped cell reduced to it's minimum volume is shown in Figure 2.5, using both the obvious 4-fold symmetry, and also the mirror symmetry of the remaining quarter. This reduces the volume of the calculation domain to  $1/8$  of the original. In the case of completely rotationally symmetric geometries, all planes are mirror symmetries, so a wedge of any opening angle works<sup>5</sup>.

For  $\text{TM}_{1,1}$ -type (dipole) modes such as shown in Figure 2.6, the electric field on a mirror plane is in the  $z$ -direction only, and for one of the two polarizations it is zero on the horizontal plane. For this polarization, the magnetic field on the horizontal plane is parallel to it, and normal to the vertical plane. These modes can therefore be solved using a combination of one horizontal electric wall and a vertical magnetic wall, or the opposite if the other polarization is wanted. This mode is often the dominating mode of the geometric transverse wakefield, as discussed in Chapter 6.

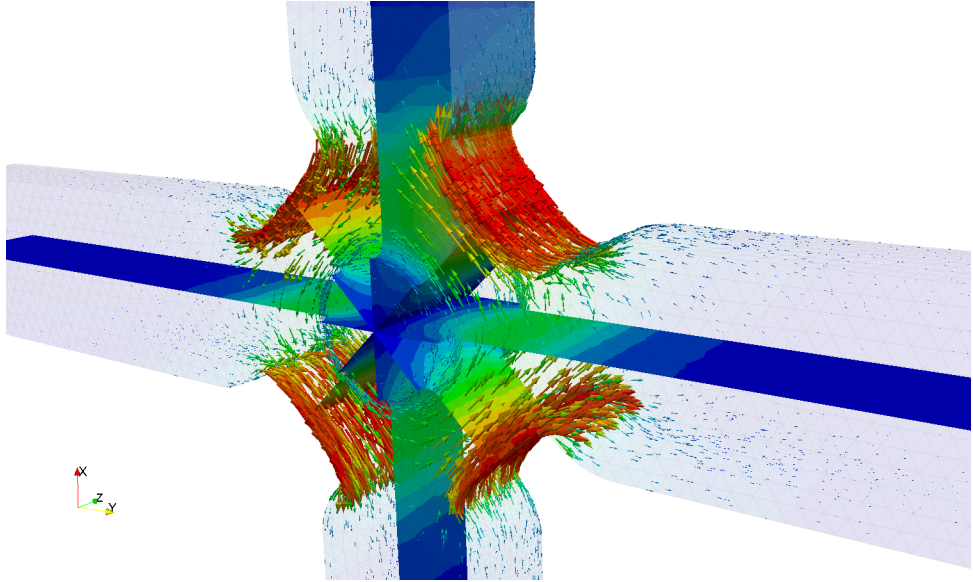
<sup>4</sup>The solver needs a “starting frequency” and the number of modes to try and locate above this frequency.

<sup>5</sup>However if the angle of the wedge is too narrow, generating a good mesh can sometimes be problematic.

## 2. RF structures for particle acceleration



(a) Electric field.



(b) Magnetic field.

Figure 2.5.: The  $TM_{1,0}$ -type eigenmode in a damped CLIC-type cell, also showing symmetry planes which can be set as magnetic walls in order to exploit the 8-fold symmetry of the cavity and field. The arrows are sampled at one given phase (same for electric and magnetic field), and the colors on the arrows and surfaces indicates the complex magnitude of the calculated fields.

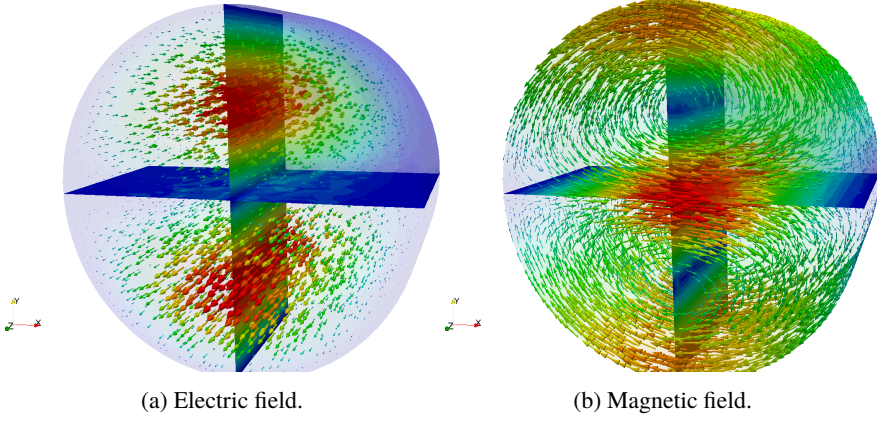


Figure 2.6.: The  $\text{TM}_{1,1,0}$  eigenmode in a pillbox cavity, with cutplanes for electric- (horizontal) and magnetic- (vertical) wall symmetry. This cavity has a length  $L = 10$  mm and radius  $R = 9.57$  mm, making the oscillation frequency  $f = 19.1$  GHz for this mode.

### 2.4.3. Extraction of RF parameters from the field pattern

Important quantities like the accelerating voltage  $V$  and average gradient  $G = V/L$ , stored energy  $U$ , power loss through surface resistance  $P$ , power flow  $P_f$  through a cell, and peak fields  $\hat{E}$ ,  $\hat{H}$  and  $\hat{S}_c$  are calculated directly from the fields. These values are then used to calculate the Q-factor, shunt impedance  $R$ , and normalized peak fields  $\bar{E}$ ,  $\bar{H}$  and  $\bar{S}_c$ , for which the global field level cancels out.

It is usually more convenient to calculate these quantities as complex numbers. As an example, while the accelerating voltage  $V$  is defined by Equation (2.3), a related complex value  $\tilde{V}$  can be defined as

$$\tilde{V} = \int_0^L \tilde{E}_z \exp\left(i\frac{\omega z}{v} + i\theta'_0\right) dz = \left(\tilde{V}_r + i\tilde{V}_i\right) \exp(i\theta'_0), \quad (2.36)$$

where  $\tilde{E}_z = \mathbf{E} \cdot \hat{z} = A(z) \exp(i\phi(z))$  is taken along the beam axis, and  $\theta'_0 = \theta_0 + \omega t_0$  an arbitrary phase offset equal to 0 in the output of the simulation. As  $V = \Re(\tilde{V})$  and  $\theta'_0$  is a free phase determined by the injection timing, it follows that the maximum possible accelerating voltage in the cavity is given as

$$V_0 = \sqrt{\tilde{V}_r^2 + \tilde{V}_i^2}. \quad (2.37)$$

The surface power dissipation  $P$  can be calculated by integrating the per-area dissipation  $\frac{dP}{dA}$  over the surface of the conductor. This is given as [72]

$$\frac{dP}{dA} = R_s H_{\parallel}^2, \quad (2.38)$$

where  $R_s = \sqrt{\mu_0 \omega / 2\sigma}$  is the RF surface resistance, and  $H_{\parallel} = \Re(\mathbf{H} \exp(i\omega t))$  is the surface magnetic field and  $\sigma$  the surface conductivity. The time-average of  $H_{\parallel}^2$  over one

## 2. RF structures for particle acceleration

oscillation period  $T$  is given as

$$\begin{aligned}
 \langle H_{\parallel}^2 \rangle &= \frac{1}{T} \int_0^T H_{\parallel}^2 dt = \frac{1}{T} \int_0^T \Re(\mathbf{H} \exp(i\omega t))^2 dt \\
 &= \frac{1}{T} \int_0^T \frac{1}{4} (\mathbf{H} \exp(i\omega t) + \mathbf{H}^* \exp(-i\omega t))^2 dt \\
 &= \frac{1}{T} \int_0^T \frac{1}{2} (\mathbf{H} \cdot \mathbf{H}^*) + \frac{1}{2} \Re(\mathbf{H}^2) \cos(2\omega t) dt = \frac{1}{2} (\mathbf{H} \cdot \mathbf{H}^*) .
 \end{aligned} \tag{2.39}$$

Thus the time-averaged power dissipation can be calculated from the complex field  $\mathbf{H}$  as

$$P = \frac{R_s}{2} \int_{\Gamma_x} (\mathbf{H} \cdot \mathbf{H}^*) d\Gamma , \tag{2.40}$$

where  $\Gamma_x$  is the part of the domain boundary declared as an *exterior* boundary in the Omega3P input file. This is for the finite element computation treated as a perfect electric conductor, and at the end of the calculation the resistive power loss  $P$  is calculated using Equation (2.40). This is then used together with  $V_0$  as defined in Equation (2.37) to calculate the effective shunt impedance using Equation (2.6).

The stored energy  $U$  is in linear media defined as

$$U = \frac{1}{2} \int_{\Omega} (\epsilon \vec{E}^2 + \mu \vec{H}^2) d\Omega . \tag{2.41}$$

For the results of Omega3P, when using the E-formulation the field is normalized such that  $U = \epsilon_0/2$ , while in the H-formulation the total stored energy is normalized as  $\mu_0/2$ .

Knowing  $U$  and  $P$  from the above discussion, as well as the angular oscillation frequency  $\omega = 2\pi f$ , the quality factor  $Q$  can easily be calculated using Equation (2.5). Similarly, knowing  $V_0$  and  $P$ , the shunt impedance  $R$  can be calculated using Equation (2.6), as can also  $R/Q$ , either directly or through Equation (2.7).

The group velocity is calculated using Equation (2.15), and for this the power flow  $P_+$  is needed. The easiest way to calculate  $P_+$  is to integrate  $\langle \vec{S} \rangle$ , the Poynting vector averaged over one oscillation period, over one of the periodic boundary surfaces  $\Gamma_p$ . Here the Poynting vector  $\vec{S}$  is given as

$$\begin{aligned}
 \vec{S} &= \vec{E} \times \vec{H} = \Re(\mathbf{E} \exp(i\omega t)) \times \Re(\mathbf{H} \exp(i\omega t)) \\
 &= \frac{1}{4} [\mathbf{E} \exp(i\omega t) + \mathbf{E}^* \exp(-i\omega t)] \times [\mathbf{H} \exp(i\omega t) + \mathbf{H}^* \exp(-i\omega t)] \\
 &= \frac{1}{2} \Re(\mathbf{E} \times \mathbf{H}^*) + \frac{1}{2} \Re(\mathbf{E} \times \mathbf{H} \exp(i2\omega t)) ,
 \end{aligned} \tag{2.42}$$

and when taking the average across one oscillation period, the 2<sup>nd</sup> term disappears. The time-averaged Poynting vector is hence given as

$$\langle \vec{S} \rangle = \frac{1}{2} \Re(\mathbf{E} \times \mathbf{H}^*) . \tag{2.43}$$

Inserting this into the integral over the periodic boundary surface  $\Gamma_p$  yields

$$P_+ = \int_{\Gamma_p} \langle \vec{S} \rangle \cdot d\vec{\Gamma} , \tag{2.44}$$



which can then be used to calculate the group velocity using Equation (2.15).

In order to estimate how high gradient can be supported by a proposed accelerator cell geometry, the normalized peak fields are used, as discussed in Chapter 3. For the electric and magnetic field, these are given as

$$\bar{E} = \frac{\hat{E}}{G} \quad \text{and} \quad \bar{H} = \frac{\hat{H}}{G}, \quad (2.45)$$

where  $\hat{E}$  is the maximum of  $\sqrt{\mathbf{E} \cdot \mathbf{E}^*}$  on the metal surface  $\Gamma_x$ , and likewise for  $\hat{H}$ . How these maxima can be located and their value estimated from the numerical results will be discussed in Section 5.4.

The modified Poynting vector [77], which is the scalar quantity that will be discussed in Section 3.2.3, is given as

$$S_c = ||\Re(\mathbf{S})|| + g_c ||\Im(\mathbf{S})||, \quad (2.46)$$

where  $\mathbf{S} = \frac{1}{2} \mathbf{E} \times \mathbf{H}^*$  is the complex Poynting vector also occurring in Equation (2.43),  $g_c$  is a weighting factor usually set to 1/6, and  $|| \cdot ||$  is the usual  $L_2$ -norm of a vector quantity. The normalized peak modified Poynting vector is given as

$$\bar{S}_c = \frac{\hat{S}_c}{G^2}, \quad (2.47)$$

where  $\hat{S}_c$  is the maximal value of  $S_c$  on the surface  $\Gamma_x$ , and is located in the same manner as for the electric field.



### 3. High gradient acceleration challenges

This chapter describes the issues which limit the gradients reachable in normal-conducting accelerating structures, such as used in CLIC. Assuming a suitable power source is available, the main limitations arise from RF breakdowns and surface fatigue from pulsed surface heating, as described below. These breakdowns are caused by high peak surface electric field and large power flows along the surface of the structure, and there are several models of the mechanisms through which these can cause breakdowns (Section 3.2). Comparing the quantities used in these models to experimental data, a set of scaling relations are found (Section 3.3), which can be used to set limits for the acceptable surface electric field and surface power flow (Section 3.3.1). Finally, the surface fatigue caused by magnetic fields is also limiting the gradient and pulse length at which a structure can be run (Section 3.4).

#### 3.1. RF breakdowns in accelerating structures

When operating an accelerating structure at very high gradients, vacuum arcs sometimes occur, forming a plasma. A vacuum arc event is often called an *RF breakdown* when it happens in an RF accelerating structure. A detailed description of these arcs is the subject of Chapter 4 and Section 1.4.

RF breakdowns are unwanted phenomena when operating an RF accelerating structure, as they can:

- Damage the surface of the structure, as seen in Figure 3.1 [78, 79, 80].
- Deflect the beam transversely by refraction at the plasma-vacuum interface [81, 82, 83] and by fields generated by the current emitted from the breakdown.
- Reflect the RF power in the structure, which results in a greatly changed field profile in the structure. This has multiple effects, including [84, 85]:
  - Increase the energy spread in the beam train, which may cause parts of it to be mismatched to the the focusing lattice after the breakdown.
  - Lack of a transverse acceleration kick which is normally present due to angular misalignment of the accelerating structures.
- May make a breakdown on subsequent pulses much more likely, making it necessary to slowly ramp up the input power [86, Sec. 4.5.5].

All of these effects are clearly negative, and must be limited to an acceptable level in order to achieve the target luminosity. For CLIC this means that the breakdown rate should be less than  $3 \cdot 10^{-7}$  events per pulse per meter [18, Sec. 2.3.2]. This limitation comes from the assumption that when there is a breakdown somewhere along the main linac, no luminosity will be produced in this pulse due to the transverse kicks mentioned above, which can result in the beams missing each other at the interaction point and not colliding. The CLIC

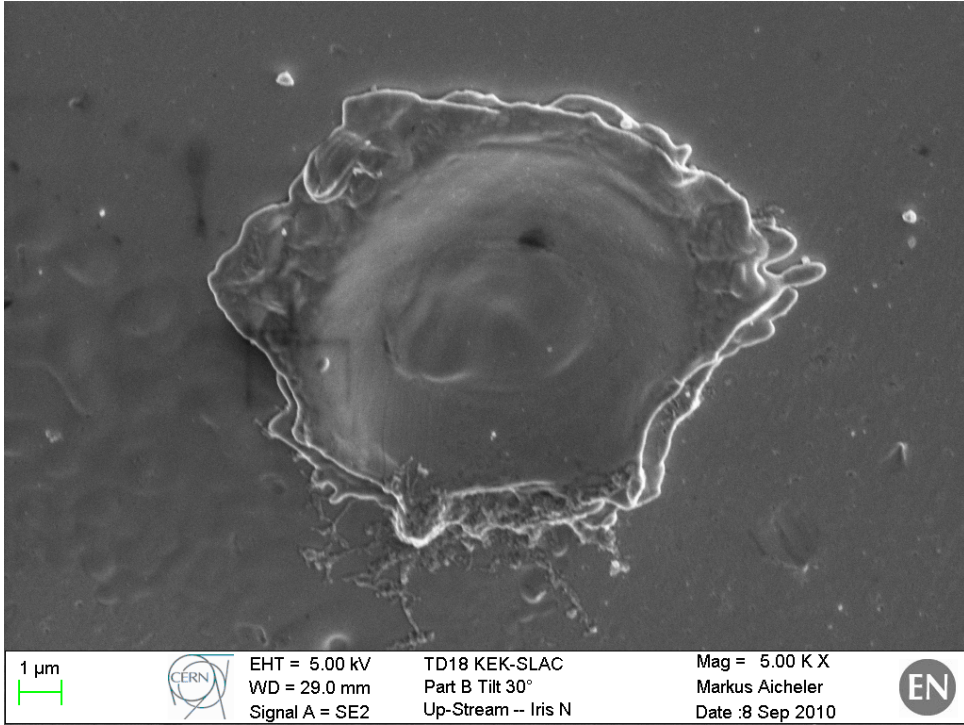


Figure 3.1.: Electron micrograph by Markus Aicheler [78] of the crater left behind from a breakdown on the iris of a TD18 accelerating structure.

parameters budget for a 1% accepted luminosity loss from this, so assuming 30 km of accelerating structures determines the maximally allowed breakdown rate through the relation  $0.01 \text{ events/pulse} = \text{BDR}_{\text{max}} \times 30 \text{ km}$ .

Achieving this low breakdown rate is done by designing and powering the structure in an optimal way, as described in Chapter 5 and 7. However, for this to be possible, models describing the breakdown probability as a function of the structure design and operating conditions are needed. This chapter describes a selection of such models.

## 3.2. Models of RF breakdowns

At the very basis of arcing in accelerator structures is the surface electric field which creates cold field emission of electrons. However, the field emission is limited by the RF power flow into the volume near the emitter or arc spot. The limits from RF breakdowns are thus related to both the peak surface electric field and the power flow.

### 3.2.1. Surface electric field and the Kilpatrick criterion

One factor which is critical for initiation of breakdowns is the surface field, as it causes cold field emission of electrons, which is an important process for vacuum arcs. Cold field

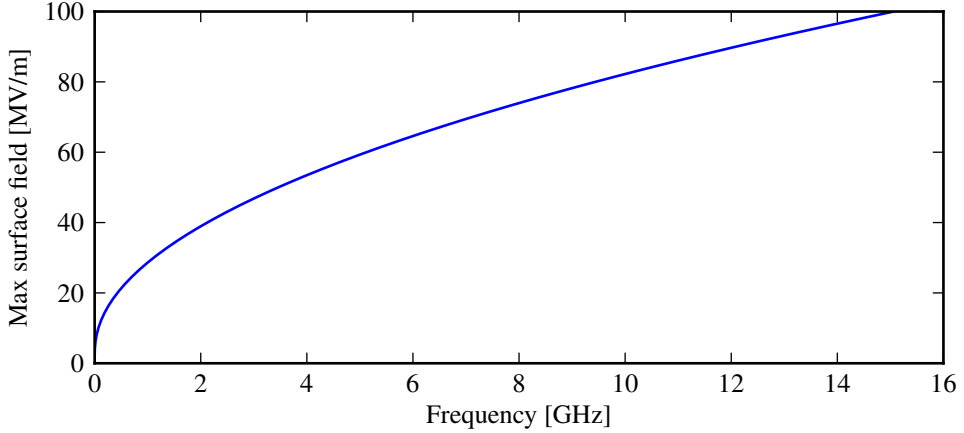


Figure 3.2.: Kilpatrick's limit on surface field as a function of frequency, as expressed in Equation (3.2).

emission of electrons is described in Section 4.1.2.

One of the earliest criteria developed for estimating the maximal gradient capability of an accelerating structure from the surface electric field is the Kilpatrick criterion [87]. This is based on the experimental observation that no arcing occurred if the maximum possible energy of ions hitting the surface  $W$  and the surface field  $E$  fulfilled the relation

$$WE^2 \exp\left(\frac{-K_1}{E}\right) \leq K_2, \quad (3.1)$$

where  $K_1 = 17 \text{ MV/m}$  and  $K_2 = 1.8 \cdot 10^{14} \text{ eV(V/cm)}^2$ . As the maximum ion energy  $W$  shrinks as the frequency increases, the maximum acceptable electric field  $E$  is greater for higher frequencies. The Kilpatrick limit was later expressed in a convenient formula [72, 88]

$$f = 1.64 \frac{\text{MHz}}{(\text{MV/m})^2} \cdot E^2 \exp\left(\frac{-8.5 \text{ MV/m}}{E}\right). \quad (3.2)$$

This expression is likely derived assuming hydrogen ions and ion energy only limited by RF frequency and not gap size, and that the field is independent of the distance from the surface. However as the original paper [88] is not available, the exact assumptions are difficult to know. The inverse of this function is plotted in Figure 3.2, showing how the maximum acceptable field increases with the frequency.

Today, the Kilpatrick criterion is viewed as unnecessary conservative, and surface field levels exceeding the maximum allowed from the Kilpatrick criterion are often seen. As an example, the CLIC accelerating cavities reach surface fields of 200–300 MV/m in short pulses (Figure 7.7). Furthermore, the Kilpatrick criterion does not include any pulse-length dependence, which we know exists as shown in Figure 3.6b. However, it is still desirable to minimize the cavities peak surface electric field.

### 3. High gradient acceleration challenges

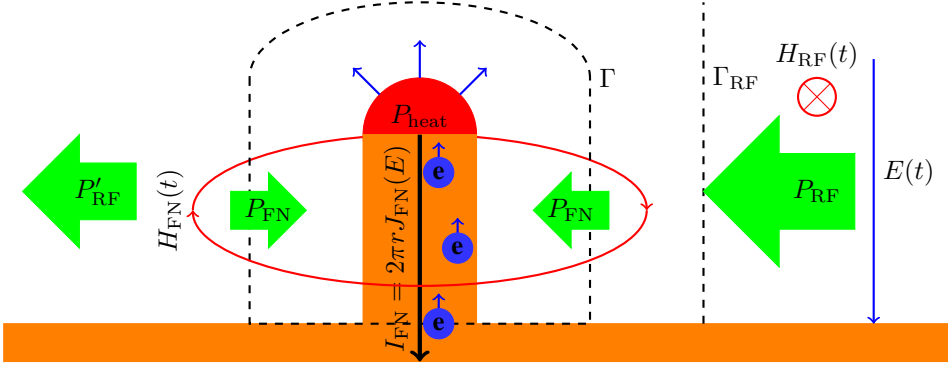


Figure 3.3.: Power flows around a field emitter tip in an RF cavity.

#### 3.2.2. Power flow through the structure and iris circumference

A newer criterion arose from the experimental observation that in traveling wave normal conducting RF structures, structures with higher power flows  $P_+$  are more prone to breakdowns. At the same time it was also observed that the structures with larger iris apertures have fewer breakdowns, even when operating at the same or higher power flows [89]. This led to the breakdown limit

$$\frac{P_+ \tau^\alpha}{C} < \mathcal{C}_{P/C} , \quad (3.3)$$

where  $\tau$  is the RF pulse length,  $C$  the iris circumference and  $\mathcal{C}_{P/C}$  a phenomenological constant. The constant  $\alpha$  describes the pulse length dependency, and is usually given as  $1/3$ .

Theoretically, this fits well with the fact that a newly formed vacuum arc needs to absorb energy, which must come from the input RF power, in order to grow. Further, in a  $TM_{01}$ -mode, much of the power in  $P_+$  is concentrated near the circumference of the iris apertures [90, Figure 2.10], which is also close to where most breakdowns occurs.

#### 3.2.3. The modified Poynting vector $S_c$

The modified Poynting vector  $S_c$  [77, 91] builds on many of the same ideas as the  $P/C$  criterion. However this is a limit on the local power flow and not  $P_+$ , which makes it applicable to standing wave structures as well as traveling wave. Further, since it is a local surface field quantity, it can be used for any geometry.

The expression for the modified Poynting vector stated in Equation (2.46) can be understood by considering the power flows around a field emitting tip, illustrated in Figure 3.3. The basic assumption is that the limiting factor is heating of the tip, which is due to the dissipated power  $P_{\text{heat}}$  caused by Ohmic heating from the current  $I_{\text{FN}}$  passing through it. This current is caused by the cold field emission of electrons from the top of the tip. The energy to heat the tip comes from the power flow  $P_{\text{FN}}$  towards the field emission current, which is mostly spent on accelerating the emitted electrons. The field emission power  $P_{\text{FN}}$  is given as

$$P_{\text{FN}} = \oint_{\Gamma} \vec{S}_{\text{FN}} \cdot d\vec{\Gamma} = \oint_{\Gamma} (\vec{E} \times \vec{H}_{\text{FN}}) \cdot d\vec{\Gamma} \propto E(t) I_{\text{FN}}(t) , \quad (3.4)$$

where  $\Gamma$  is a surface completely containing the field emitter, as shown in Figure 3.3, and  $I_{\text{FN}}$  is the current of electrons in the tip which is emitted through cold field emission, creating the magnetic field  $H_{\text{FN}}$ .

The power taken by the field emitter  $P_{\text{FN}}$  must come from the RF power  $P_{\text{RF}}$ . Assuming a time-harmonic field such as for a single eigenmode in an accelerating cavity and near a metal surface, the fields are given as

$$\vec{E}(t) = \hat{y}E_0 \sin(\omega t) \quad (3.5)$$

$$H_{\text{RF}}(t) = \Re(\mathbf{H}_{\text{RF}} \exp(i\omega t)) = \hat{x}H_{\text{SW}} \cos(\omega t) + \hat{x}H_{\text{TW}} \sin(\omega t), \quad (3.6)$$

where  $\hat{x}$  is a unit vector parallel to the metal surface, and  $\hat{y}$  is another unit vector perpendicular to the surface. In Equation (3.6), the magnetic field is split into a standing-wave component  $H_{\text{SW}} \cos(\omega t)$  which is  $90^\circ$  out of phase with the electric field, and a traveling-wave component  $H_{\text{TW}} \sin(\omega t)$  which is in phase with the electric field, as was discussed in Section 2.4.1. Using this, the flow of RF power through the surface  $\Gamma_{\text{RF}}$  towards the emitter is given as

$$\begin{aligned} P_{\text{RF}}(t) &= \int_{\Gamma_{\text{RF}}} \vec{S}_{\text{RF}} \cdot d\vec{\Gamma} = \int_{\Gamma_{\text{RF}}} (\vec{E} \times \vec{H}_{\text{RF}}) \cdot d\vec{\Gamma} \\ &\propto E_0 H_{\text{SW}} \sin(\omega t) \cos(\omega t) + E_0 H_{\text{TW}} \sin^2(\omega t). \end{aligned} \quad (3.7)$$

In the second line of this expression, the first term describes a net power flow through  $\Gamma_{\text{RF}}$  that is always positive, while the second term describes the reactive power flow which is oscillating back and forth through this surface every RF cycle. Since the field emitter couples to this power, regardless of which direction it is coming from, the power  $P_{\text{IN}}$  inbound on the emitter is proportional to

$$P_{\text{IN}}(t) \propto |E_0 H_{\text{TW}} \sin^2(\omega t)| + |E_0 H_{\text{SW}} \sin(\omega t) \cos(\omega t)| = S_{\text{TW}} + S_{\text{SW}}. \quad (3.8)$$

Here  $S_{\text{TW}}$  and  $S_{\text{SW}}$  are power flux densities corresponding to the traveling-wave and standing-wave component of  $P_{\text{IN}}$ .

Similarly, since the field emission current  $I_{\text{FN}}$  from copper is (as will be discussed in Section 4.1.2) is proportional to

$$I_{\text{FN}}(E) \propto \begin{cases} E^2 \exp\left(\frac{-62 \text{ GV/m}}{\beta E}\right) & \text{for } E \geq 0 \\ 0 & \text{for } E < 0 \end{cases}, \quad (3.9)$$

the field emission power  $P_{\text{FN}}$  (Equation (3.4)) is proportional to

$$P_{\text{FN}}(t) \propto ||\vec{S}_{\text{FN}}|| \propto \begin{cases} E_0^3 \sin^3(\omega t) \exp\left(\frac{-62 \text{ GV/m}}{\beta E_0 \sin(\omega t)}\right) & \text{for } \sin(\omega t) > 0 \\ 0 & \text{for } \sin(\omega t) \leq 0 \end{cases}. \quad (3.10)$$

As shown in Figure 3.4, the traveling wave RF power  $P_{\text{TW}}$  is in phase with the power used by the field emission, while  $P_{\text{SW}}$  is  $90^\circ$  out of phase. It is therefore expected that the traveling wave is more effective at supplying energy to the heating of the tip. This can be quantified by the “coupling integral” between  $P_{\text{FN}}$  and  $P_{\text{IN}}$ , such that the average power

### 3. High gradient acceleration challenges

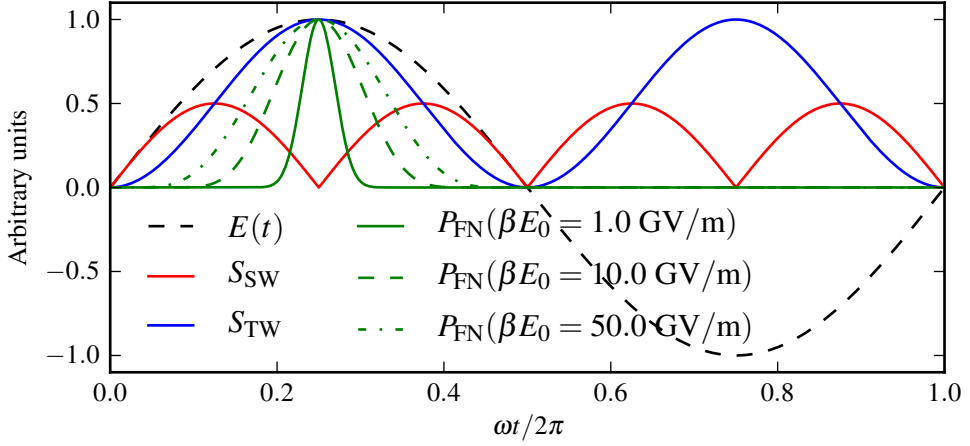


Figure 3.4.: Time-dependence of the electric field, traveling- and standing-wave RF power (all normalized such that  $E_0 = H_{SW} = H_{TW} = 1$ ) and the field emitter power for different values of  $\beta E_0$  (normalized such that the peak value equals 1).

$P_{\text{heat}}$  heating the tip is proportional to

$$\begin{aligned}
 P_{\text{heat}} &\propto \frac{\int_0^T P_{\text{IN}} P_{\text{FN}} dt}{\int_0^T P_{\text{IN}} dt \int_0^T P_{\text{FN}} dt} \propto \frac{\int_0^T \sin^2(\omega t) P_{\text{FN}} dt}{\int_0^T P_{\text{IN}} dt \int_0^T P_{\text{FN}} dt} |E_0 H_{\text{TW}}| \\
 &+ \frac{\int_0^T |\sin(\omega t) \cos(\omega t)| P_{\text{FN}} dt}{\int_0^T P_{\text{IN}} dt \int_0^T P_{\text{FN}} dt} |E_0 H_{\text{SW}}| \\
 &\equiv C_{\text{TW}} |E_0 H_{\text{TW}}| + C_{\text{SW}} |E_0 H_{\text{SW}}|,
 \end{aligned} \tag{3.11}$$

where  $T = 2\pi/\omega$  is one oscillation period. In the small volume in the immediate vicinity of an emitter, the field pattern in a RF cavity is constant and everywhere given by Equation (3.5) and (3.6). Thus  $P_{\text{heat}}$  is proportional to

$$\begin{aligned}
 P_{\text{heat}} &\propto |E_0 H_{\text{TW}}| + \frac{C_{\text{SW}}}{C_{\text{TW}}} |E_0 H_{\text{SW}}| \\
 &= |E_0 H_{\text{TW}}| \frac{2}{T} \int_0^T \sin^2(\omega t) dt \\
 &\quad + g_c(\beta E_0) |E_0 H_{\text{SW}}| \frac{\pi}{T} \int_0^T |\sin(\omega t) \cos(\omega t)| dt \\
 &= 2\langle S_{\text{TW}} \rangle + g_c \pi \langle S_{\text{SW}} \rangle,
 \end{aligned} \tag{3.12}$$

where  $\langle f(t) \rangle$  means the average of the function  $f(t)$  across one oscillation period  $t \in (0, T)$ .



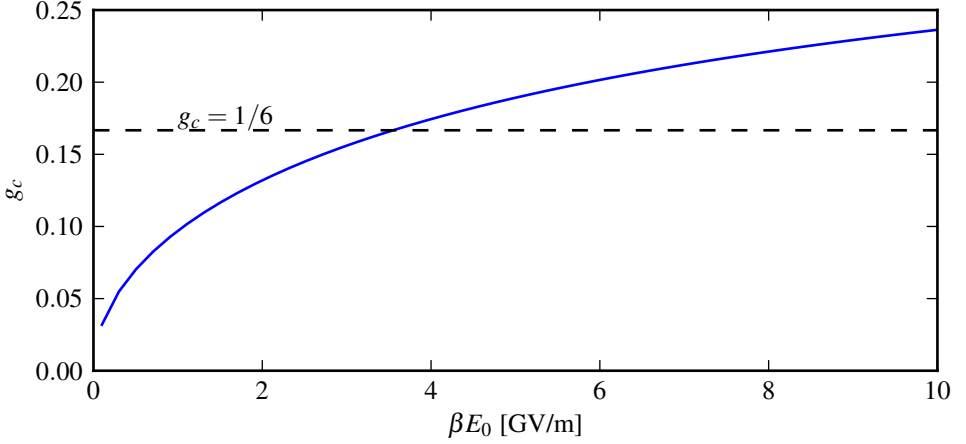


Figure 3.5.: Plot of  $g_c$  (defined in Equation (3.13)) as a function of the local field at the emitter  $\beta E_0$ , used in the modified Poynting vector  $S_c$ .

The field-dependent factor  $g_c(\beta E_0) = \frac{C_{SW}}{C_{TW}}$  is defined as

$$g_c(\beta E_0) = \frac{\int_0^T |\cos(\omega t) \sin(\omega t)| P_{FN}(\beta, E_0, t) dt}{\int_0^T \sin^2(\omega t) P_{FN}(\beta, E_0, t) dt} = \frac{\int_0^{T/2} |\cos(\omega t)| \sin^4(\omega t) \exp\left(\frac{-62 \text{ GV/m}}{\beta E_0 \sin(\omega t)}\right) dt}{\int_0^{T/2} \sin^5(\omega t) \exp\left(\frac{-62 \text{ GV/m}}{\beta E_0 \sin(\omega t)}\right) dt}. \quad (3.13)$$

This function is plotted in Figure 3.5. The dependency of  $g_c$  on  $\beta E_0$  can be understood from Figure 3.4, as a higher value means the field emitter is active for a longer part of the cycle, and thus being able to receive relatively more power from the standing wave component. A value of  $g_c = 1/6$  is generally used [77], as this results in the smallest scatter of  $S_c$  in the tested structures.

Starting from Equation (3.12), a power flux density  $S_c$  which is proportional to  $P_{IN}$  can be defined. This is normalized such that  $S_c = \langle S_{TW} \rangle$  in the case that  $g_c \langle S_{SW} \rangle = 0$ . This quantity is the modified Poynting vector, and is defined as

$$S_c = \langle S_{TW} \rangle + \frac{g_c \pi}{2} \langle S_{SW} \rangle. \quad (3.14)$$

When working with the output of a frequency domain eigensolver like Omega3P, the output is typically provided as complex vectors  $\mathbf{E}$  and  $\mathbf{H}$ . Including the global phase  $\exp(i\varphi)$ , the complex Poynting vector  $\mathbf{S} = \frac{1}{2} \mathbf{E} \times \mathbf{H}^*$  is

$$\begin{aligned} \mathbf{S} &= \frac{1}{2} \vec{E}_0 \exp(i\varphi) \times \left( \vec{H}_{TW} \exp(i\varphi) + i \vec{H}_{SW} \exp(i\varphi) \right)^* \\ &= \frac{1}{2} \vec{E}_0 \times \vec{H}_{TW} - \frac{i}{2} \vec{E}_0 \times \vec{H}_{SW}. \end{aligned} \quad (3.15)$$

In a small volume close to the surface, the electric field is always normal to the surface and the magnetic field is parallel to the surface, and given as in Equation (3.5) and (3.6). The

### 3. High gradient acceleration challenges

absolute values of the real and imaginary parts of the complex Poynting vector are thus given as

$$||\Re(\mathbf{S}_c)|| = \frac{1}{2}|E_0 H_{TW}| = \langle S_{TW} \rangle \quad (3.16)$$

$$||\Im(\mathbf{S}_c)|| = \frac{1}{2}|E_0 H_{SW}| = \frac{\pi}{2}\langle S_{SW} \rangle . \quad (3.17)$$

Inserting these into the definition of  $S_c$  given in Equation (3.14) yields

$$S_c = \langle S_{TW} \rangle + \frac{g\pi}{2}\langle S_{SW} \rangle = ||\Re(\mathbf{S}_c)|| + g_c ||\Im(\mathbf{S}_c)|| , \quad (3.18)$$

which can be used to directly calculate  $S_c$  from the output of a frequency domain eigenmode solver.

### 3.3. Scaling phenomenology for RF breakdowns

Through the course of the CLIC program and also the previous NLC/JLC program [86], a large number of different accelerating structures have been tested at high powers [92]. The different structures were ran at many different input powers and pulse lengths, achieving different gradients and break down rates. While the data has a large spread, it was noticed that the break down rate BDR is proportional to the accelerating gradient  $G$  to a high power, such that

$$\text{BDR} = k_G G^x , \quad (3.19)$$

where  $k_G$  is a scaling constant that varies between different structures, pulse lengths etc. The exponent  $x$  is typically found to be on the order of 25–30. Similar behavior is also observed at the DC spark experiment [93].

Further, it is also observed that the break down rate follows a similar dependence with the pulse length  $\tau$ . Including this in the model as

$$\text{BDR} = k G^x \tau^y , \quad (3.20)$$

also fits the data well. Such a fit is shown in Figure 3.6, where the measured break down rate of each point has been scaled to a pulse length  $\tau = 200$  ns or a gradient  $G = 100$  MV/m. The fit was done using a normal linear model in the statistical software package R [94], fitting  $\log(\text{BDR}) = \log(k) + x \log(G) + y \log(\tau)$  under the assumption that all points have a Gaussian uncertainty with the same width in  $\log(\text{BDR})$ .

While the fitted parameters  $x$  and  $y$  of Equation (3.20) varies between different data sets and structures, the values  $x = 30$  and  $y = 5$  are commonly used. It is also useful to rearrange the expression such that the scaling constant  $K$  becomes an index of performance of a certain structure under test, where a higher constant signifies a higher maximum tolerance for field and pulse length. The typical form of Equation (3.20) is thus

$$K \equiv k^{-1} = \frac{G^{30} \tau^5}{\text{BDR}} . \quad (3.21)$$

These values for the exponents are used in the rest of this thesis.

One issue with this model is that while it predicts how a structure behaves once its break down rate has been measured for one combination of gradient and pulse length, the spread

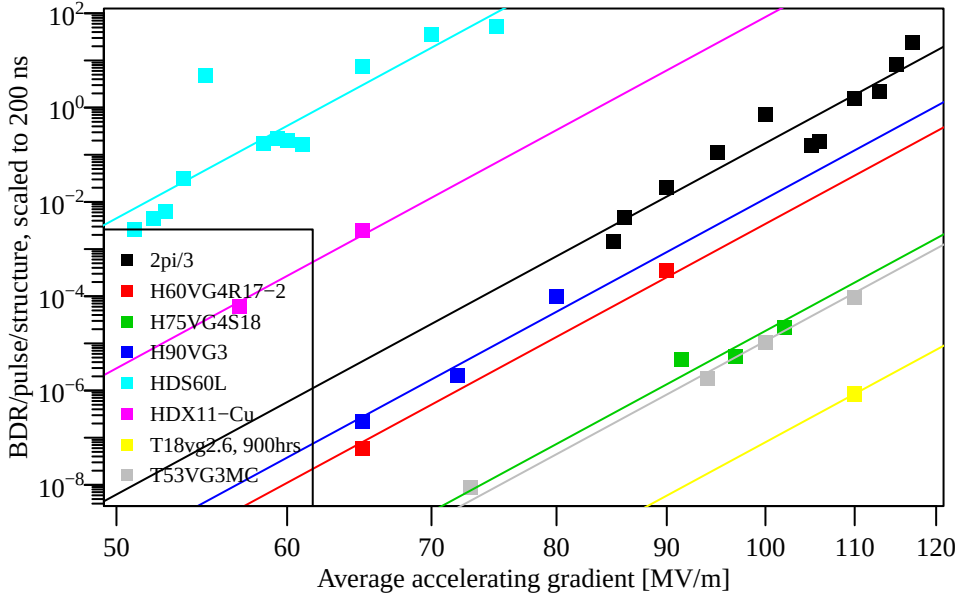
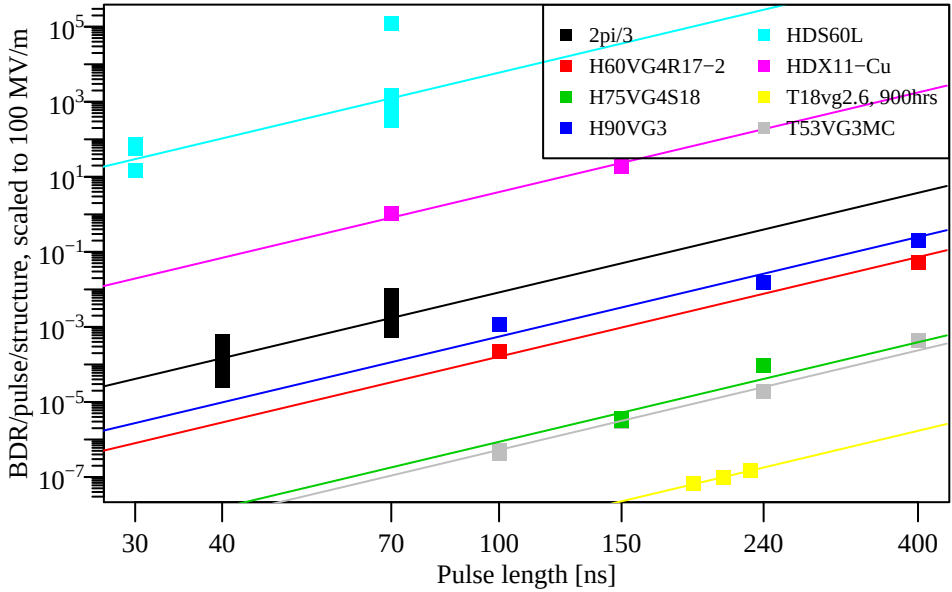

 (a) BDR as function of accelerating gradient  $G$ , scaled to  $\tau = 200$  ns.

 (b) Scaled BDR as function of pulse length  $\tau$ , scaled to  $\tau = 100$  MV/m.

Figure 3.6.: A fit of Equation (3.20) to a set of test data for different structures [95]. The exponents were here found to be  $x = 24.75 \pm 3.3$  and  $y = 4.4 \pm 0.9$ . The break down rate is scaled to a standard pulse length or gradient, as both the gradient and especially the pulse length are usually changed simultaneously in the experiments. It clearly shows that the structures follow the same scaling for the BDR as a function of  $\tau$  and  $G$ , with  $k$  varying between different structures. As some of the structures were never able to reach  $G = 100$  MV/m or  $\tau = 200$  ns, they are scaled to a BDR  $> 1$ .

### 3. High gradient acceleration challenges

in  $K$  is too large for it to usefully predict the achievable gradient and pulse length of a new and untested structure design. However, this can to a certain extent be remedied by not comparing accelerating gradients, but rather use peak field levels, as will be discussed in Section 3.3.1. Another process that is observed but not included in this model is the conditioning of accelerating structures, where they improve over time such that  $K$  and thus the achievable gradient and pulse length at the same break down rate increases. This process tend to be rapid at first, before slowing down as the number of RF pulses sent to the structure increases [96, 97, 98]. This effect is therefore most important for newly built accelerating structures.

However, when applied within a relatively small range of parameters and for fully conditioned structures, the scaling relation of Equation (3.21) still provides a method for scaling the measured performance of a structure to another combination of pulse length, gradient, and break down rate. It is therefore used as the basis for the high gradient limits described below.

#### 3.3.1. High gradient limits

While Equation (3.21) does not predict the achievable gradient in an accelerating structure, it does predict how it scales with the pulse length  $\tau$  and accelerating gradient  $G$ . This can be used to compare the achieved gradient between several different accelerating structures, and thus also compare quantities which are directly related to the gradient.

Three such quantities which is commonly taken to be limiting the achievable accelerating gradient, is the peak surface electric field  $\bar{E}$ , power over iris aperture circumference  $P_+/C$ , and the peak modified Poynting vector  $S_c$ . These quantities were described in Section 3.2. They can be inserted into Equation (3.21), providing a method for directly comparing them.

The peak surface electric field is proportional to the gradient, which implies that *normalized* peak surface electric field  $\bar{\bar{E}} = \frac{\bar{E}}{G}$  can be defined. This is purely function of the structure geometry, and can be calculated as described in Section 5.4.2. This can be inserted into Equation (3.21) as

$$K \rightarrow K_E \frac{\left(\hat{E}/\bar{E}\right)^{30} \tau^5}{\text{BDR}} \Rightarrow K_E \bar{E}^{30} = \frac{\left(\hat{E}\right)^{30} \tau^5}{\text{BDR}}, \quad (3.22)$$

relating the peak surface electric field to the pulse length and breakdown rate. Here  $K_E$  is a scaling constant equivalent to and with the same units as  $K$ , but specifically referring to the surface electric field.

Similarly, for the peak modified Poynting vector, a similar normalized quantity  $\bar{\bar{S}}_c = \frac{\hat{S}_c}{G^2}$  can be defined. This is also inserted into Equation (3.21), yielding

$$K \rightarrow K_{S_c} \frac{\left(\hat{S}_c/\bar{S}_c\right)^{15} \tau^5}{\text{BDR}} \Rightarrow K_{S_c} \bar{S}_c^{15} = \frac{\hat{S}_c^{15} \tau^5}{\text{BDR}}. \quad (3.23)$$

Finally, for the power flow per circumference  $P_+/C$ , Equations (2.5), (2.6) and (2.15) can be combined to

$$G^2 = \frac{P_+ \omega R' / Q}{v_g}, \quad (3.24)$$

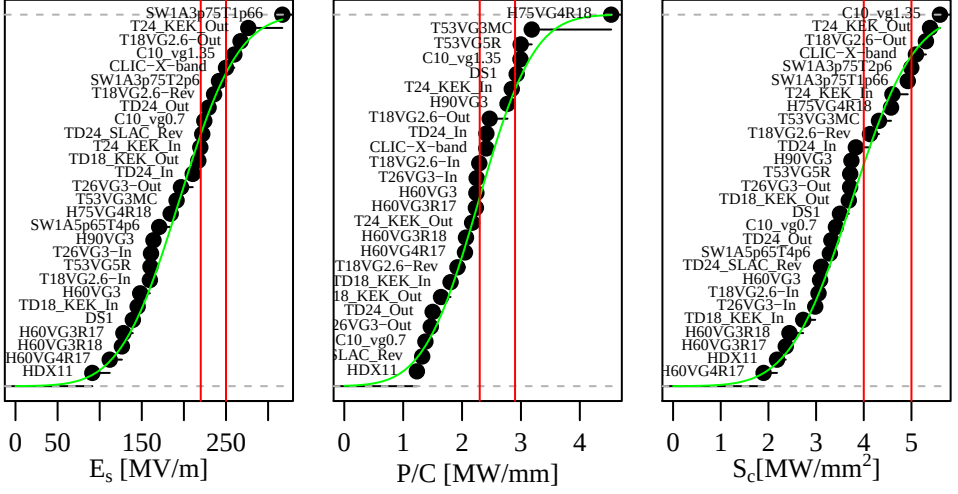


Figure 3.7.: Rescaled peak fields  $\hat{E}$ ,  $\hat{S}_c$  and  $P/C$  for a range of different structures. The curved green lines are the cumulative distribution functions for Gaussian distributions with  $\mu$  and  $\sigma$  given by the mean and sample variance of the data. The vertical red lines are the chosen “pessimistic” and “optimistic” limits.

where  $R'$  is the shunt impedance per unit length. Inserting this into Equation (3.21) yields

$$\begin{aligned}
 K &\rightarrow K_{P/C} = \frac{\left( \frac{P_+ \omega R' / Q}{v_g} \cdot \frac{C}{C} \right)^{15} \tau^5}{\text{BDR}} \\
 &\Rightarrow K_{P/C} \left( \frac{v_g}{\omega R' / QC} \right)^{15} = \frac{(P_+ / C)^{15} \tau^5}{\text{BDR}}.
 \end{aligned} \tag{3.25}$$

Using the scaling relations from Equation (3.22), (3.23) and (3.25), the peak fields can be re-scaled to *standard conditions* of  $\tau_0 = 200$  ns and  $\text{BDR}_0 = 10^{-6}$  breakdowns/pulse/meter. The unit of BDR has here been changed to include a normalization for the structure length. These re-scaled fields are shown in Figure 3.7. Using this data, a set of limits can be set for each of the three re-scaled limiting quantities. It is assumed that as long as all three quantities stay below this limit,  $\text{BDR}_0$  is not exceeded. The chosen limits are  $\hat{E}_0 = 220 - 250$  MV/m,  $\hat{S}_{c0} = 4 - 5$  MW/mm<sup>2</sup> and  $(P/C)_0 = 2.3 - 2.9$  MW/mm, the higher end of this range later called the optimistic limits and the lower end the pessimistic limits [92]. These limits are set such that they should be reachable for a well-made structure, while keeping within  $\tau \geq \tau_0$  and/or  $\text{BDR} \leq \text{BDR}_0$ . It is also possible that some of the structures which does not reach one of the limits do so due to running into problems with another limit first, i.e. non-optimal design, or due to fabrication defects related to the individual structure rather than the design.

These limits can be used to fix the scaling constant  $K_E$ ,  $K_{S_c}$  and  $K_{P/C}$  for a specific structure, by assuming that it should at least be able to reach the field limits at standard

### 3. High gradient acceleration challenges

conditions. Thus when operating at the limit, the inequalities

$$K_E \bar{E}^{30} = \frac{\hat{E}_0^{30} \tau_0^5}{\text{BDR}} \leq \frac{\hat{E}_0^{30} \tau_0^5}{\text{BDR}_0} \quad (3.26)$$

$$K_{S_c} \bar{S}_c^{15} = \frac{\hat{S}_{c0}^{15} \tau_0^5}{\text{BDR}} \leq \frac{\hat{S}_{c0}^{15} \tau_0^5}{\text{BDR}_0} \quad (3.27)$$

$$K_{P/C} \left( \frac{v_g}{\omega R'/QC} \right)^{15} = \frac{(P_+/C)^{15} \tau_0^5}{\text{BDR}} \leq \frac{(P/C)_0^{15} \tau_0^5}{\text{BDR}_0} \quad (3.28)$$

turns into the equalities

$$K_E = \frac{\hat{E}_0^{30} \tau_0^5}{\text{BDR}_0} \bar{E}^{-30} = \frac{\hat{G}_E^{30} \tau_0^5}{\text{BDR}_0} \quad (3.29)$$

$$K_{S_c} = \frac{\hat{S}_{c0}^{15} \tau_0^5}{\text{BDR}_0} \bar{S}_c^{-15} = \frac{\hat{G}_{S_c}^{30} \tau_0^5}{\text{BDR}_0} \quad (3.30)$$

$$K_{P/C} = \frac{(P/C)_0^{15} \tau_0^5}{\text{BDR}_0} \left( \frac{\omega R'/QC}{v_g} \right)^{15} = \frac{\hat{G}_{P/C}^{30} \tau_0^5}{\text{BDR}_0}, \quad (3.31)$$

where

$$\hat{G}_E = \frac{\hat{E}_0}{\bar{E}} \quad (3.32)$$

$$\hat{G}_{S_c} = \sqrt{\frac{\hat{S}_{c0}}{\bar{S}_c}} \quad (3.33)$$

$$\hat{G}_{P/C} = \sqrt{(P/C)_0 \frac{C\omega R'/Q}{v_g}} \quad (3.34)$$

are the maximum gradients allowed by each of the limits. Thus, as long as the accelerating gradient at standard conditions stays below

$$\hat{G} = \min \left( \hat{G}_E, \hat{G}_{S_c}, \hat{G}_{P/C} \right), \quad (3.35)$$

none of the rescaled peak fields will exceed their limits. To find the maximally allowed gradient at a given break down rate and pulse length, one may thus rescale  $\hat{G}$  using Equation (3.21).

This method provides a logically consistent method for comparing the different high gradient limits considered in this thesis. Especially, it predicts what the maximally acceptable gradients are for a given cell design, as used for the cell optimization method described in Chapter 5 and [23]. It is also used for the overall structure optimization described in Chapter 7 and [24]. The method itself was published in [99].

The main issue of this method is the dependency on the choice of the limits  $\hat{E}_0$ ,  $\hat{S}_{c0}$  and  $(P/C)_0$ , which are based on data extracted from a diverse range of experiments not directly aimed at testing these limits. A specialized set of experiments similar to [100, 101], mapping out the breakdown rate while varying the electric field and the power flow separately, might increase the understanding of these limits and how they interact. Such a specialized

experiment would also be beneficial, in that the surface treatment could be kept constant and under control.

Another issue is the normalization to structure length, which strictly speaking is only correct if the peak fields are the same along the structure. As seen in Fig. 7.7, this is often not the case, however the length of the structure enters the scaling equations at the same power as the break down rate, i.e.  $1/30$ . This normalization is therefore of relatively minor concern, however normalizing by structure area exposed to high fields might lead to a slightly better method.

### 3.4. Pulsed surface heating from magnetic fields

Another issue for high gradient accelerator structures is *pulsed surface heating*. In this process, the magnetic field induces a current in the metal surface on the inside of the accelerating cavity, which heats it up through Ohmic heating. For high field levels such as seen in the CLIC accelerating structures, this heating can be quite intense, and the thickness of the layer absorbing the power is only on the order of one skin depth. While some cooling is obtained by the conduction of heat into the wall (away from the surface), the short and intense pulses seen in machines like CLIC mean that the surface temperatures can rise very quickly and by significant amounts. This results in a temperature profile that changes very quickly as a function of depth in the material. The rapid heating and resulting thermal expansion of the surface every single RF pulse causes fatiguing of the surface, which can lead to surface roughening and formation of cracks [102] which may degrade the structures Q-factor. This degradation is a problem as it reduces the lifetime of the machine, however it does not directly limit the achievable gradient in a single pulse.

To quantify this effect, the basic number is the power density  $\langle \frac{dP}{dA} \rangle$  from an RF field on a conductor, averaged over one oscillation period. This is given as [72]

$$\left\langle \frac{dP}{dA} \right\rangle = \frac{\sqrt{\mu_0 \omega / 2 \sigma}}{2} |H_{\parallel}|^2, \quad (3.36)$$

where  $H_{\parallel}$  is the surface magnetic field over the area,  $\mu_0 = 4 \cdot 10^{-7} \pi$  (V s)/(A m) the vacuum permeability,  $\omega$  the oscillation frequency of the field in radians per unit time, and  $\sigma = 5.8 \cdot 10^7$  S/m the electrical conductivity of copper, which is the material used for the RF structures under consideration.

Since the the power density is proportional to the surface magnetic field, the point with the peak surface magnetic field  $\hat{H}$  also sees the largest power density. The peak power dissipation per area is thus given as

$$\left\langle \frac{dP}{dA} \right\rangle = \frac{\sqrt{\mu_0 \omega / 2 \sigma}}{2} \bar{H}^2 G^2, \quad (3.37)$$

where  $\bar{H} = \frac{\hat{H}}{G}$  is the normalized peak surface magnetic field. This can be used to calculate the maximum change of temperature  $\Delta T$  on the surface of the accelerating structure after a time  $t$ , using the specific heat capacity of the material and Fourier's law of heat conduction.

### 3. High gradient acceleration challenges

Assuming that  $t \gg \frac{2\pi}{\omega}$ , this yields [103]

$$\begin{aligned}\Delta T(t) &= \frac{1}{\sqrt{\rho c_\epsilon \pi k}} \int_0^t \left\langle \frac{dP(t')}{dA} \right\rangle \frac{dt'}{\sqrt{t-t'}} \\ &= \frac{1}{\sqrt{\rho c_\epsilon \pi k}} \frac{\sqrt{\mu_0 \omega / 2\sigma}}{2} \bar{H}^2 \int_0^t G(t')^2 \frac{dt'}{\sqrt{t-t'}} ,\end{aligned}\tag{3.38}$$

where  $\rho = 8.95 \cdot 10^3 \text{ kg/m}^3$  is the material density,  $c_\epsilon = 385 \text{ J/(kg} \cdot \text{K)}$  the specific heat capacity, and  $k = 391 \text{ W/(m} \cdot \text{K)}$  the thermal conductivity. Further,  $G(t)$  is the gradient as a function of time, which as seen in Section 7.8.2 includes the shape of the RF pulse to the structure.

A limit for the maximum acceptable pulsed surface heating is found from experimental data [78]. Taking the damage in cell 9 as a limit of what is acceptable [92] and scaling [104] it to the number of pulses expected to be seen though the lifetime of the CLIC machine, a limit of  $\Delta T \leq 50 \text{ K}$  is reached [92].

## 3.5. Summary and conclusions

This chapter presents a review of the most relevant models for predictign the probability of a vacuum arc breakdown in a given RF structure and operating conditions. These are given as phenomenological scaling laws, relating the actual value of the breakdown-correlated quantity ( $\hat{E}$ ,  $\hat{S}_c$  or  $P_+/C$ ) with a reference level at a given break down rate and pulse length. The scaling laws were then rewritten to a form which directly gives the predicted maximum accelerating gradient from each of the three criteria, given a typical pulse length and BDR. This allowed quickly estimating how high a gradient could be reached by a given design, and also facilitated direct comparison of the three different criteria. For structure design, the smallest of the three was assumed to be one limiting the structure's performance.

In addition to the criteria primarily related to vacuum arcs, the fattigue of metal is mainly caused by the temperature rise during the pulse. This temperature rise is given by the pulse shape and surface magnetic field, and can be limited by reducing either of these. For practical structures, a longer max allowable pulse shape and higher field levels are desirable, so minimizing the normalized peak surface magnetic field is important. As will be seen in Chapter 5, this optimization is mostly orthogonal to the optimization neccessary to reduce the breakdown rate.



## 4. Simulation of vacuum arcs

As described in Chapter 3, vacuum arcs breakdowns have some probability of occurring in accelerating structures when operating at high gradients. These can be described statistically, and one finds that the breakdown probability in a given pulse to some degree be predicted by the field strength, pulse shape, and structure geometry. These predictions are made through quantities connecting these parameters, such as  $\tilde{E}$ ,  $P_+/C$  and  $\hat{S}_c$ , as described in Chapter 3. However, this does not answer some fundamental questions: What is a “breakdown”, how do they start, and how and why do they occur?

If we can better understand the basic process, it might be possible to both make better models for predicting the likelihood of an arc to start in a given RF structure and pulse, and improving and/or explaining the mostly phenomenological models presented in Section 3.2. This would lead to a better understanding of how to build structures (i.e. materials, geometry, and materials processing) that can reach higher gradients or pulse lengths without suffering from vacuum arcs.

We therefore study breakdowns in high-voltage DC devices as well as the RF that is used in accelerating structures. The main difference between the RF and DC experiments is obviously that in DC, the electromagnetic fields are static from the beginning of the pulse up until the appearance of the arc; while in RF they reverse sign multiple times within the typical rise time of the arc, which is on the order of a nanosecond. This affects the transfer of energy from the field into the emitter, which in the case of RF is interrupted once every cycle as seen in Section 3.2.3. Furthermore, while a strong material dependence was observed in the DC experiment [105], this was not reproduced to the same degree in RF experiments [106]. It was however observed that the break down rate in the DC spark experiment scales with the field in the same way as in the RF measurements, i.e. following Equation (3.19). Furthermore, both the time distribution of the breakdowns within a pulse and the effect of pulse length on break down rate is also the same [27]. This indicates that some of the underlying mechanisms are the same. As mentioned in Section 1.4, we therefore study breakdown in DC along with RF because the DC spark experiments are easier to build, modify and instrument in order to test different effects. The comparative simplicity of the experiments also means that it is easier to separate parameters such as field level, material, surface treatment, temperature, magnetic field etc. Further, this experiment has a higher repetition rate which means it is possible to get more statistics in a shorter time frame. High voltage DC experiments are therefore useful in order to better understand the underlying physics of the breakdowns, which are believed to be mostly the same for RF and DC.

This chapter discusses the processes in vacuum arcs, and presents simulations of how they start and the early stages in their evolution. Some dependencies on some model parameters are also discussed. The simulation model was created based on first principles, starting from model of a collisional plasma which was combined with a surface model and a circuit model. From these building blocks we were able to create a realistic model of the initial stages of a vacuum arc, reproducing several phenomena seen in experiments.

#### 4. Simulation of vacuum arcs

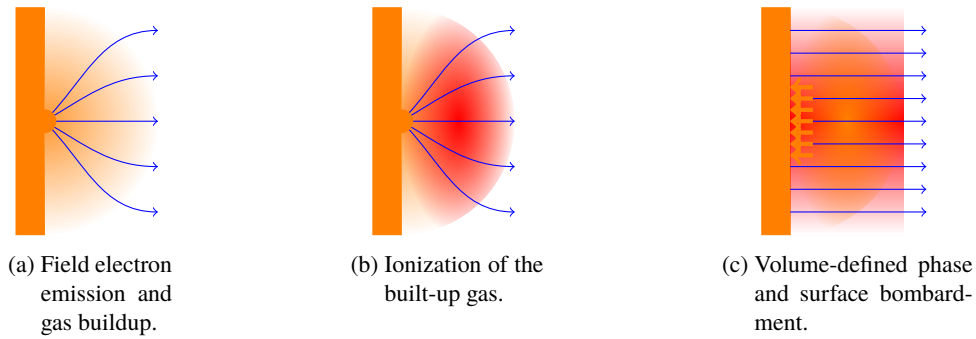


Figure 4.1.: Important stages in the ignition of a vacuum arc.

### 4.1. Vacuum arcs

Vacuum arcing is a phenomena that occurs on metal surfaces in vacuum under high field conditions, which extracts electrons and atoms from it. These atoms form a gas, which can be ionized to create into a plasma. This plasma can be detected when it emits light (Figure 1.5), conducts a current which may be very large, damages the surface (Figure 3.1), reflects electromagnetic waves, or kicks a passing beam.

A vacuum arc is a plasma discharge that starts in vacuum, in contrast to a “normal” arc, which starts in an already existing medium. Both types need a source of free electrons, such as an atom ionized by radiation, or field emission from the cathode (Section 4.1.2). Similarly for both types of arcs, these electrons are accelerated by the electric field. Once they gain enough energy, they are able to ionize gas atoms on impact, which creates a plasma. However, the source of the gas is different – in a normal arc the gas is already present everywhere in the volume, while in a vacuum arc there must be a local source for the gas, typically on the cathode surface (Section 4.1.3). Further, once the vacuum arc has started, if the arc is to grow then the gas production must be able to quickly ramp up to a larger flux. This can happen due to sputtering on the surface (Section 4.1.4), where ions from the plasma are accelerated across the plasma sheath, bombarding the surface, releasing neutrals. If the conditions are right, this bombardment can release more atoms than the ions removed, increasing the amount of gas and enabling the arc to grow.

The main events during the ignition of a vacuum arc are outlined in Figure 4.1. This illustrates how it can, as explained above, start with field emission from a small area on the cathode, and an associated production of neutrals through evaporation or a similar mechanism. The field emission can for example be enabled by a geometrical field enhancement, such as a protrusion on the surface. Such a protrusion may be present at before the field is switched on, however since they are never directly observed it seems more likely that they are created by an interaction between the field and the material (Section 4.1.1). This may for example happen by slowly pulling a void towards the surface until it “bursts open”, creating the necessary geometrical feature.

Once the neutral density reaches a critical value, an ionization avalanche can be triggered, creating a plasma within about 10 ns. This plasma creates a plasma sheath above the metal surface, with a potential on the order of 50 V and a thickness in the order of a few  $\mu\text{m}$ . When the sheath is established, a much larger area is exposed to a high field and will start emitting

electrons, which makes the current increase by many orders of magnitude. At the same time, ions are continuously diffusing from the plasma volume and into the sheath region, where they are accelerated towards the surface. This leads to a continuous ion bombardment of the surface, which creates more neutrals and also damages the surface. These neutrals are then injected into the plasma, where they are ionized by collisions with electrons, expanding the plasma.

#### 4.1.1. The origin of the emission site

As stated above, an imperfection that enhances the surface field must be present in order for the field emission to start. There are several potential sources for these, both pre-existing defects on the surface, and defects that are created during operation of the RF structure or the high voltage DC electrodes.

The pre-existing “weak points” can for example be surface irregularities, contamination such as dust, or surface oxides. This is supported by that during the initial pulses seen by a newly created surface, a rapid fall in break down rate is observed, and this initial fast conditioning is strongly influenced by the surface treatment undergone prior to testing [27]. However, after the initial fast conditioning, the break down rate does keeps falling, however at a slower rate which is mostly independent of the surface treatment. Furthermore, the conditioning appears to be a function of the number of RF pulses, not the number of break-downs, which further reduces the support for the idea that the break down rate is dropping because the breakdowns are “cleaning” the surface [98].

It is therefore likely that field emission spots are created continuously during operation of the structure. One proposed mechanism for this is that the pull on the surface from the electric field strains the material, bringing defects such as voids or inclusions up to the surface [107], and even creating new such defects [108]. These defects can then be pulled out to tips, forming a field emission site [109]. This yields a theoretical prediction which is approximately compatible with the field strength scaling discussed in Section 3.3, and also the fact that the break down rate is affected by the pulse length even if the breakdowns are approximately uniformly distributed throughout the pulse.

#### 4.1.2. Cold field emission of electrons

Cold field or Fowler-Nordheim emission of electrons is the emission of electrons from a relatively cold metal into vacuum. To reach the vacuum, the electrons must tunnel through the potential barrier

$$V(x) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{4x} - eFx, \quad (4.1)$$

where  $x$  is the distance from the metal surface, and  $F$  is the field strength [110]. This function is plotted for a few values of  $F$  in Figure 4.2, illustrating that the barrier becomes much lower and narrower when the field increases, making tunneling more likely. Thus once a strong electric field is present, the emitted current density can become very large, as shown in Figure 4.3.

The emitted current density can using the Wang and Loew approximation [111] be calculated as

$$j(E_{loc}) = \kappa_1 E_{loc}^2 \exp\left(\frac{-\kappa_2}{E_{loc}}\right), \quad (4.2)$$

#### 4. Simulation of vacuum arcs

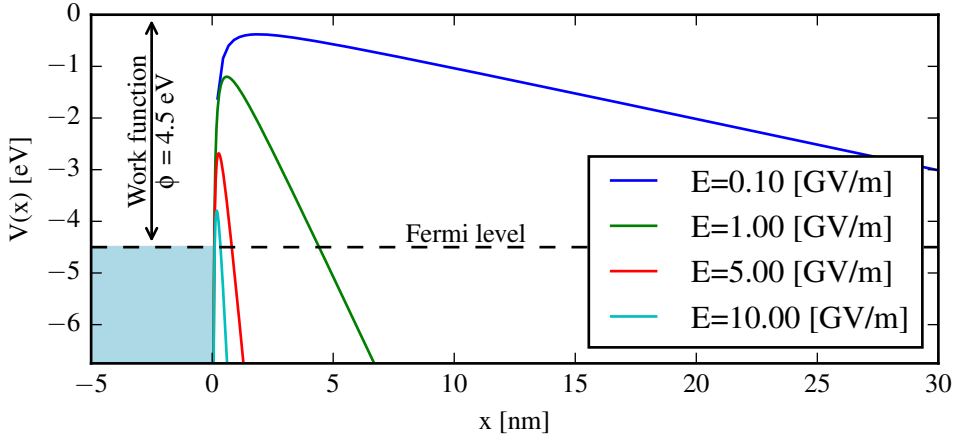


Figure 4.2.: Electric potential seen by an electron as a function of the distance  $x$  from the metal surface (Equation (4.1)), for three different external electric field strengths. The no-field vacuum level is set to 0 V.

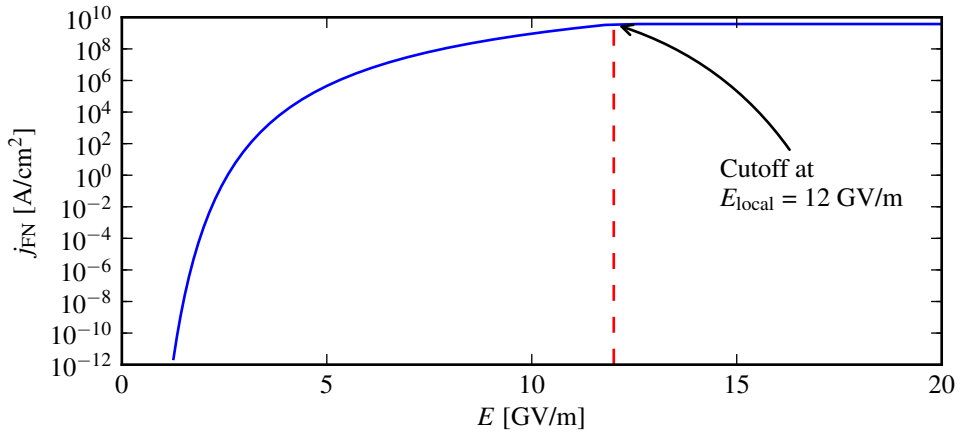


Figure 4.3.: Current density from cold field emission as a function of the local surface field (Equation (4.2)).

where  $E_{\text{loc}}$  is the electric field on the surface of the metal. The two constants are given as  $\kappa_1 = 4.7133 \text{ A/GV}^2$  and  $\kappa_2 = 62.337 \text{ GV/m}$  [112] in the case of a work function  $\phi = 4.5 \text{ eV}$  (which is typical for copper metal) and a small temperature. This model is valid for temperatures below  $\approx 1000 \text{ K}$  and up to a field of  $12 \text{ GeV}$  [110].

In experimental studies, it is often measured [113] that the surface field  $E_{\text{loc}}$  is locally enhanced by a factor of 30–60 [105]. This enhancement factor is normally called  $\beta$ , and may arise due to an irregularity on the surface such as a tip. Such high enhancement factors corresponds to relatively sharp tips, and while they are seen in field emission measurements they have not been directly observed on Cu surfaces using for example scanning electron microscopy [114, 27, 115]. This may be explained if they are relatively unstable, disappearing or changing into duller features quickly after they are created. However, recent results indicate that they may not only be created by the high field (as discussed in Section 4.1.1), but that they are also stabilized by this field until either breakdown happens and melts the tip, or the field switches off [116].

#### 4.1.3. Evaporation of neutral atoms

Another process that is important for vacuum arc is the evaporation of neutral atoms from the surface. This process is necessary if an arc is to start, since the plasma requires a source of gas in order to form.

A closely related process that has been much studied – especially in the context of Atom Probe (AP) techniques – is field evaporation. Here, neutrals or ionized atoms are removed from a tip by a combination of an electric field and thermal excitation [117, 118, 119]. However it is normally assumed that the evaporating sample is the anode, releasing neutral or positive ions; while in our case the sample is the cathode, and the field would push any positive ions back towards the source. This means that while field evaporation in the traditional sense might be relevant for RF [120], it is likely less important for DC. Still, simulations indicate that neutrals are released from the surface near field emitters due to the strong electric field close to the emitter, electron transport, and high temperatures [121, 122, 123].

The exact functional form and full set of dependencies for neutral evaporation in the region around a field emitter is currently not completely understood. A rather simple model is used in the simulations presented in this chapter, where it is assumed that the rate of emission for the neutral atoms is proportional to the field emission current. The same model as was also used in [124]. Such a model is expected to provide a sufficiently realistic density distribution to start the arc; once the arc has started, sputtering also becomes important (as seen in Figure 4.12b).

#### 4.1.4. Sputtering

Sputtering is a surface process where atoms are released from a material that is struck by high-velocity projectiles, in the form of ions or other atoms. This is important for expanding and sustaining a vacuum arc, as it is one of the main sources of gas that can be ionized to create the plasma.

The sputtering yield, i.e. the number of atoms released due to the impact of a single atom, mainly depends on the impact energy. For ions hitting a solid surface a normal incidence, the average yield as a function of energy is given by Yamamura and Tawara [125], who created and fitted an empirical formula based on a large collection of experimental data.

#### 4. Simulation of vacuum arcs

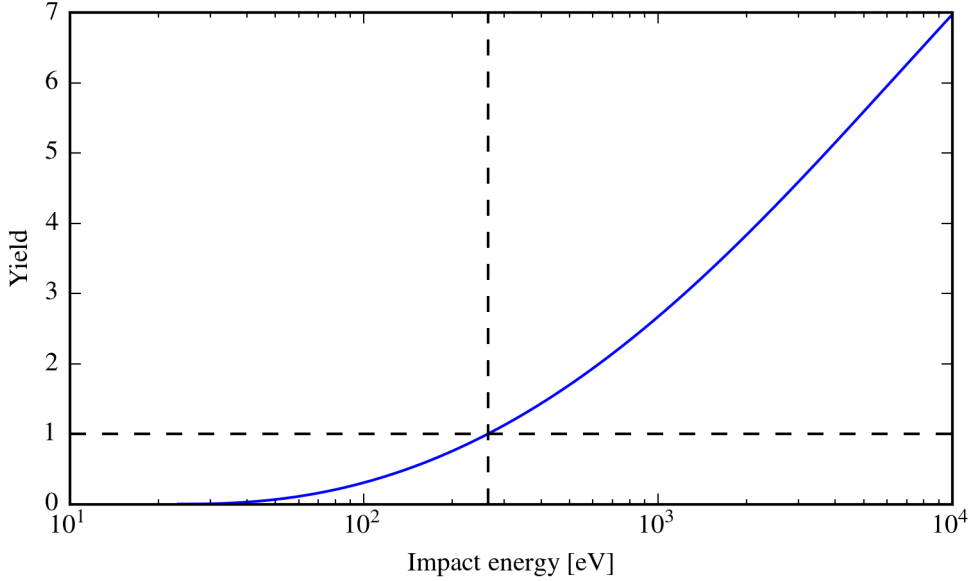


Figure 4.4.: Average sputtering yield for Cu→Cu calculated using empirical formula [125]. The dashed lines indicates where the yield crosses 1.0, which happens at an impact energy of 264 eV.

The curve for copper on copper is shown in Figure 4.4. Note that a yield greater than 1.0 is only seen for an impact energy greater than 264 eV. This means that if the energy of the ions is mainly determined by the sheath potential (as is indicated by the simulations presented in Section 4.3, see especially Figure 4.15b), the ion bombardment is on average removing ions from the plasma, reducing it's volume and density.

However, if the number of impinging atoms is very large, this can modify the sputtering yield. This can be due to a heat spike, which is mainly relevant for high-energy bombardments, or it can be due to local heating effects [80]. In both cases, the effect is a large increase in average sputtering yield for large ion bombardment fluxes. This increased yield has been taken into account in the model presented in this chapter as described in Section 4.2.7.

## 4.2. Simulation methods

While vacuum arcs are at CERN being studied in experiments such as DC spark and XBox RF structure test stand at CERN (Sec. 1.4), there are many processes which are too fast or otherwise inaccessible in such experiments. Furthermore, some hypotheses are more accessible by simulations than experiments, such as when comparing the importance of different processes happening on the plasma-surface interface or model parameters. Simulation is therefore helpful, as it gives us full access to observe all physical parameters of the system at all points in time, and also full control over which physics processes can happen and with which parameters.

### 4.2.1. 2D ArcPic and The Particle in Cell (PIC) method

For the simulations presented in this chapter, the particle in cell (PIC) method (this Section) with Monte Carlo collisions (Section 4.2.2) was used. Additionally, the interactions between the plasma and the surface (Section 4.2.7) and the effects of the circuit (Section 4.2.6) were included in the model. These are all implemented in the 2D ArcPIC code [31]. This code simulates the evolution of the plasma between two cylindrical electrodes, which matches the geometry of the CERN DC spark fixed gap experiment.

Three species are considered: Electrons ( $e^-$ ), singly ionized copper ( $\text{Cu}^+$ ), and neutral copper (Cu). The phase-space density of these are tracked in a cylindrically symmetric coordinate system, keeping track of all three velocity components ( $v_r, v_z, v_\theta$ ) and two position components ( $r, z$ ). Further, the charged particles are interacting electrostatically with each other and with two electrodes, and the potential of these electrodes are calculated based on a model of the connected circuit, as shown in Figure 4.9. The geometry of the system is as illustrated in Figure 4.10.

In order to discretize the problem, the density distribution in the 5-dimensional phase-space is sampled by a set of macro particles, each representing some fixed number of physical particles. Each of these particles is affected by the electromagnetic field, and the equations of motion for a single particle are thus

$$\frac{d\vec{v}}{dt} = \frac{q}{m} \left( \vec{E} + \vec{v} \times \vec{B} \right) \quad \text{and} \quad \frac{d\vec{r}}{dt} = \vec{v}.$$

Since the magnetic field induced by the beam current is small and its effect can be disregarded, the equations of motion are discretized with a time step  $\Delta t$  using the leapfrog method. This gives the following discrete-time equation of motion:

$$\frac{\vec{v}_{k+1/2} - \vec{v}_{k-1/2}}{\Delta t} = \frac{q}{m} \vec{E}_k \quad \text{and} \quad \frac{\vec{r}_{k+1} - \vec{r}_k}{\Delta t} = \vec{v}_{k+1/2}.$$

The case of a non-vanishing and constant external magnetic field is also supported by the code, and in this case the Boris method is used [31]. Since the simulations use a cylindrically symmetric coordinate system, the centrifugal forces on a particle having a nonzero  $v_\theta$  is taken into account by “rotating” the particle pack onto the plane, updating its  $r$ -position.

Once the particle positions have been updated, the potential is updated to take the new charge distribution into account. This is done by first weighting the charge of each macro particle onto the four nearest grid points  $\vec{r}_i = z_i \hat{z} + r_i \hat{r}$  using a weighting function  $S_i(\vec{r}_j)$ ,

#### 4. Simulation of vacuum arcs

where  $j$  is the particle index. Using the cloud in cell weighting scheme, this can be written as

$$S_i(\vec{r}_j) = \left(1 - \frac{|z_j - z_i|}{\Delta z}\right) \left(1 - \frac{|r_j - r_i|}{\Delta r}\right). \quad (4.3)$$

This is equivalent to assuming that the particle is represented by a rectangle of constant density with area  $\Delta z \Delta r$  that is centered on the particle's position. The partial charge  $q_{i,j}$  which is weighted to the grid point is then the total charge of particle  $j$ , multiplied by the fraction of its rectangle which is inside the rectangle that is centered on that grid point. This is done for all particles and all grid points.

To then compute the volume density  $\rho_i$  at each grid point, the effective volume  $V_i$  of the grid point with index  $i$  is then found using the Verbonceaur method [126], such that  $\rho_i = q_i/V_i$ , where  $q_i = \sum_j q_{i,j}$  is the total charge deposited on that grid point. This takes into account that the size of the volume element  $2\pi r dr dz$  depends on  $r$  such that the density represented by each macro particle is reduced at larger  $r$ , and the special cases for the edge cells with  $r = 0$  and  $r = r_{\max}$ .

The field solver then runs, using an implicit finite-difference method to solve Poisson's Equation with the relevant boundary conditions. These boundary conditions are generally Neumann on  $r = 0$  and  $r = r_{\max}$ , and Dirichlet on the cathode ( $z = 0$ ) and anode ( $z = z_{\max}$ ). The potential on the cathode and anode are adjusted at each time step, according to the potential that is set by the circuit model. In order to avoid excessive memory usage and enable relatively fast calculation times by saving the partially inverted matrix, the sparse linear system is then solved using SuperLU [127, 128].

This yields a value for the potential  $\phi$  in all grid points, of which the gradient can be numerically calculated in order to find the electric field on these grid points. For the pusher, the same weighting function (Equation (4.3)) is then used to interpolate the fields back to the position of the particle in the next time step.

The order of the actions which are completed in each time-step of the simulation is illustrated in Figure 4.5. This shows where collisions, surface physics and output are done in addition to the "basic PIC" steps described above, changing and reacting to the particle distributions and the boundary conditions for the field solver.

##### 4.2.2. Monte-Carlo collisions

Several collision processes are implemented in 2D ArcPIC. Some of these are crucial for vacuum arcs, such as the ionization of neutral gas through inelastic collisions with electrons. The following processes are used, grouped by the implementing routine: [31]:

- Elastic Coulomb collisions between the pairs ( $\text{Cu}^+$ ,  $\text{Cu}^+$ ) and ( $\text{e}^-$ ,  $\text{e}^-$ )
- Elastic collisions between between the pair ( $\text{Cu}$ ,  $\text{Cu}$ )
- Elastic collisions between between the pair ( $\text{Cu}$ ,  $\text{e}^-$ )
- Elastic collisions between between the pair ( $\text{Cu}$ ,  $\text{Cu}^+$ )
- Impact ionization  $\text{e}^- + \text{Cu} \rightarrow \text{Cu}^+ + 2 \text{e}^-$

The algorithms implementing these collisions have been adapted from a 1D PIC code developed at the Max-Planck Institut für Plasmaphysik [129, 130, 131].

While the exact details vary, the algorithms all follow a similar scheme:



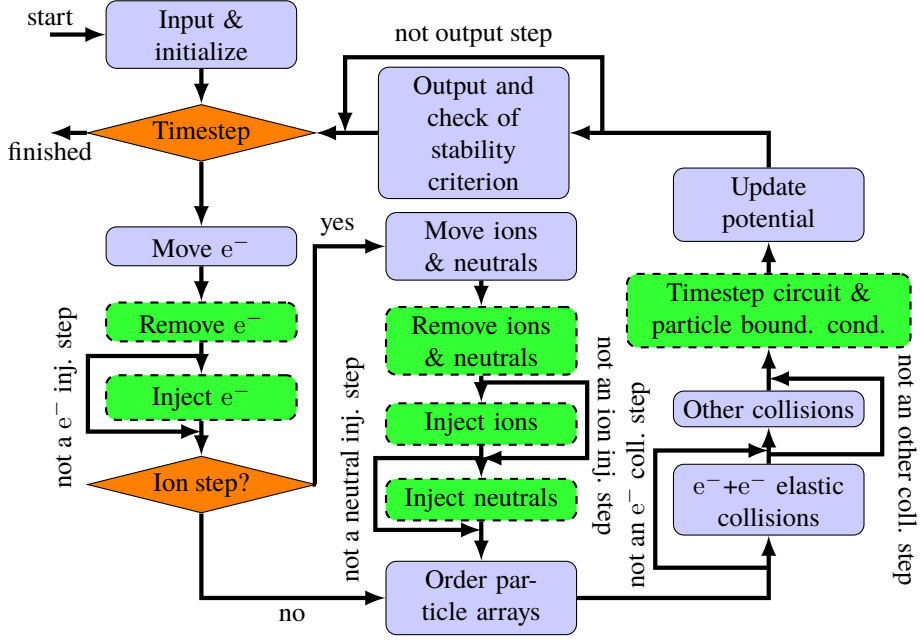


Figure 4.5.: The main sequence of the 2D ArcPIC code. The green rectangles with dashed border indicates modular components, i.e. the currently loaded circuit- or surface model.

```

for all cells  $i,j$  in the domain do
  if the number of particles in the cell  $n_{i,j} \leq 1$  then
    Skip this cell
  end if
  Generate a random pairing of the particles in the cell
  for all pairs of particles in the cell do
    Collide the two particles
  end for
end for

```

There are some of the variations in the pairing of particles, due to the differences in colliding a species with itself and colliding particles from two different species [132]. Another source of differences is how of the collision processes are handled; for Coulomb all pairs are collided but the scattering angle is sampled [132, 133]. For other collisions the null-collision method is used [134, 129], where the cross-section is used to determine whether a collision happens at all, and if so the angle is then sampled.

#### 4.2.3. Parallelization of collisions

As some of the simulations needed a very large amount of time to complete – in some cases several months, even after the improvements – some measures were required to improve the performance of the code. The long running times were due to the large span in particle den-

#### 4. Simulation of vacuum arcs

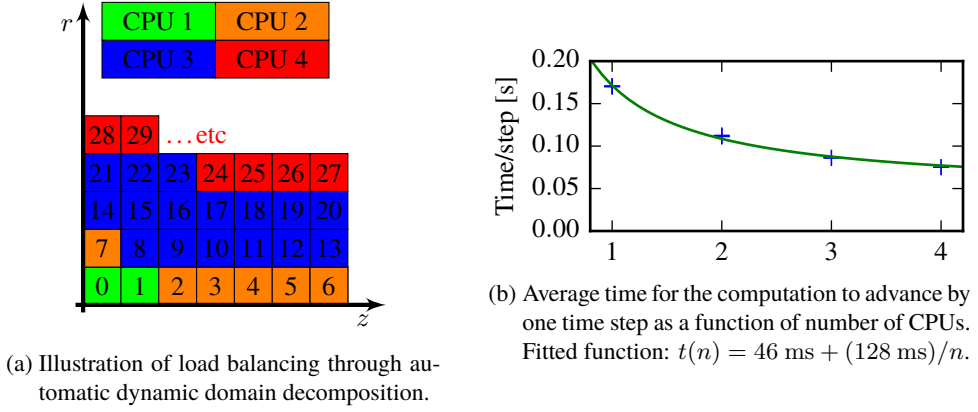


Figure 4.6.: Paralellization of the Cu+Cu elastic scattering process in 2D ArcPIC, as described in Section 4.2.3.

sities seen in each single simulation, requiring simulation settings (particle weighting, grid and time step etc.) which were not optimal for the simulation performance during either the field emission phase at the beginning of the simulation, or for the high-density plasma created by the arc. This reflects reality – while a field emitter may carry a current of a few nA, a mature arc can carry multiple kA. Spanning over such a range of currents and densities resulted in the simulations containing a large number of super-particles, and initial simulations indicated that the neutrals were the dominating species. When measuring with the profiling tool *gprof*, it was thus found that for an arc simulation the Cu+Cu elastic collisions routine dominated the CPU time usage. Later simulations, such as the one described in Section 4.3, would most likely have benefited more from parallelizing the charged particle collisions.

This routine was therefore parallelized, splitting the load over several CPUs using OpenMP [32]. OpenMP is a compiler-based multithreading, which enables the process to spawn several threads which share the same memory, complete some task in parallel, and later merge back to a single thread. While this type of implementation might require some restructuring of the algorithms that is to be parallelized, it does not need large changes to the overall structure of an already existing program, as would be required by message passing frameworks such as MPI [135]. The parallelization was done over the number of cells, as the collision algorithm (described in Section 4.2.2) runs independently in each cell. Since the number of particles per cell varies greatly (see Figure 4.14), the algorithm splits the work such that each CPU handles an approximately equal number of particles. This way, some CPUs handles few but highly-populated cells, while other handles many cells but with fewer particles in each, balancing the work between the CPUs as illustrated in Figure 4.6a. This split is updated at every call to the collision routine.

The parallelization worked well: As shown in Figure 4.6b, the time to complete one time-step is well described as  $t_{\text{step}}(n) = A + B/n$ , where  $n$  is the number of CPUs available, and  $A$  and  $B$  two constants. This means that the processing speed of the parallelized part scales linearly with the number of CPUs. The test shown in Figure 4.6b was run on a system filled with a gas of neutrals, so while the values of the fitted constants are not representative for a more typical simulation, the good fit of the model shows that the parallelized routine scales well within the typical number of CPUs available.

While scaling to more CPUs could provide a larger speedup, scaling to more CPUs than what is typically found in a single machine would require the use of a different parallelization method such as MPI, triggering an extensive rewrite of the code. It might also be possible to parallelize other parts of the code (and a parallel version of the particle pusher was implemented but then discarded as the benefit was too small), however one of the remaining main bottlenecks was found to be the implicit field solver, which does not lend itself to parallelization. Furthermore, there are several possible other avenues of code optimization which may yield a larger effect, such as changing the particle weighting over the course of the simulation.

#### 4.2.4. Accuracy of the field solver near the emitter at $r = z = 0$

During the early field emission phase of the simulations, the simulated field emission current tend to oscillate over very short time scales (a few picoseconds). In this phase, few or no ions are present in the system and the emission is completely dominated by the tip at  $r = 0$ . It was understood that this instability was due to the space charge of the emitted electrons reducing the field seen at the emitter, as the emission current (Equation (4.2)) is highly sensitive to the field. The hypothesis was strengthened when it was found that the period of this instability corresponded to the time an electron took to travel a distance  $\Delta z$  from the emitter. This was explained by looking at the how the field calculated by the PIC method depends on the particle position. Essentially, the PIC method is not particularly accurate for estimating the field at short distances, as is shown in Figure 4.7. It was also found that unless the particle weight was excessively increased, the emitted current was unchanged, which ruled out a statistical effect (shot noise).

In order to compare the field seen at the emitter with the analytical case, an expression was found. In free space, the field observed at  $\vec{r} = \vec{0}$  from a charge “ring”  $q$  at position  $\vec{r} = r\hat{r} + z\hat{z}$  is given as

$$\vec{E}_0(z) = \frac{-qz}{4\pi\epsilon_0|\vec{r}|^3} . \quad (4.4)$$

The conducting surfaces of the anode and cathode at  $z = 0$  and  $z = z_{\max}$  can be modeled as an infinite set of mirror charges. The field can thus be expressed as

$$\vec{E}(z) = \vec{E}_0(z) + \sum_{i=1}^{\infty} \left( (-1)^n \vec{E}_0(z_{-i}) + (-1)^n \vec{E}_0(z_{+i}) \right) , \quad (4.5)$$

where

$$z_i = -i z_{\max} + \begin{cases} z_{\max} - z & \text{for } i \text{ odd} \\ z & \text{for } i \text{ even} \end{cases} . \quad (4.6)$$

In practice, the sum in Equation (4.5) must be truncated at some level; for the plots in Figure 4.7 the sum was truncated after  $i = 15$ .

While some steps were taken to mitigate the effect of this inaccuracy inherent in the PIC method, it was eventually assumed to be relatively un-important for the particle injection processes. Further, the current used for the circuit is anyway effectively smoothed by the Shockley-Ramo theorem as described in Section 4.2.5.

Another possible source of field error is the boundary condition at  $r = r_{\max}$ . This was addressed simply by making the simulation domain significantly larger than the expected maximum radius of the arc.

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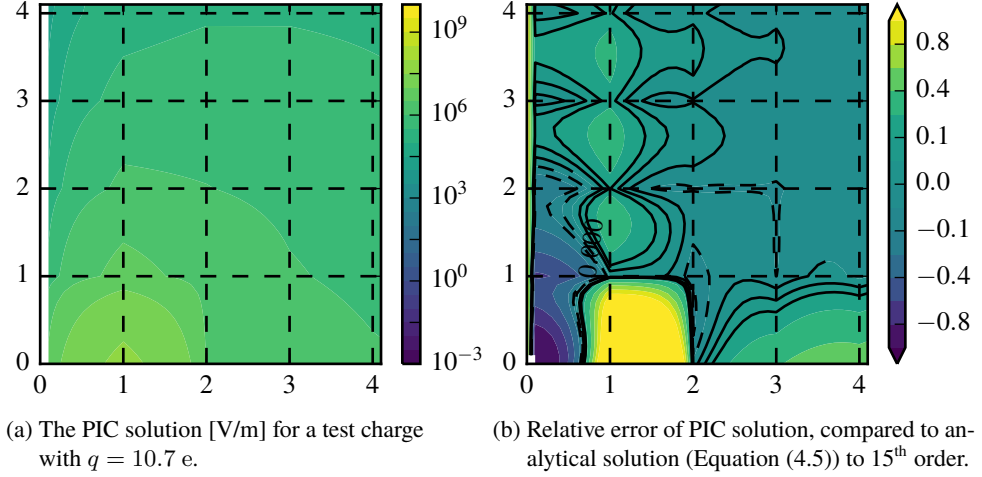


Figure 4.7.: Field from a test particle on  $r = z = 0$  as a function of the test particle position. The grid is the PIC grid,  $\Delta z = 50$  nm. Field boundary condition BC=4 [31].

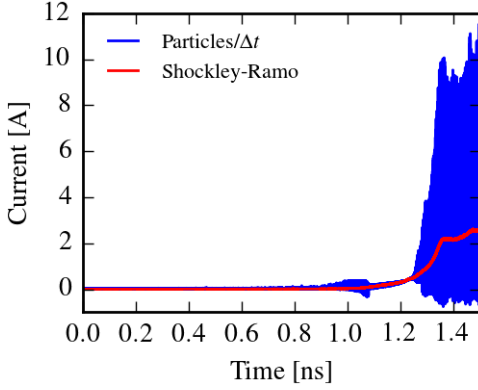
##### 4.2.5. Shockley-Ramo

In order to run the circuit models, a good estimate for the gap currents is needed. As shown in Figure 4.8a, the naive method of counting the amount of charge as it are absorbed or injected at the walls and dividing with the time step  $\Delta t$  does not work well, as it creates large amounts of noise. This problem can be solved by looking at the actual amount of charge being transported in or out of the system comprised of the gap and the electrodes, including the image charges. When a negative charge  $-q$  is emitted from the cathode, it is gradually replaced by new negative charges as the emitted charge distances itself from the surface. This happens as the mirror charges on the surface are weakened, and as illustrated in Figure 4.8b the “replacement current” can also be described as a flow of positive charges out of cathode. A similar process occurs on the anode, where the approaching negative charge generates positive image charges as it approaches, which again must be supplied by the circuit.

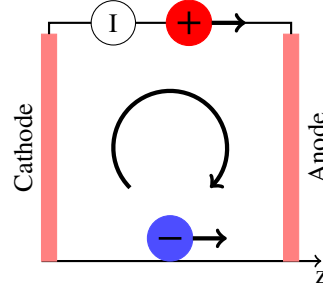
The Shockley-Ramo theorem [136, 137] describes how this induced charge can be calculated, by introducing a “weighting field” for each electrode. The weighting field  $\varphi_c$  for the cathode is calculated by solving Laplace’s equation  $\nabla^2 \varphi_c = 0$  with the boundary conditions  $\varphi_c = 1$  on the cathode and  $\varphi_c = 0$  on the anode. In the same way, the weighting field  $\varphi_a$  for the anode is found by setting the boundary conditions to  $\varphi_a = 1$  on the anode and  $\varphi_a = 0$  on the cathode. Using this weighting field, the charge induced on a given electrode is  $Q_{\text{ind}} = -q\varphi(\vec{r})$ , where  $\vec{r}$  is the position of the inducing charge  $q$  and  $\varphi(\vec{r})$  is the weighting field evaluated at  $\vec{r}$ .

For the geometry used in this simulations, the solutions to Laplace’s equation are simply

$$\varphi_c(\vec{r}) = 1 - \frac{z}{z_{\text{max}}} \quad \text{and} \quad \varphi_a(\vec{r}) = \frac{z}{z_{\text{max}}} . \quad (4.7)$$



(a) Naive wall current implementation and Shockley-Ramo calculation. The data is from the simulation presented in Section 4.3.



(b) The S.R. gap current and the particle flow in the gap. The circular arrow indicates the positive current direction.

Figure 4.8.: Shockley-Ramo gap current calculation.

The total charge induced on the cathode is thus given by

$$Q_{c,\text{ind.}} = - \sum_{\forall i} q_i \varphi_c(z_i), \quad (4.8)$$

and the cathode current as

$$I(t) = \frac{\Delta Q_c}{\Delta t} = -1 \frac{(Q_{c,\text{ind.}}(t) - Q_{c,\text{ind.}}(t - \Delta t)) + Q_{c,\text{inj}} - Q_{c,\text{abs}}}{\Delta t}, \quad (4.9)$$

where  $Q_{c,\text{inj}}$  is the total charge injected into the system from the cathode, and  $Q_{c,\text{abs}}$  the total charge removed at the cathode. The factor -1 comes from that a positive charge going from the cathode to the anode is seen as a negative current, as illustrated in Figure 4.8b.

Note that when injecting e.g. an electron superparticle with charge  $q_e < 0$  from the cathode, the injection current  $-Q_{c,\text{inj}}/\Delta t = -q_e/\Delta t > 0$  counts as a positive current  $q_e/\Delta t$ . This positive current is then initially almost canceled by the induced current  $q_e \varphi(z(t))/\Delta t = q_e(1 - z(t)/z_{\text{max}})/\Delta t \approx q_e/\Delta t < 0$ .

This current is given to the circuit model, which may use it to update the gap voltage before the next time step. Finally, since the current is the same throughout a circuit loop, the cathode and anode currents are identical. It is therefore sufficient to calculate only one of them.

#### 4.2.6. Circuit model

The 2D ArcPIC code supports several circuit models, which are implemented as classes. The selection of which class to instantiate and load, as well as its parameters, is controlled from the input file. Common for all of these circuit models is that they are provided with the gap current  $I_{\text{gap}}$  after each time step, and uses this to update the gap voltage  $V_{\text{gap}}$  before the next time step. The gap current is always calculated (in the main code) using Equation (4.9).

The circuit model is an important part of the simulation, as it controls how the gap voltage drops when the arc starts to pull a large current. This again effects the processes inside the

#### 4. Simulation of vacuum arcs

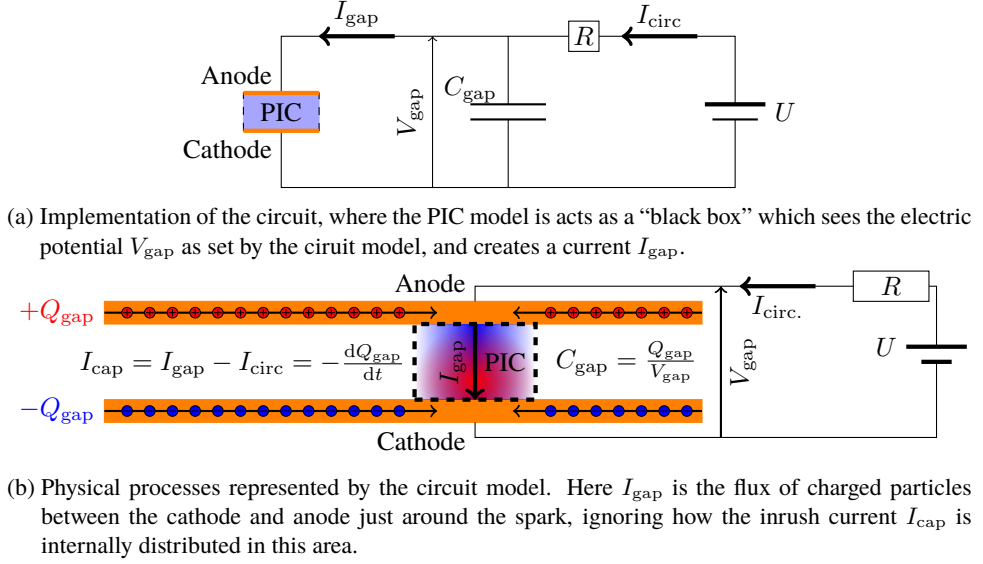


Figure 4.9.: The circuit model used in the presented simulations.

arc, such as the maximum energy of the particles and thus the energy of the ions hitting the electrodes.

The circuit model used in the presented simulations is made to emulate the circuit used in the DC spark experiments (Section 1.4) at CERN. It is consisting of a local capacitance  $C_{\text{gap}}$  and a constant-voltage power-supply with a voltage  $U$  and an internal resistance  $R$ , as illustrated in Figure 4.9. The external power supply is meant to emulate the effect of the PFL cable, which provides a pulse that is much longer than the length of the simulation.

Every time step, the voltage is updated as

$$V_{\text{gap}}(t) = V_{\text{gap}}(t = 0) + \frac{1}{C_{\text{gap}}} \int_0^t I_{\text{circ}}(t) - I_{\text{gap}}(t) dt \quad (4.10)$$

and the circuit current as

$$I_{\text{circ}}(t) = \frac{U - V_{\text{gap}}(t)}{R}. \quad (4.11)$$

The initial condition for the voltage is that  $V_{\text{gap}}(t = 0) = U$ . All of these quantities are written to file, and are plotted for one simulation in Figure 4.11. Note that  $I_{\text{circ}}$  is the current that can be measured in the real external circuit, while  $I_{\text{gap}}$  is only seen inside the gap and in the circuit model, as illustrated in Figure 4.9b.

### 4.2.7. Surface physics

Similar to the circuit models, the 2D ArcPIC code supports several surface physics models, which are selected and controlled from the input file. These classes handle injection of new particles into the simulation domain from the anode and cathode. Also handled by the surface physics model classes are particle removals, as this can influence the injection via for example sputtering. Figure 4.10 illustrates the surface physics model used in the simulations presented in this chapter. As is seen from this figure, both electrons and neutral copper are injected according to several different models.

For electrons, the main source is field emission (described in Section 4.1.2). This is broken up in two parts with different parameters, the first being field emission from the “tip”, using the field at  $r = 0$ . A large field enhancement factor  $\beta_{\text{tip}}$  is assigned to this area, but a relatively small radius  $R_{\text{tip}}$  is used to convert the current density to the actual current. The current emitted from the tip is then injected over an area with a slightly larger radius  $R_{\text{emit}}$ , which reduces the numerical stability problems described in Section 4.2.4. Outside of the tip region, a much smaller field enhancement factor  $\beta_{\text{flat}}$  is applied.

Another source of electrons is the secondary electron yield, i.e. electrons emitted from the surface due to hard impacts (above 100 eV) of ions; however as seen in Figure 4.12, this is a relatively small proportion of the emitted electrons.

For neutrals, two sources are taken into account: Evaporation and sputtering. The evaporation of neutral Cu atoms (Section 4.1.3) is taken to be proportional to the field emission current of electrons, with a constant of proportionality  $r_{\text{Cu/e}}$  setting how many Cu atoms are emitted per electron as discussed in Section 4.1.3. The choice of this value is mainly affecting the time to breakdown in the simulations [124], and a value that caused the breakdown to start within a few ns after the beginning of the simulation was chosen.

The sputtering (Section 4.1.4) is divided in two components: Single-particle sputtering, where the sputtering yield is given by the energy using the empirical formula plotted in Figure 4.4, and high-flux sputtering. Only particles with  $E_k > 23.383$  eV are counted for sputtering, as this is the lower threshold for the energy-dependent sputtering. The high flux sputtering is only active where and when the ion bombardment flux exceeds a threshold of  $j_{\text{enhanced}}$ , averaged across the last neutral injection step  $= 5\Delta t$ . When this happens, the yield from the ions hitting the cathode at a position inside the radius  $\hat{r}_{\text{enhanced}}$  is increased by a constant value  $Y_{\text{enhanced}}$ , on top of any yield from energy-dependent sputtering. This radius is the radius of the outermost edge of the outermost cell with a flux above the threshold. These extra sputtered particles are injected with an initial position following a Gaussian distribution with  $\sigma = r_{\text{enhanced}}$ .

Adding this high-flux sputtering was necessary for vacuum arcs to increase in size once the initial ionization has happened. Further, simply increasing the value of  $r_{\text{Cu/e}}$  yields unreasonably large evaporation rates before the breakdown. The exact nature of both of these processes are interesting subjects of further study.

For both evaporation and sputtering, the neutral particles are injected with a thermal velocity distribution corresponding to a temperature of 14.5 eV, while 0.29 eV was used for the electrons. This neutral temperature was chosen in order to match the typical temperature of sputtered atoms [112].

#### 4. Simulation of vacuum arcs

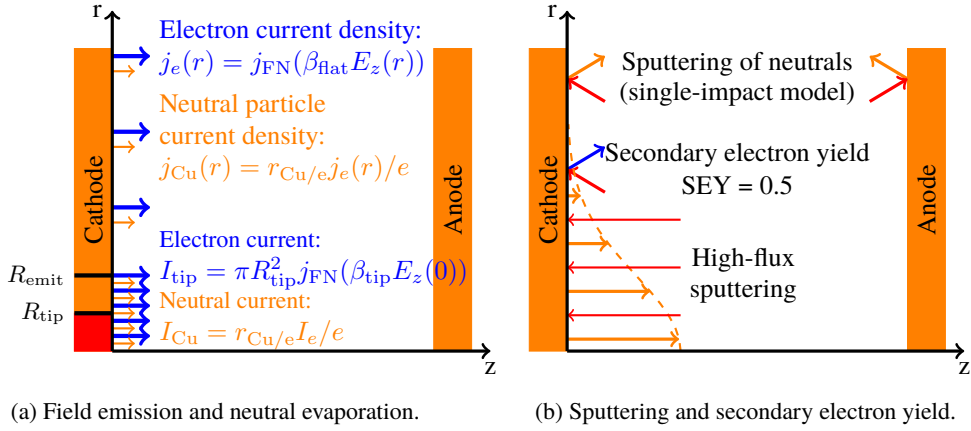


Figure 4.10.: The geometry of the simulation domain, and the surface physics process models used for particle injection in the presented simulations.

|         | Parameter             | Value          | Unit                          | Comment                                    |
|---------|-----------------------|----------------|-------------------------------|--------------------------------------------|
| General | $\Delta t$            | 0.886          | fs                            | Time step                                  |
|         | $\Delta z$            | 50             | nm                            | Grid spacing                               |
|         | $N_{\text{sp}}$       | 10.68          |                               | Particle/super-particle weighting ratio    |
|         | $Z$                   | 6 (120 cells)  | $\mu\text{m}$                 | Domain size                                |
|         | $R$                   | 24 (480 cells) | $\mu\text{m}$                 |                                            |
| Surface | $\beta_{\text{tip}}$  | 35             |                               | Field enhancement factor for “tip”         |
|         | $\beta_{\text{flat}}$ | 2              |                               | Field enhancement factor outside “tip”     |
|         | $R_{\text{tip}}$      | 56.4           | nm                            | Radius used for calculating “tip” current  |
|         | $R_{\text{emit}}$     | 400            | nm                            | Radius used for injection of “tip” current |
|         | $Y_{\text{SEY}}$      | 0.5            |                               | Secondary electron yield                   |
|         | $r_{\text{Cu/e}}$     | 0.015          |                               | Cu/e <sup>-</sup> injection ratio          |
|         | $j_{\text{enhanced}}$ | $10^{25}$      | $\text{cm}^{-2}\text{s}^{-1}$ | Enhanced (high-flux) sputtering threshold  |
| Circuit | $Y_{\text{enhanced}}$ | 1              |                               | Enhanced (high-flux) sputtering yield      |
|         | $U$                   | 1740           | V                             | Supply and initial gap voltage             |
|         | $E_z$                 | 290            | MV/m                          | $E_z(t=0) = U/Z$                           |
|         | $R$                   | 1000           | $\Omega$                      | Series resistance                          |
|         | $C$                   | 1.0            | pF                            | Gap capacitance                            |

Table 4.1.: Parameters for the simulation presented in Section 4.3.



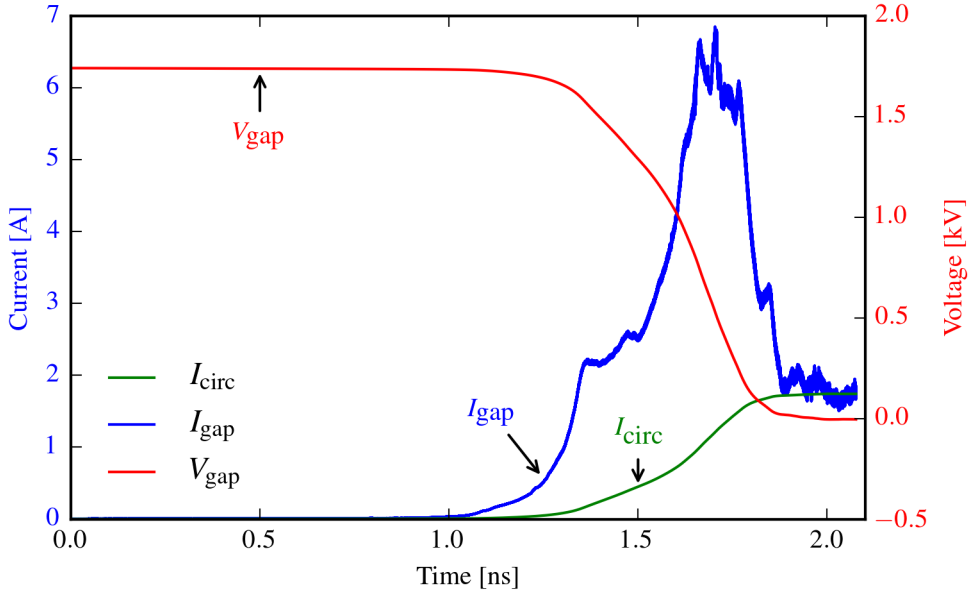


Figure 4.11.: Typical simulated current and voltage for the simulation described in Section 4.3. The symbols are as defined in Figure 4.9.

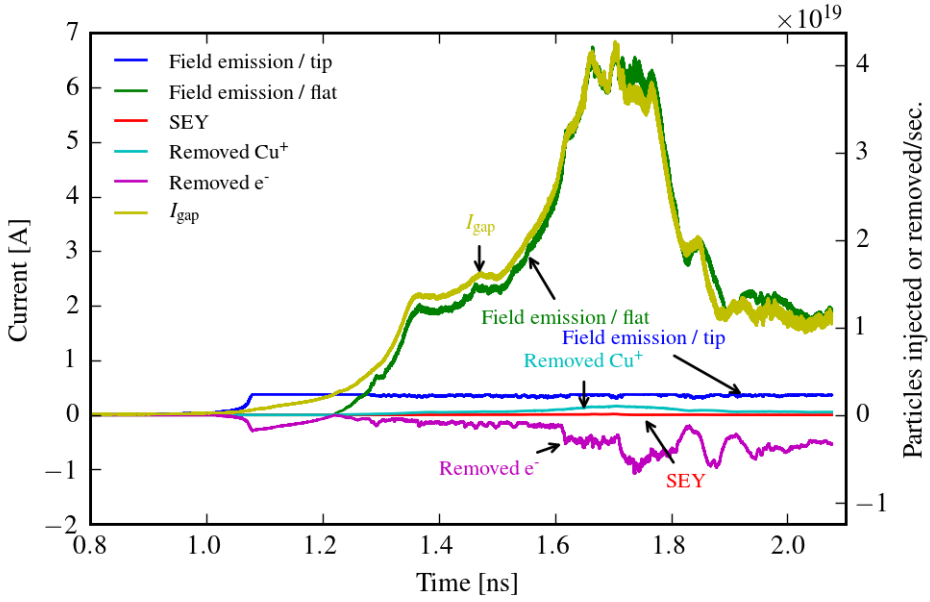
### 4.3. Simulation results

While a full description of the results are found in [112], some of the main results are described in this section. Here, only the “reference” run from the paper is described, while Section 4.3.1 describes the effects of changing some parameters. The reference values for the simulation parameters are given in Table 4.1.

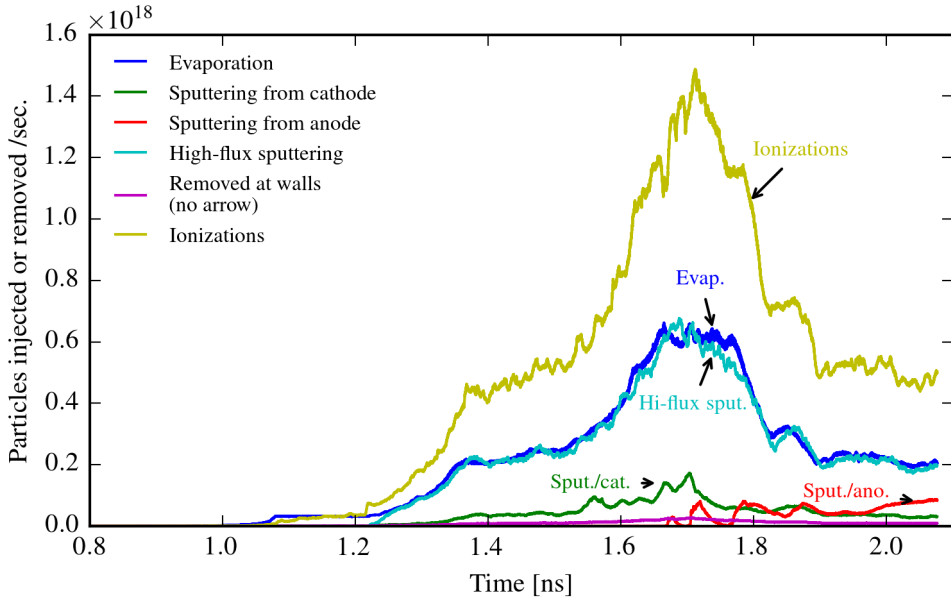
The simulated arc follows the same behavior as described in Section 4.1 and Figure 4.1. Again, it starts with field emission and evaporation of neutrals, slowly building up the number and density of neutrals as shown in Figures 4.13a and 4.14. Around  $t = 1.0$  to  $1.2$  ns, a large number of ions are rapidly created by ionization of the gas (Figure 4.12b), creating the plasma sheath which greatly increases the surface field in a region around the initial emitter. As a result of this, the electron emission current and neutral evaporation increases rapidly, and ion bombardment of the cathode (Figure 4.15) becomes strong. The plasma then grows rapidly (Figure 4.17) until  $I_{\text{circ}}$  has reached the maximum current that can be supported by the circuit (Figure 4.11),  $U/R$ . Note that the gap current, which is also drawing on the charge stored on the gap capacitance, can overshoot the circuit current for a brief moment until the charge on the gap capacitance is depleted.

The simulation results are in good agreement with experimental data reported in literature. Especially, the current density under the arc of  $1.0 \text{ A}/\mu\text{m}^2$  (Figure 4.18) and plasma density of  $\approx 10^{20} \text{ cm}^{-3}$  (Figure 4.13) are the same as reported in [138]. Furthermore, the expansion velocity of  $2.3 \text{ km/s}$  (Figure 4.17) is slightly lower but in the order of magnitude as the measurement reported in the same paper. Also seen was a plasma sheath voltage of  $10\text{--}100 \text{ V}$  (Figure 4.16), which is in the expected range. Finally, the time scale and shape of the current- and voltage curves are similar to those typically seen in the CERN DC spark

#### 4. Simulation of vacuum arcs



(a) Flow of charged particles through the cathode surface.



(b) Sources and sinks of neutrals.

Figure 4.12.: Injected and removed particles from different processes as a function of time. All plots are smoothed over a  $1000 \Delta t = 0.886$  ps time window using a boxcar smoother.

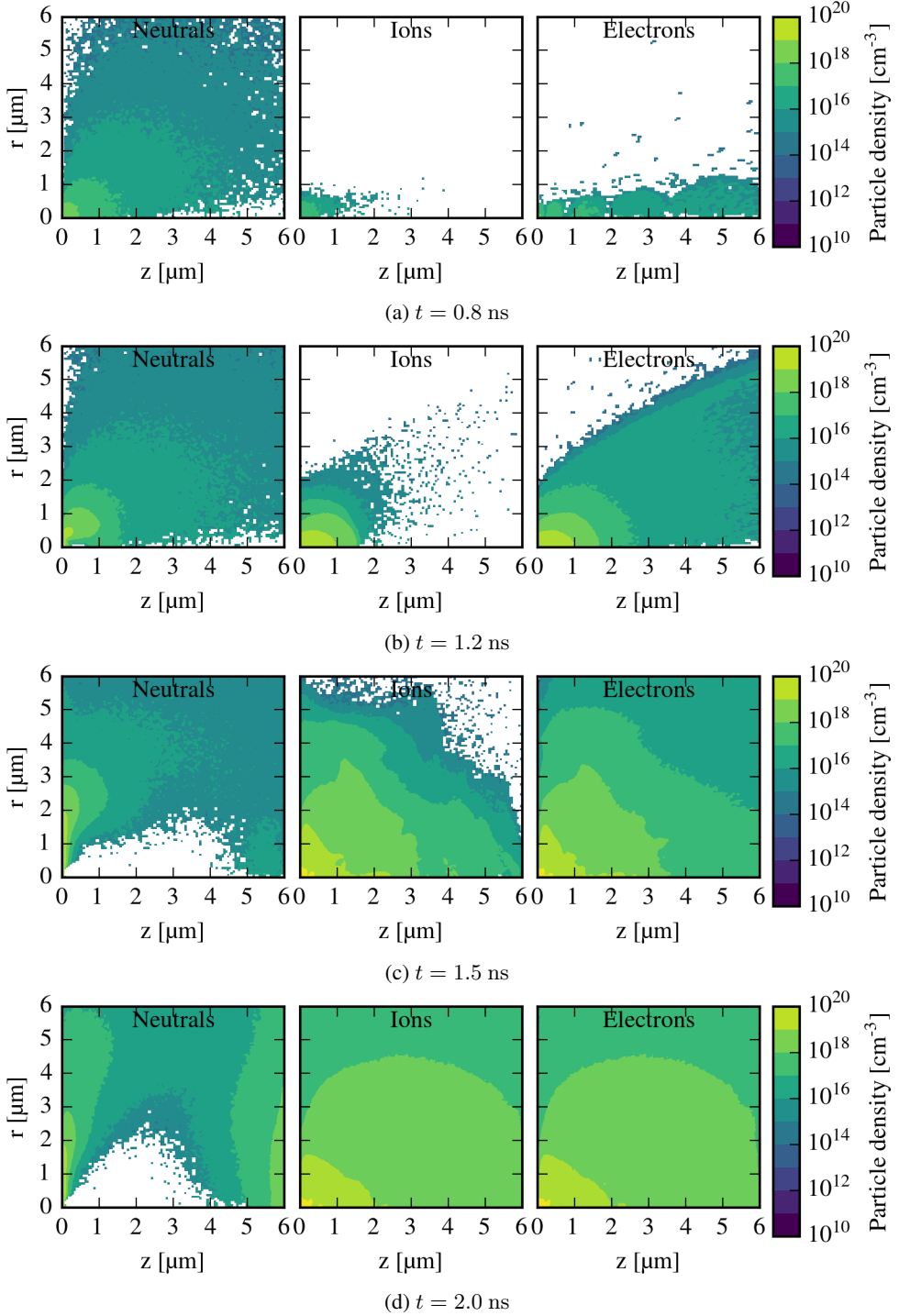


Figure 4.13.: Density plots (zoom on central region) for copper, copper ions, and electrons for the simulation described in Section 4.3.

#### 4. Simulation of vacuum arcs

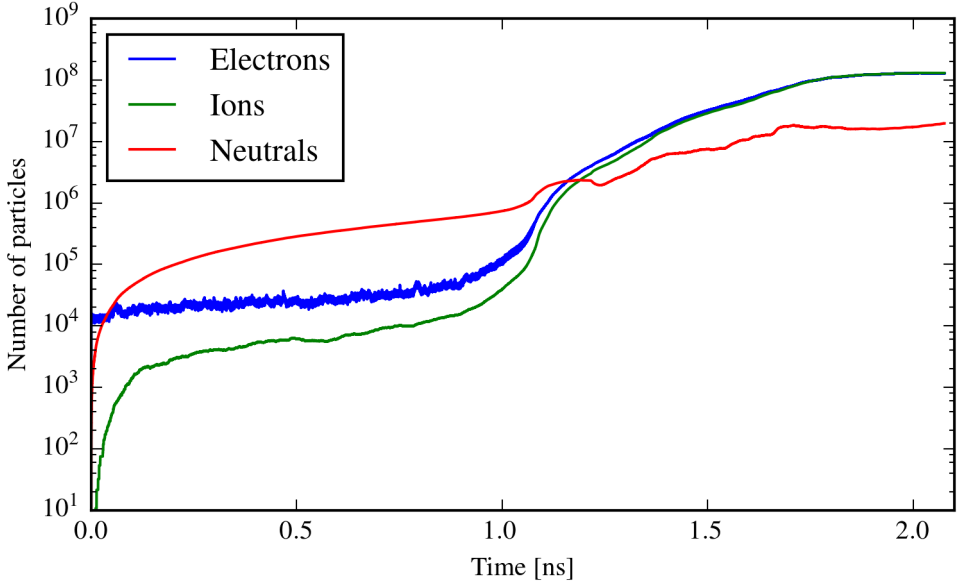
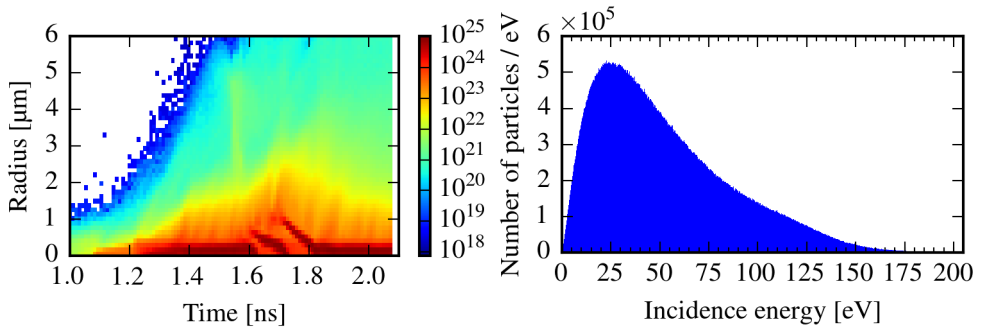


Figure 4.14.: Particle populations as a function of time. Data from the simulation described in Section 4.3.



(a) Flux density [ions/s/cm<sup>2</sup>] as a function of time and  $r$ . (b) Energy spectrum integrated over total simulation time.

Figure 4.15.: Statistics for ions arriving on the cathode surface, from the simulation described in Section 4.3.

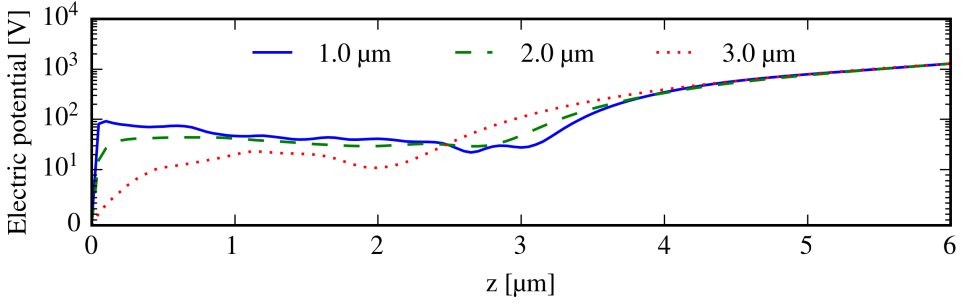


Figure 4.16.: The electric potential as a function of  $z$  at three different values of  $r$  at  $t = 1.5$  ns. Note the semi-logarithmic scale on the y-axis, which is linear from 0 to 10 V, then logarithmic above 10 V. Data from the simulation described in Section 4.3.

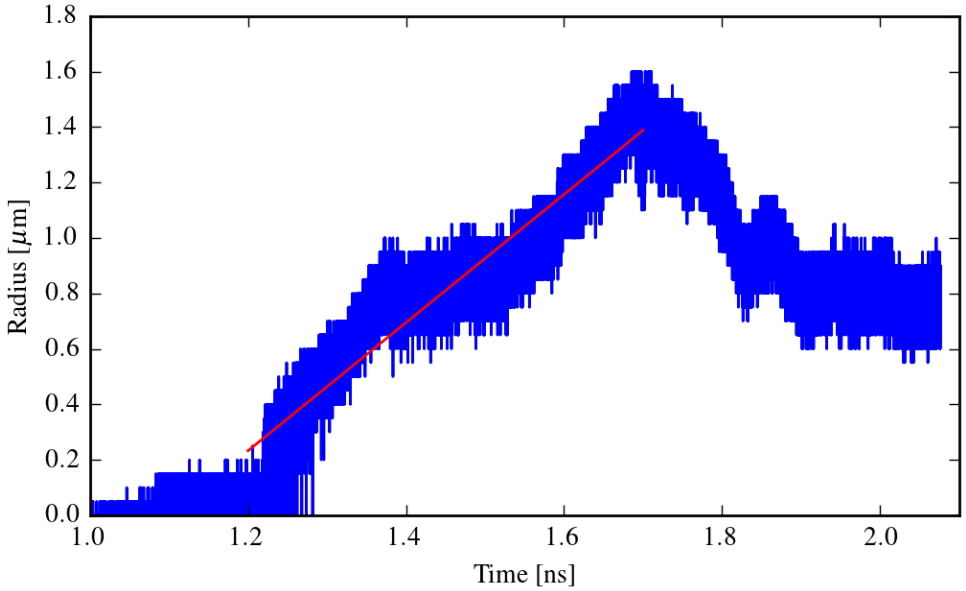


Figure 4.17.: Arc radius (measured as the radius  $r_{\text{enhanced}}$  affected by the high-flux sputtering) as a function of time. Fit in range  $t \in [1.2, 1.7]$  ns:  $r(t) = 2.3 \text{ km/s} * t - 2.5 \text{ } \mu\text{m}$ . Data from the simulation described in Section 4.3.

#### 4. Simulation of vacuum arcs

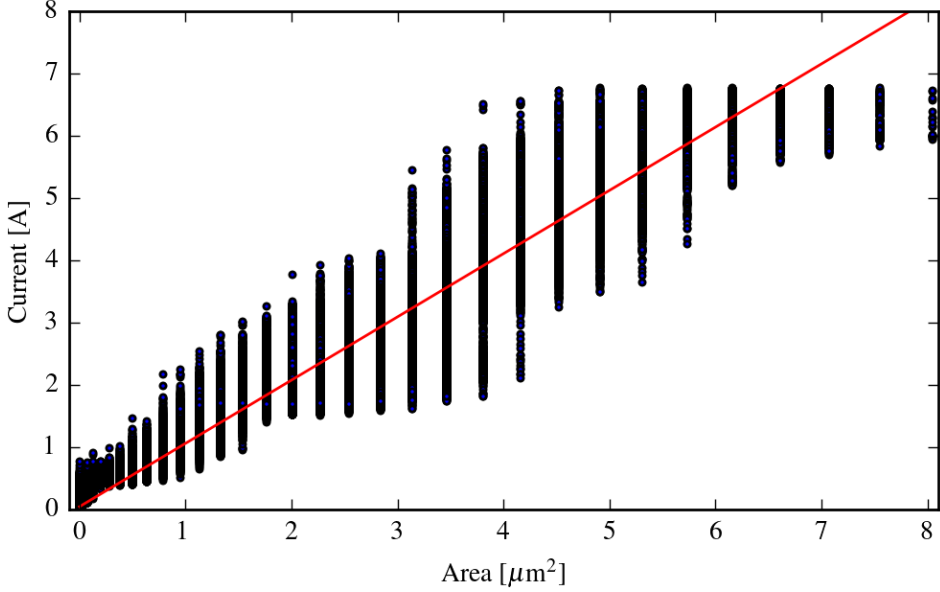


Figure 4.18.: Current as a function of area of the arc. The area covered by the arc is calculated from the radius  $r_{\text{enhanced}}$  affected by the enhanced emission. The fit gives the current density as  $1.0 \text{ A}/\mu\text{m}^2$ . Data from the simulation described in Section 4.3. Visible discretization of x-value due to the  $r_{\text{enhanced}}$  being measured as a multiple of  $\Delta r$ .

experiment, and much of the remaining differences can be explained by differences between the experimental and simulated circuit [112].

The ion bombardment flux of  $10^{23}$ – $10^{25}$  ions/cm<sup>2</sup>/s (Figure 4.15a) is in the same range as found by an earlier 1D version of the code [80], and the impact energy (Figure 4.15b) of  $\approx 25$  eV indicates that it is accelerated over plasma sheath potential.

When measuring the size of the arc’s footprint as in Figure 4.17 and 4.18, the radius  $r_{\text{enhanced}}$  (defined in Section 4.2.7) was used rather than the field. This was done because this radius was a much less noisy measure than the point where the field dropped below some threshold value. However, the two different measures were generally in good agreement. Furthermore, while the surface field was quite noisy near  $r = 0$  (as discussed in Section 4.2.4), further out it was much more smooth both in time and space.

It is also interesting to observe how the neutral emission from the evaporation and hi-flux sputtering are strongly correlated in time (Figure 4.12b). This is likely due to that the area which sees a strong surface field is the same as the area which sees a heavy bombardment. Further, evaporation from the high-field area is proportional to the field emission current, and the field emission current density is mostly constant.

### 4.3.1. Effects of varying the model parameters

In addition to the run discussed above, several others were ran with slightly changed parameters.

In one experiment, the sputtering threshold  $j_{\text{enhanced}}$  were changed to  $10^{24}$  and  $10^{26}$  while keeping the other parameters as listed in Table 4.1. With this heightened threshold, the rapid growth of the arc never started, and it kept being a small, low-current cathode spot since the bombardment intensity was now below the threshold of the enhanced sputtering. With the lowered threshold, the development was similar to the usual case. In a similar experiment, the enhanced sputtering yield  $Y_{\text{enhanced}}$  was set to 0 or 2. This resulted in similar effects as changing the threshold – with  $Y_{\text{enhanced}} = 0$  the enhanced sputtering was disabled, so again the rapid growth never happened. When the enhanced sputtering yield was increased to 2, the development of the current and voltage was again similar to what was seen with nominal parameters. In yet another simulation, the value of  $\beta_{\text{flat}}$  was reduced from 2.0 to 1.0. While this simulation was ran for a relatively short time, it showed the beginning of a development which was very similar to the nominal case, including the transition into a growing arc where the electron emission is dominated by the flat surface.

In addition to changing the parameters of the surface physics model, the gap capacitance  $C_{\text{gap}}$  and the resistance  $R$  were also varied. Further, some simulations were ran with a changed initial voltage (870 V or 5700 V). For these simulations, the time  $t_{90\%/10\%}$  for the voltage to drop from 90% to 10% of the starting value was observed, as was the peak gap current  $\hat{I}_{\text{gap}}$ . A weak dependence was seen for the time  $t_{90\%/10\%}$  on  $C_{\text{gap}}$ , where a larger capacitance allowed the arc to develop for longer before needing to draw on the external supply. Similarly, reducing the resistance in the current path from the external supply allowed a longer growth phase, as the maximum sustainable current and the amount of charges which can be delivered from the supply (and thus not from the gap capacitance) is larger.

## 4.4. Discussion, conclusions, and outlook

The presented model generally agrees with the features and timescales expected from the initiation of a vacuum arc. It successfully describes the expansion of an arc, starting from a tiny cathode spot and growing into a much larger, multi-Ampere discharge. This is done with a model composed of a variety of processes known to occur in such arcs.

An interesting feature is the relative insensitivity of the arc development to the surface model parameters, as shown in Section 4.3.1. When changing the circuit parameters, the arc responded in a way that is in agreement with what has been seen experimentally.

While significant uncertainties surround the enhanced high-flux sputtering model, it is clear that a process similar to that described in this paper is necessary for the arc to develop. This is due to the energy-dependent single-particle sputtering process having an average yield much less than one for the ion energies most commonly seen. Such a process is likely to be present, as the area under the arc receives a significant flow of energy from the ion bombardment. “Heat-spike” type models are not appropriate for this, as they assume much larger impactor energies [80].

The 2D ArcPIC code includes some elements not commonly seen in plasma codes, such as calculation of the current using the Schockley-Ramo theorem, which is more commonly used in semiconductor device simulation [139]. Another way of taking this effect into account would be to use a full EM field solver and including at least the spark gap’s connection to the

#### 4. *Simulation of vacuum arcs*

circuit in the simulation domain, however by using the SR theorem we were able to avoid this.

As the simulation time progresses, the presented model becomes less accurate, as it does not include effects like recombination, further species and higher charge states, surface modification, droplets, or the full external circuit. Another limitation is the 2D nature of the code – for longer time periods it may be interesting to study the interaction of multiple emitter spots in close proximity. For this, a large increase in the computing power and techniques is necessary, however this could likely be achieved with advanced computing techniques such as implemented in Aleph [140]. So while the model presented in this chapter is a good starting point for modeling vacuum arc discharges, there is still room for large improvement both on the surface physics and on the computational side.

In addition to what is mentioned above, some ideas for code improvements are listed in [31, Chapter 4], discussing for example dynamic particle weighting. One technical limitation that was not listed there but could be improved is the field solver; changing the current implicit scheme for an iterative one may make it possible to increase the system size and make better use of parallel computing resources. On the physics side, one may want to look into keeping track of the temperature distribution in the cathode. This could include both the temperature in the surface and bulk, and also of the initial field emitter. While this emitter is not directly resolved by the simulation grid, its temperature could be kept track by the surface physics model. Tracking the temperature is motivated by that it may affect both the evaporation that supplies the initial gas, and also the field emission from the tip [123]. In a similar direction, it may also be interesting to study the effect of a changed work function, which may occur due to add-atoms and other rough surface features [141]. Such features may make strong electron emission possible without requiring very sharp surface features. In the field emission model presented in Section 4.1.2, the effect of a changed work function would be a change in the parameters  $\kappa_1$  and  $\kappa_2$  used in the approximation for the field emission. One way to implement a temperature- and work-function dependency may be to couple to the new field emission model presented in [142], which also takes into account how the tunneling probability is affected by the local surface geometry around the tip.



## 5. Cell geometry optimization

In order to maximize the gradient capability of the accelerating structure designs for CLIC, the geometry of the accelerating cells for these traveling wave structures must be optimized. This is done for several typical iris apertures  $a$  and thicknesses  $d$ , producing a database of optimized cells. These cells are used by the structure parameter estimation method that will be presented in Chapter 7 for quickly calculating the parameters of a structure with the specified apertures, tapering, length etc.

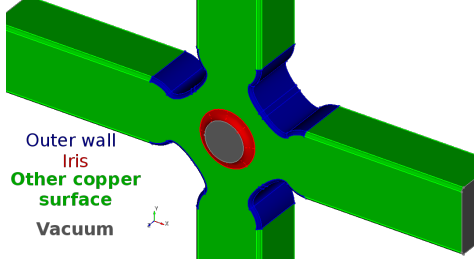
This chapter first describes the basic cell geometry (Section 5.1), the method used for optimizing this geometry (Section 5.2), and the goal functions used for the optimization (Section 5.3). Then the underlying tools such as the algorithm for extraction of peak fields (Section 5.4) and the AcdOptiGUI software (Section 5.5) are presented. Finally, results for a typical optimized accelerating cell are presented in Section 5.6, and the complete cell database in Section 5.7.

### 5.1. Cell geometry

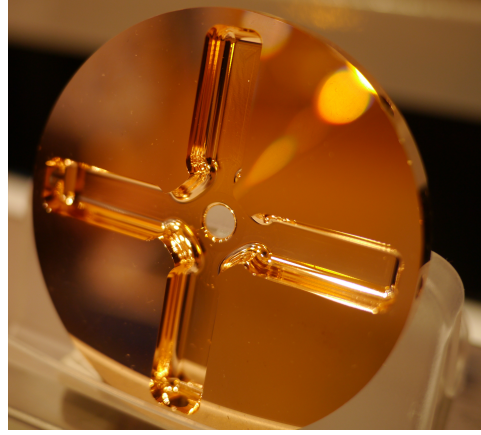
The geometry of the vacuum volume in a single accelerating cell is shown in Figure 5.1a. This volume is created by removing material through turning and milling of a copper disk (Figure 5.1b) and then stacking and brazing such disks in order to form an accelerating structure (Figure 1.4) [18, 143]. This geometry consists of a central volume which traps the accelerating mode, and four narrow waveguides allowing higher frequency modes excited by the beam (Chapter 6) to radiate out of the central volume. The design avoids radiation of the fundamental mode, as its frequency is below the cutoff frequency of the four damping waveguides. As was discussed in Section 2.3, the periodic loading of the irises forces the field to be periodic, causing it to form space harmonics. The structure can then be tuned such that the phase velocity of the principle wave is synchronized with the electrons which should be accelerated.

When optimizing the cells for high gradient, the topic of this chapter, the geometry is varied. This is possible by parameterizing the geometry of the cells, as shown in Figure 5.2. Here, the length of the cell (and also the period of the accelerating structure)  $h$  is determined by the frequency and phase advance per cell, such that the phase velocity of the first space harmonic matches the speed of the particles (Section 2.3). The iris aperture  $a$  and thickness  $d$  is also fixed at the beginning of the cell optimization. These are commonly listed as the normalized values  $a/\lambda$  and  $d/h$ , where  $\lambda = c/f$  is the free space wavelength of the accelerating mode. Other fixed parameters are the width of the damping waveguide  $adw$ , the aperture of the damping waveguide entrance  $idw$ , and the round-off  $rr$ . This round-off is due to the radius of the milling tool used to carve the outer part of the cavity from the blank disk. The length of the damping waveguide  $ldw$  is not important for the simulation of the main mode, as long the waveguide length is long enough for the main mode's below-cutoff wave to decay to an insignificant level before reaching the end of the waveguide.

## 5. Cell geometry optimization



(a) Vacuum volume of an accelerating cell. Annotations indicate where the cavity is open, and a copper surface is present. Of the copper surface, the “iris” and “outer wall” regions are specially marked.



(b) An accelerating cell disk, photographed at the VDL stand at IPAC'12, New Orleans.

Figure 5.1.: The geometry of a single accelerating cell.

The varied parameters for the iris are the ellipticity  $e = ae/be$  and the fraction of the iris thickness  $sFrac = s/d$  which is flat-tipped. For the outer wall, the varied parameters are the length of the flat part  $2 \cdot c$  and the ellipticity  $eow = ac/bc$ . Also varied is the cell radius  $b$ . Together, the fixed and varied parameters define the geometry of the cell. However, in order to construct a cell in a 3D modeling program such as CUBIT, the helper variables  $ae$ ,  $be$ ,  $ac$ ,  $bc$ ,  $rdw$  and  $ldw'$  are also needed.

For the iris, one of the ellipse half-axis are found by the relation  $d = 2 \cdot be + s$  such that  $be = (d - s) / 2$ . The other half-axis is then  $ae = e \cdot be$ .

For the outer wall, a relation between  $ac$  and  $idw'$  can be found by considering the isosceles right triangle with sides  $ac + c$  and  $b + bc - idw' / \sqrt{2}$ . These sides being equally long leads to the relation

$$b + bc - \frac{idw'}{\sqrt{2}} = ac + c = eow \cdot bc + c, \quad (5.1)$$

which relates  $bc$  to the known geometrical parameters  $b$  and  $c$ , and also  $idw'$ . The auxiliary parameter  $idw'$  must then also related to the other, known, parameters. This can be done through the equation

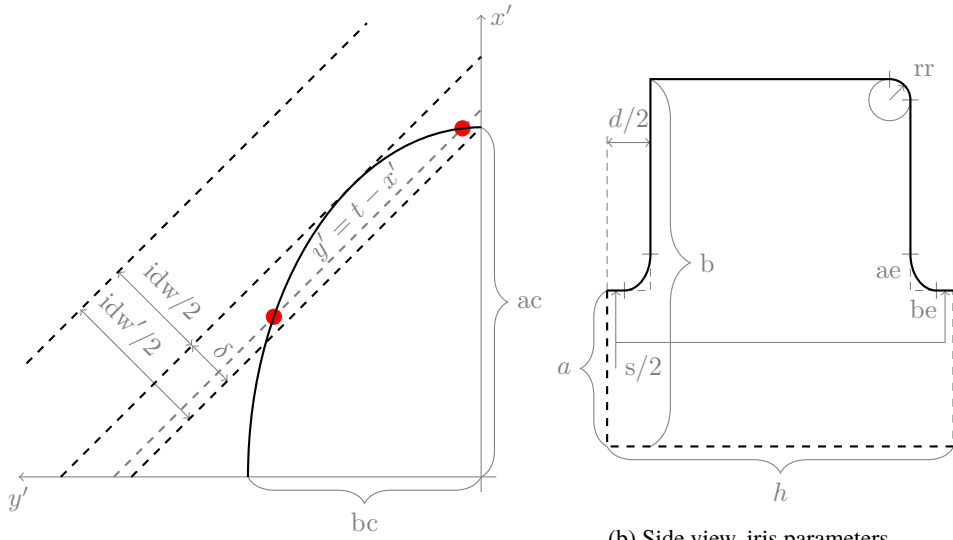
$$\frac{idw'}{2} = \frac{idw}{2} + \delta, \quad (5.2)$$

where  $\delta$  is the offset between the line which is tangent to the ellipse and parallel to the damping waveguide center line, and the line which goes through the point separating the  $(ac, bc)$ -ellipse and the  $45^\circ$  circle segment with radius  $rdw$ . In the coordinate system of Figure 5.2a, the  $(ac, bc)$ -ellipse is given as

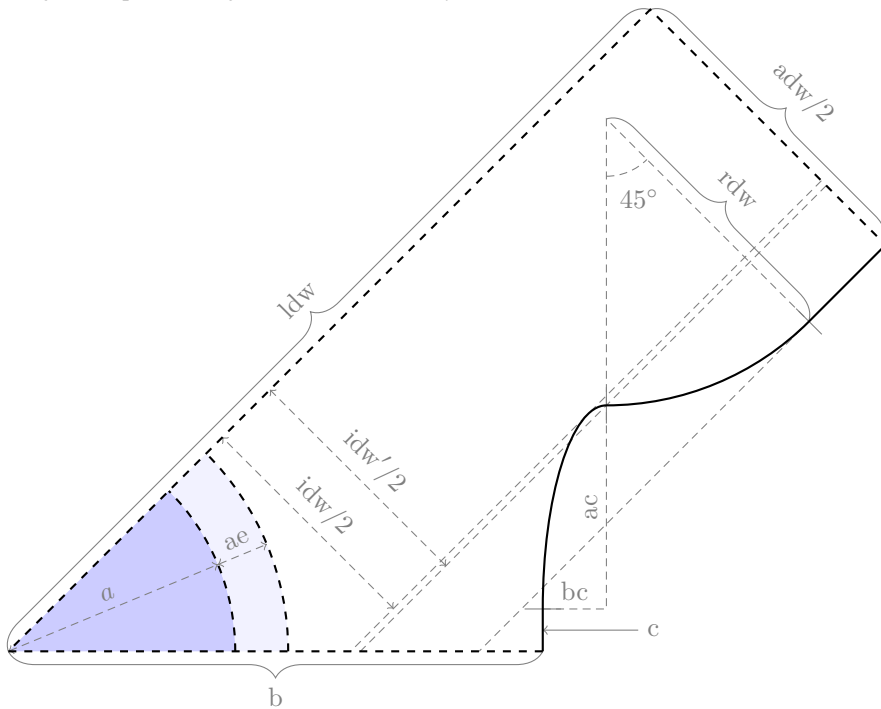
$$\frac{y'^2}{bc^2} + \frac{x'^2}{ac^2} = 1 \quad (5.3)$$

and the  $idw'/2$  line as

$$y' = ac - x'. \quad (5.4)$$



(a) Helper figure for outer wall. Some parameters changed compared to Figure 5.2c for readability.



(c) End view, outer wall parameters.

Figure 5.2.: Definition of the geometry parameters used for the traveling wave waveguide damped cell geometry.

## 5. Cell geometry optimization

Defining a line  $y' = t - x$  which intersects the ellipse, the intersections between this line and the ellipse can be found by inserting this expression into Equation (5.3). The values of  $x'$  at the intersections are then found as

$$x' = \frac{t}{1 + \left(\frac{bc}{ac}\right)^2} \pm \frac{\sqrt{4t^2 - 4\left(1 + \left(\frac{bc}{ac}\right)^2\right)(t^2 - bc^2)}}{2\left(1 + \left(\frac{bc}{ac}\right)^2\right)}, \quad (5.5)$$

and if the square root on the right hand side is zero, then this equation has only one solution, corresponding to the tangent idw/2 line. This occurs at

$$t^2 = ac^2 + bc^2, \quad (5.6)$$

and the idw/2 line is thus given as

$$y' = t - x = \sqrt{ac^2 + bc^2} - x'. \quad (5.7)$$

From this it can be shown that

$$\delta = \cos(45^\circ)(t - ac) = \frac{ac}{\sqrt{2}} \left( \sqrt{1 - \left(\frac{bc}{ac}\right)^2} - 1 \right), \quad (5.8)$$

which when inserted into Equation (5.1) yields the wanted relation

$$bc = \frac{b - c - \frac{idw'}{\sqrt{2}}}{\sqrt{eow^2 + 1} - 1}. \quad (5.9)$$

The other half axis is then found as  $ac = bc \cdot eow$ .

The radius rdw can similarly be found by the examination of the line marked with a brace and rdw in Figure 5.2c. This yields the equation

$$rdw \cdot \cos(45^\circ) = rdw - \frac{adw - idw'}{2}, \quad (5.10)$$

which after using Equation (5.1) to remove idw' yields

$$rdw = \frac{1}{\sqrt{2} - 1} \left( \frac{adw}{\sqrt{2}} - b + c - bc + ac \right). \quad (5.11)$$

When running the eigenmode solver to find the RF parameters (Section 2.4.3), the boundary conditions must be specified. The copper surface (marked green, red, and blue in Figure 5.1a) are assigned to surface  $\Gamma_x$ , which is represented by a perfect conductor boundary condition in the finite element simulation. A value for the conductivity is also assigned to  $\Gamma_x$ , and is used in the post-processing for calculating the Q-factor. The ends of the damping waveguides are also included in  $\Gamma_x$ , as they are long enough for the field to decay to almost zero. The beam apertures uses periodic boundary conditions, as was explained in Section 2.4.2. Finally, perfect magnetic conductor boundary conditions are applied to mirror symmetry planes in order to reduce the size of the numerical problem to be solved, as seen in Figure 2.5.

## 5.2. Optimization algorithm

The objective of the cell geometry optimization is to maximize the accelerating gradient which can be obtained in the cell, and the pulse length for which this gradient can be maintained at a given break down rate. The gradient and pulse length are limited by the peak surface fields, as was discussed in Chapter 3. These peak fields are therefore minimized by variation of the geometry parameters (Section 5.1), and finally the cells are tuned for the correct frequency at the chosen phase advance.

The general procedure for geometry optimization is to first optimize the iris by varying the geometry parameters  $sFrac$  and  $e$ , and then optimize the outer wall by varying  $eow$  and  $c$ . This produces two mostly independent two-parameter optimization problems, which are solved by scanning the geometry parameters so that the dependency of the variables of interest as a function of the geometry parameters can be mapped out. This scanning is done iteratively by first scanning some area of the parameter space, and then manually picking a new area based on the accumulated results from earlier calculations. These areas may be both inside and/or outside of previously selected areas.

In order to compare the variables of interest between different geometry parameter points, all points taken into consideration are tuned to the target frequency  $f_0 = 11.9942$  GHz by variation of the cell radius  $b$ . When tuning, the accepted margin was either  $f_0 \pm 0.2$  MHz or a range of 11.993–11.995 GHz. This variation is either done within a single geometry point using linear 1D fit tuning (Section 5.2.1), or by predicting the cell radius of new parameter point(s) using 2D surface fit tuning (Section 5.2.2). A combination of the two methods were also often used. This tuning is the main source of coupling between the iris and outer wall optimization, as the correctly tuned cell radius may change by up to 1.5 mm during iris parameter variation. This causes the optimum outer wall geometry to change significantly, as seen for the cells for which there exist two different iris optimization points (cell database version 1 and 2 [23]). For this reason the outer wall is optimized after the iris is considered to be finished.

The selection of new areas in parameter space is continued until adding more data points yields little more information about the location of the optimum. This happens when the noise in the variables of interest are on the order of the real change in the variable itself due to the small change of geometry parameters. In cases where the optimum is close in geometry parameter space to an “edge”, a point is selected which is close to the optimum, but slightly away from the edge. An *edge* in parameter space is the border between two regions, in which the gradient of the variable of interest is very different and changes very rapidly when transitioning between two regions of parameter space. This is most commonly seen for the peak magnetic field as function of  $(eow, c)$ , as shown in Figure 5.11c and will be discussed in Section 5.4.1.

## 5. Cell geometry optimization

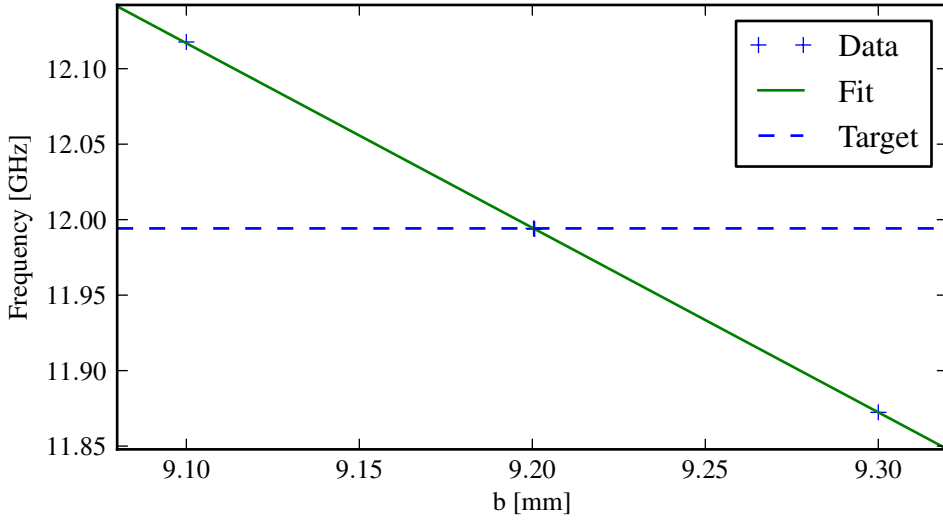


Figure 5.3.: A straight line fitted to  $(b, f)$  data points for 1D fit tuning, in order to predict the correctly tuned  $b$ .

### 5.2.1. 1D fit frequency tuning

This method works inside a single parameter point by fitting the frequency  $f$  as a function of the cell radius  $b$  for otherwise identical geometry parameters. The starting point is two or more cells with different values of  $b$ . The radius  $b$  is then fitted as a linear function of the frequency, and this fit is then used to predict the correct  $b$  for the target frequency  $f_0$ , as illustrated in Figure 5.3. Linear 1D fit tuning works best when the initial guesses for  $b$  are close to correct. If one or more of the initial guesses for  $b$  produced a frequency far away from  $f_0$ , it is usually beneficial to remove them from the fit when more accurate points become available.

### 5.2.2. 2D surface fit frequency tuning

This method is used when creating new parameter points, and predicts the correct radius  $b$  for the new parameter points based on data from the old points. It works by selecting calculations that fall within a narrow frequency range, and then fitting the radius  $b$  as a function of two scan parameters such as  $e_{ow}$  and  $c$  or  $sFrac$  and  $e$ . The resulting quadratic surface is then used to predict the correctly tuned radius  $b$  when creating new scan points. This is illustrated in Figure 5.4. The accuracy of the predictions made by this method depends on how well tuned the fitted points are, and it tends to work better over small ranges and when interpolating, than over larger ranges or when extrapolating.

In cases where the estimated radius corresponds to a frequency outside of the chosen tolerance, it can still provide a very good starting point for 1D fit tuning. The typical usage is then to add one more point which goes in the wanted direction, i.e. a point with a few  $\mu m$  smaller radius if the frequency is too low, and opposite for too high frequencies. The original and the added points are then used to predict the correct radius via a 1D tune fit.

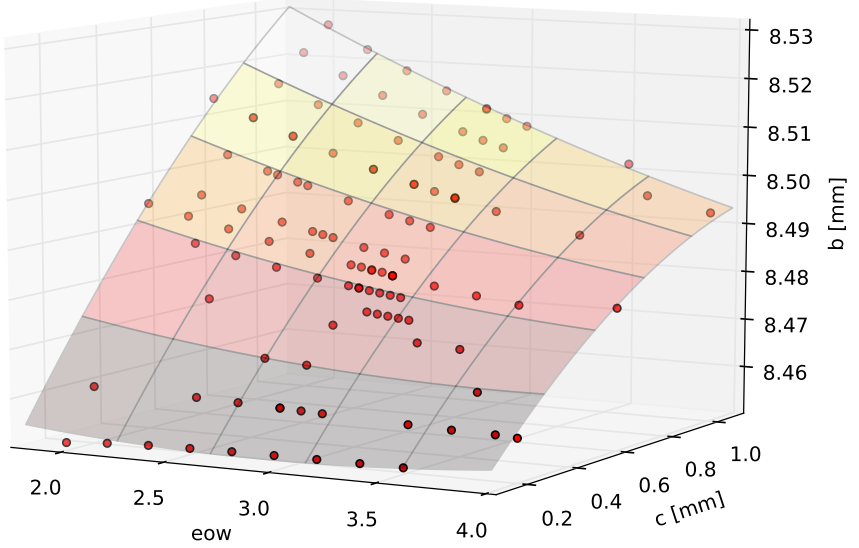


Figure 5.4.: A quadratic surface fitted to  $(eow, c, b)$  data points for 2D surface fit tuning, in order to predict the correct  $b$  as function of (in this case)  $eow$  and  $c$  when creating new  $(eow, c)$  points.

### 5.3. Optimization goals

As was discussed in Section 5.2, the parameter space is searched for an optimal cell geometry. The criterion used to find the optimum geometry parameters for the iris ( $sFrac, e$ ) will be defined in Section 5.3.1, and the criterion for the outer wall geometry parameters ( $eow, c$ ) will be defined in 5.3.2. This variation of parameters is done while maintaining the frequency of the cavity within certain tolerances. The criteria are based on the peak surface field limits which were discussed in Chapter 3.

#### 5.3.1. Minimizing the break down rate

The geometry of the iris affects the achievable gradient and pulse length by determining how the peak surface electric field  $\hat{E}$ , the peak modified Poynting vector  $\hat{S}_c$  and the power flow by circumference  $P_+/C$  scale with the accelerating gradient  $G$ . These peak limiting factors are given as  $\hat{E} = \bar{E}G$ ,  $\hat{S}_c = \bar{S}_c G^2$  and  $P_+/C = \frac{v_g G^2}{C\omega R'/Q}$ , where  $\bar{E}$ ,  $\bar{S}_c$ ,  $v_g$ ,  $R'$  and  $Q$  can be extracted from the calculated field pattern (Section 2.4.3 and 5.4). As discussed in Section 3.3.1, increasing any of these limiting factors increases the breakdown probability, and they should thus all be minimized. However, each of the three different quantities to minimize often favor significantly different geometries. One example of this

## 5. Cell geometry optimization

is seen in Figure 5.11a and 5.11b, where the minimum electric field is found at  $e = 1.2$ , and the minimum modified Poynting vector at  $e = 1.3$ , both with  $sFrac \approx 0$ . Note that the difference in  $(sFrac, e)$  is often much larger than what is seen for this cell.

A different approach is to use the predicted maximum accelerating gradient at standard conditions  $\hat{G}$  (Equation (3.35)). In this formalism, the predicted gradients  $\hat{G}_E$ ,  $\hat{G}_{S_c}$  and  $\hat{G}_{P/C}$  provides a very convenient way of directly comparing the importance of the three limiting factors. Maximizing  $\hat{G}$  is therefore the goal when picking the optimum values for  $(sFrac, e)$ .

### 5.3.2. Minimizing pulsed surface heating

As was discussed in Section 3.4, the surface magnetic field causes pulsed surface heating, which over time degrades the surface of the structure through material fatigue. It is therefore necessary to minimize this heating without sacrificing the accelerating gradient. This can be done by minimizing the normalized peak surface magnetic field  $\bar{H} = \hat{H}/G$ , as  $\Delta T \propto \bar{H}^2$  (Equation (3.38)). As  $\hat{H}$  is mainly determined by the outer wall geometry, minimizing  $\hat{H}$  is the goal when picking the optimum values for  $(eow, c)$ .

## 5.4. Peak field extraction

When optimizing the outer wall and iris, the primary goal is to minimize the normalized peak surface magnetic field  $\bar{H}$  on the outer wall, and to maximize predicted maximum gradient  $\hat{G}$  for the iris. In order to this, a reliable and accurate way of extracting  $\bar{E}$ ,  $\bar{S}_c$  and  $\bar{H}$  from the calculated field patterns is needed.

As the finite element field calculations with moderate mesh sizes often have a few overestimated points, the global maximum of the surface fields is very often overestimated, especially if the geometry contains sharp curves in high-field regions. This results in not finding the true optimum geometry for the cell [23, Section 2.6]. The other RF parameters that were discussed in Section 2.4.3 are defined by integrals, and are therefore much more robust to noise in the calculated field patterns.

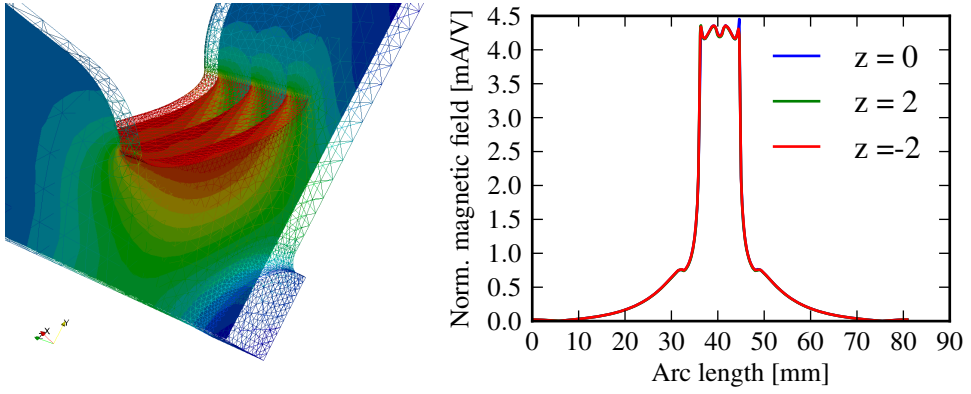
A method which reduces this problem is to define a plane which intersects the surface, and extract the field along the intersection curve. As long as the correct cut plane position is chosen and the extracted field profile is not strongly dependent on the exact position of the cut plane, this method reduces the chance of hitting a highly overestimated point, and thus produces more accurate estimates [23, Section 2.6].

### 5.4.1. Outer wall

For the magnetic field, a plane normal to the  $z$ -axis was chosen, as shown in Figure 5.5. The plane was positioned exactly in the middle of the cell ( $z = 0$  mm). However, as demonstrated by the data in the Figure 5.5b, the estimated peak field is quite insensitive to the precise positioning of the plane.

From plots of the peak surface magnetic field as a function of  $eow$  and  $c$ , such as shown in Figure 5.11c, it is clear that the peak magnetic field increases slowly when decreasing  $eow$  and  $c$  relative to the optimum location (i.e. towards the lower left corner of the plot), and increases rapidly when  $eow$  and  $c$  is increased (towards upper right corner). When plotting





(a) Field map for on planes intersecting the volume (plotted as surfaces) and on the cell surface (plotted as mesh). (b) Field as a function of the position along the three intersection curves. The  $z$ -positions are in units of mm.

Figure 5.5.: Surface magnetic field on three curves described by intersections of the outer wall with planes. Data from the cell described in Section 5.6.

the surface magnetic field on intersection curves, such as shown in Figure 5.5b, there are two sets of peaks visible – the sharp peaks at the edge of the distribution (approximately at arc length 35 and 45 mm), and the rounder peaks near the center of the distribution (at approximately 40 mm arc length). In the case of larger than optimum  $eow$  or  $c$ , the height of the sharp peaks at the edges of the distribution (at the entrance to the damping wave guides) increase very rapidly. Similarly, for smaller than optimum  $eow$  or  $c$ , the central peaks (near the flat part of the outer walls) grow slowly, while the sharp peaks at the edges disappear. For the optimum geometry, the two sets of peaks tend to be roughly the same height.

#### 5.4.2. Iris

For the electric field and the modified Poynting vector, three cut planes are used, all parallel to the beam axis and with normal vectors  $\vec{n}_x = \hat{x}$ ,  $\vec{n}_y = \hat{y}$  and  $\vec{n}_{45^\circ} = (\hat{x} - \hat{y}) / \sqrt{2}$ . These cut planes are shown in Figures 5.6 and 5.7. For the electric field, the cut planes with normal vectors  $\vec{n}_x$  and  $\vec{n}_y$  often reach slightly higher peak values than the cut plane with normal vector  $\vec{n}_{45^\circ}$ . For the modified Poynting vector, the intersection curve of the  $\vec{n}_{45^\circ}$  cut plane has a clearly higher peak, as the presence of the outer wall makes the magnetic field penetrate deeper into the cell.

### 5.5. The AcdOptiGUI optimization tool

In order to do a detailed optimization and tuning of an accelerating cell, a large number of simulation must be run before arriving at the final geometry. As an example, the cell databases presented in Chapter 5.7 required in total just over 14'000 separate Omega3P [22, 75] simulations. While each of these simulations are relatively small, usually running within a single node of the HPC cluster, the sheer number of them makes correctly setting up and running all the simulations a very large, tedious and potentially error-prone task. The tool

## 5. Cell geometry optimization

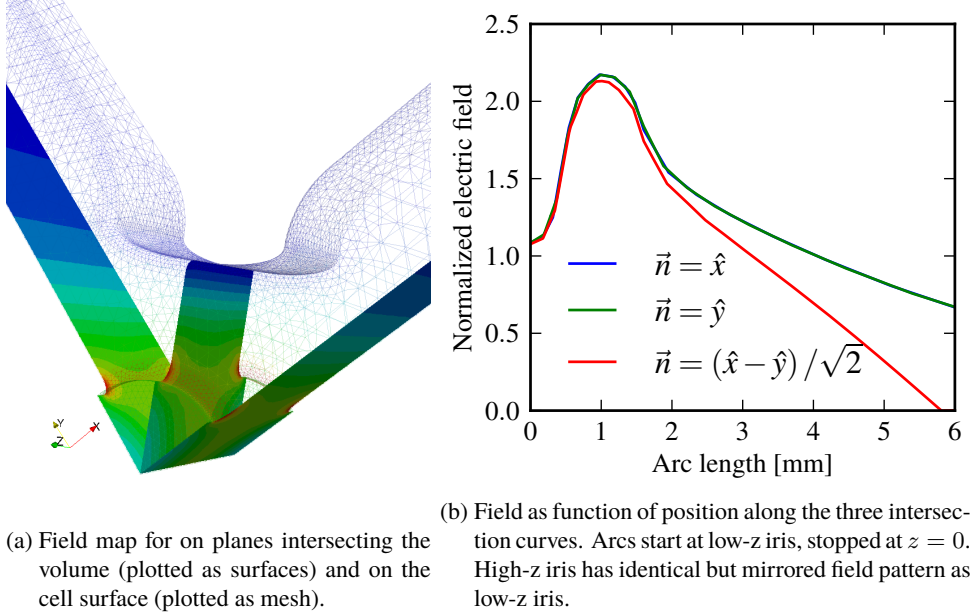


Figure 5.6.: Normalized electric field  $\bar{E}$  on three curves described by the intersection of the outer wall with planes through origo and normal vectors  $\hat{x}$ ,  $\hat{y}$ , and  $(\hat{x} - \hat{y}) / \sqrt{2}$ . Data from the cell described in Section 5.6.

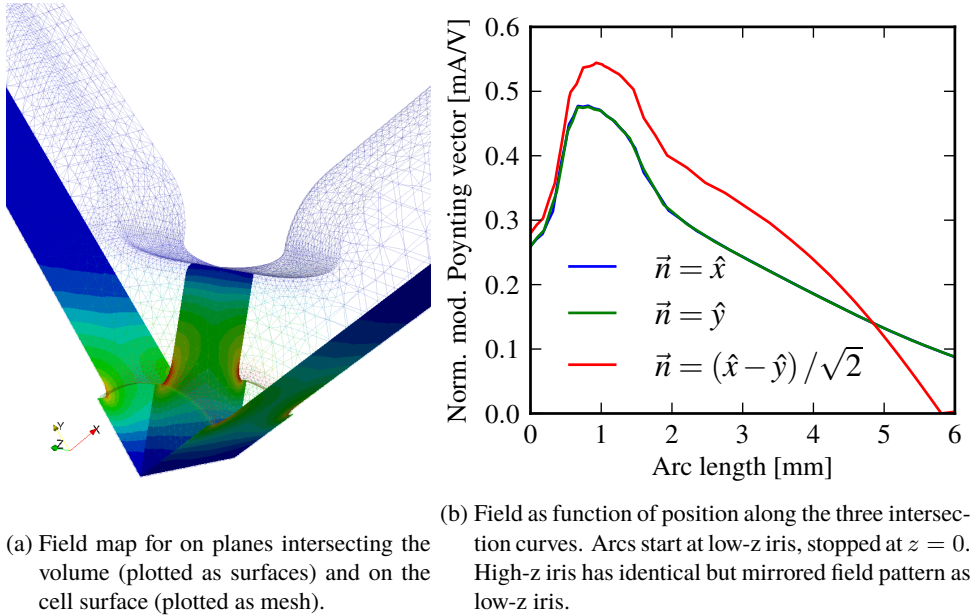


Figure 5.7.: Normalized modified Poynting vector  $\bar{S}_c$  on three curves described by the intersection of the outer wall with planes through origo and normal vectors  $\hat{x}$ ,  $\hat{y}$ , and  $(\hat{x} - \hat{y}) / \sqrt{2}$ . Data from the cell described in Section 5.6.

AcOptiGUI, which is described in detail in [23, 29], was therefore developed to handle this automatically, as well as systematically handling and presenting the resulting output data.

AcOptiGui is a graphical program written in the Python programming language, using PyGTK [144] and Matplotlib [145] for the user interface. Some screenshots of the user interface are shown in Figure 5.8. It sits on top of the library AcOpti, which manages the simulation input- and output data and communication with the remote facility. Access to the data and operations on it are provided through an object-oriented API. AcOpti and AcOptiGUI is available in source-code form from <https://github.com/kyrsjo/AcOpti> under the GNU GPL version 3 license [146].

In general, the use of AcOptiGUI follows the optimization algorithm outlined in Section 5.2 closely. The data structure in AcOpti is centered around a “project”, which represents one type of accelerator cell. For the cell database presented in Section 5.7, the optimization for each iris aperture/thickness combination is done in one such project. The cornerstone of a project is a parametric description of the cell geometry, such as shown in Figure 5.2. The parameters of the geometry can then be automatically varied and the frequency tuned using a “scan” (Figure 5.8a), generating a large number of “geometry instances”. The interface for editing the parameters of one such instance is shown in Figure 5.8b. These geometry instances can then be automatically meshed, input files with boundary conditions etc. for Omega3P automatically generated, and the resulting set of files submitted to the remote HPC cluster. Once the calculation is finished, the files can be automatically downloaded from the cluster, analyzed, and the resulting data extracted back into AcOpti (Figure 5.8c). This data can then be plotted as will be seen in Section 5.6, used for 1D- and 2D-fit tuning, or exported for further analysis in an external program.

## 5.6. A typical optimized cell

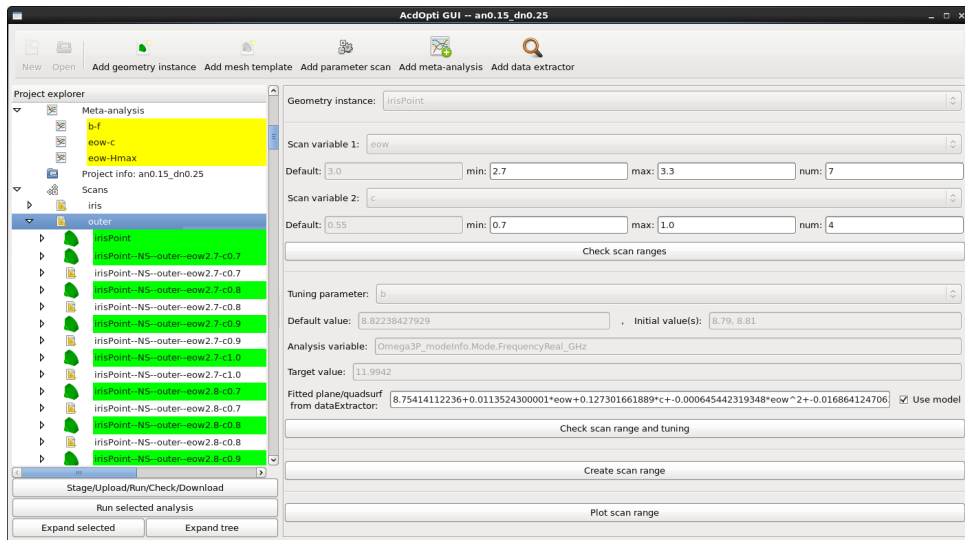
One example of an accelerating cell which was optimized using the methods presented in this chapter, is the cell from the cell database version 1 (Section 5.7) with  $a/\lambda = 0.15$  and  $d/h = 0.25$ . The geometry parameters of this cell are listed in Table 5.1a, and the final geometry and field patterns are shown in Figure 5.9. More details are available in [23, Section 4.11 and 4.12].

The dependence of  $\bar{E}$  and  $\bar{S}_c$  on the geometry parameters (sFrac, e) are shown in Figure 5.11a and 5.11b. As is the case for most cells optimized for this database, the smallest values are found at a small (but not necessarily zero) value of sFrac, and a moderately low value of e. Note that the two minima do not occur at the same geometry parameters.

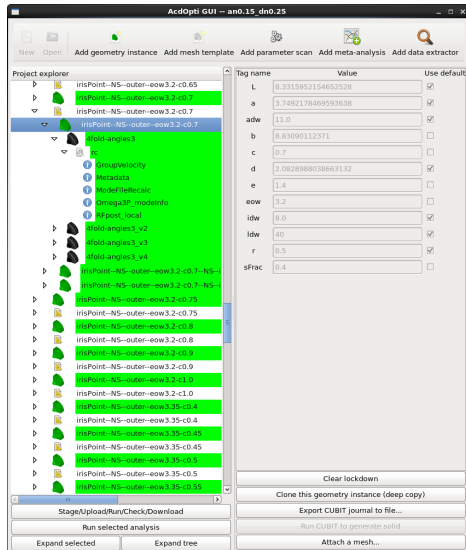
Moving away from the optimum for the surface electric field, its peak value increases as the iris becomes “pointier” towards the middle of the cavity (see Figure 5.9b), enhancing the surface electric field. For the modified Poynting vector, moving away from the optimum can increase its peak value through two mechanisms – either by increasing the surface electric- or magnetic field, or by increasing their overlap.

As seen in Figure 5.10a, this iris is dominated by both the modified Poynting vector and  $P_+/C$ , while the surface electric field plays a very minor role. A compromise was found at (sFrac = 0.4, e = 1.4). If  $P_+/C$  is ignored (as in the database version 2), it is completely dominated by  $S_c$ , and the minimum is found at (sFrac = 0.01, e = 1.3), which is the point of minimum  $S_c$ . In either case, the chosen optimum is robust between the choice of optimistic or pessimistic high gradient limits.

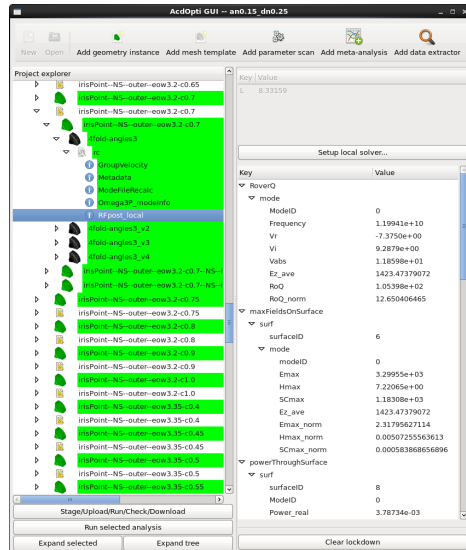
### 5. Cell geometry optimization



(a) Control panel for Scan2D\_tune.



(b) GeomInstance panel.



(c) Post analysis results from one geometry.

Figure 5.8.: Screenshots of the AcdOptiGui interface.

| Variable | Value    | Unit |
|----------|----------|------|
| $h$      | 8.331595 | mm   |
| $a$      | 3.749218 | mm   |
| adw      | 11.0     | mm   |
| $b$      | 8.830901 | mm   |
| $c$      | 0.7      | mm   |
| $d$      | 2.082899 | mm   |
| $e$      | 1.4      |      |
| eow      | 3.2      |      |
| ldw      | 8.0      | mm   |
| rr       | 0.5      | mm   |
| sFrac    | 0.4      |      |

(a) Geometry parameters.

| Variable    | Value     | $\pm$ Error           | Unit          |
|-------------|-----------|-----------------------|---------------|
| $f$         | 11.994080 | $\pm 2 \cdot 10^{-6}$ | GHz           |
| $Q$         | 5433.7    | $\pm 2 \cdot 10^{-1}$ | -             |
| $R'/Q$      | 12.65032  | $\pm 6 \cdot 10^{-5}$ | k $\Omega$ /m |
| $v_g$       | 2.37597   | $\pm 7 \cdot 10^{-5}$ | %c            |
| $\bar{E}$   | 2.19      | $\pm 2 \cdot 10^{-2}$ | -             |
| $\bar{S}_c$ | 0.56      | $\pm 1 \cdot 10^{-2}$ | mA/V          |
| $\bar{H}$   | 4.37      | $\pm 1 \cdot 10^{-2}$ | mA/V          |

(b) Main mode RF parameters.

Table 5.1.: Parameters for the accelerating cell presented in Section 5.6.

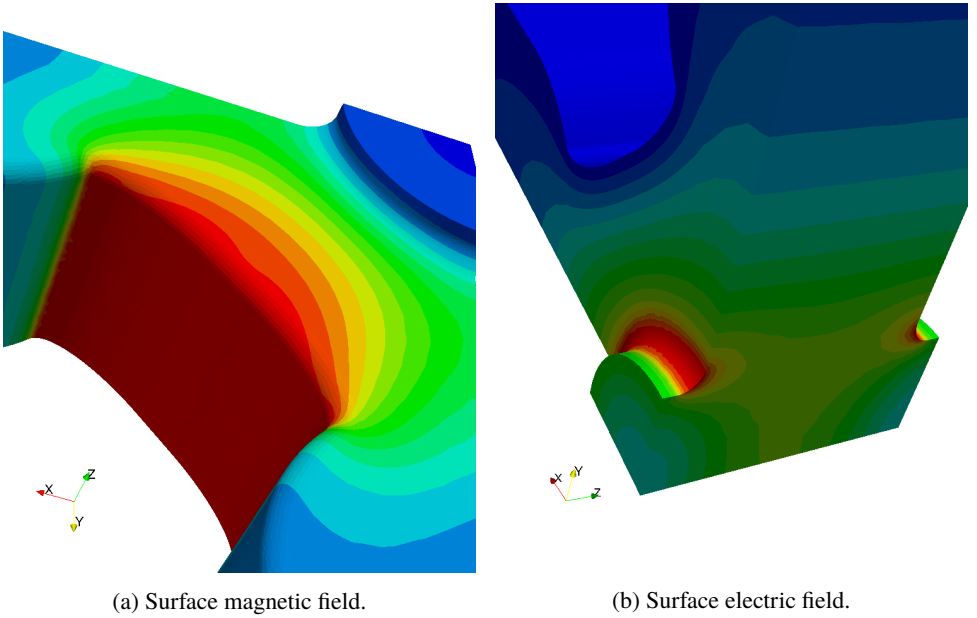


Figure 5.9.: Cell geometry and fields for the accelerating cell presented in Section 5.6.

## 5. Cell geometry optimization

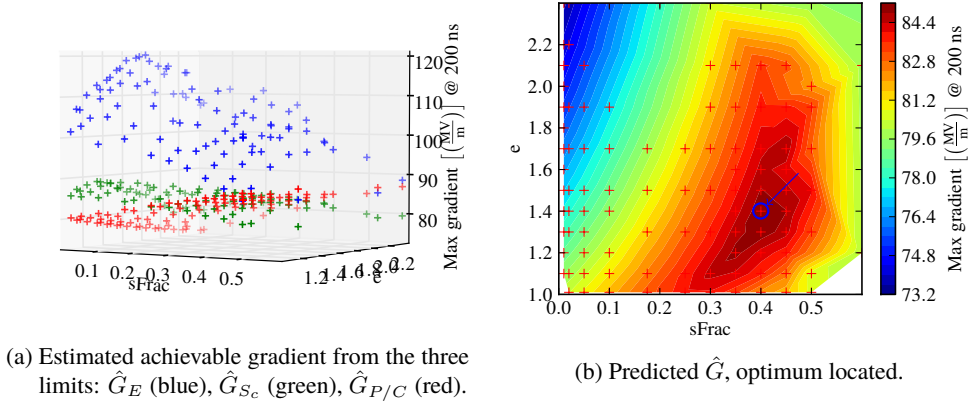


Figure 5.10.: Estimated achievable gradient at standard conditions  $\hat{G}$  as a function of geometry parameters for the accelerating cell presented in Section 5.6, using pessimistic high gradient limits as defined in Sec. 3.3.1.

After selecting the iris point, the geometry parameters for the outer wall is also varied in order to minimize the peak surface electric field. The result of this parameter scan is shown in Figure 5.11c, which shows that the peak surface magnetic field is slowly decreasing as eow and c increases, until it hits an edge where it starts to increase rapidly. As explained in Section 5.4.1, this is due to a concentration of the magnetic field on the entrance of the damping wave guides.

Changing the outer wall geometry from (eow = 3.0, c = 0.55 mm) as used during the iris scan also changes the cell radius b and the RF parameters slightly. Before outer wall optimization, the parameters were  $Q = 5453$ ,  $R'/Q = 12.678 \text{ k}\Omega/\text{m}$ ,  $v_g = 2.381 \%c$ ,  $\bar{E} = 2.2$ ,  $\bar{S}_c = 0.55 \text{ mA/V}$ ,  $\bar{H} = 4.37 \text{ mA/V}$ , and the outer wall radius was  $b = 8.822384 \text{ mm}$ . Since these parameters were quite similar to the final parameters, no second iteration of iris optimization was necessary.

## 5.7. The cell database

As stated in the beginning of this chapter, the goal for the cell optimization was to produce a database of highly optimized RF accelerating cells. Such a cell database was created using the methods that were described earlier in the chapter, and the final geometry and RF parameters of the cells in the database are listed in Table 5.2.

In this database, all the cells have a phase advance of  $\psi = 120^\circ$ . This choice was originally made after considering both  $120^\circ$  and  $150^\circ$  degree phase advances in a full machine optimization study for both cost and performance [147]. This study resulted in the CLIC\_G structure, and was the starting point for the database presented in this chapter. In the cells presented here, the phase advance was kept, while the exact cell geometry was optimized for high gradient reach.

As seen from Figure 5.12, the RF parameters vary quite a bit over the parameter range, as does the high gradient capability (Figure 5.13). The main effect observed is that the larger iris aperture cells suffer from higher peak fields and smaller shunt impedance, but

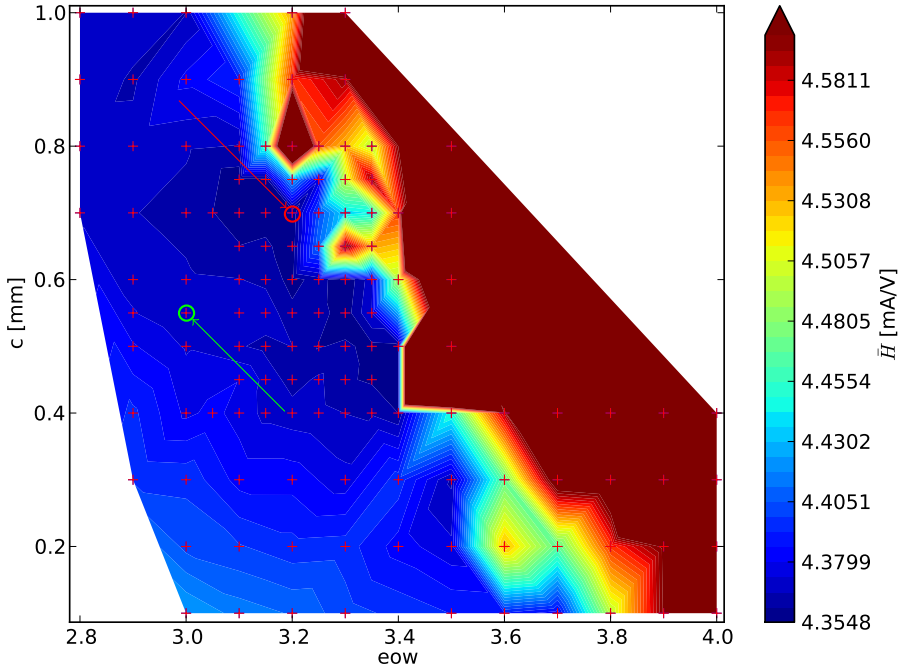
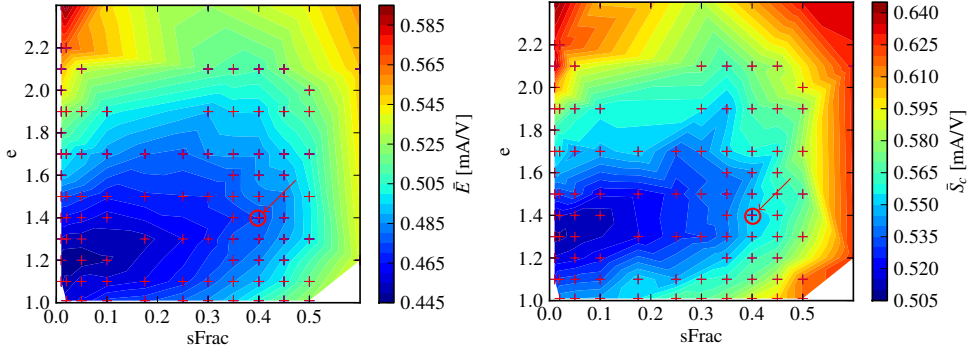


Figure 5.11.: Normalized peak fields for the accelerating cell presented in Section 5.6 as a function of geometry parameters.

## 5. Cell geometry optimization

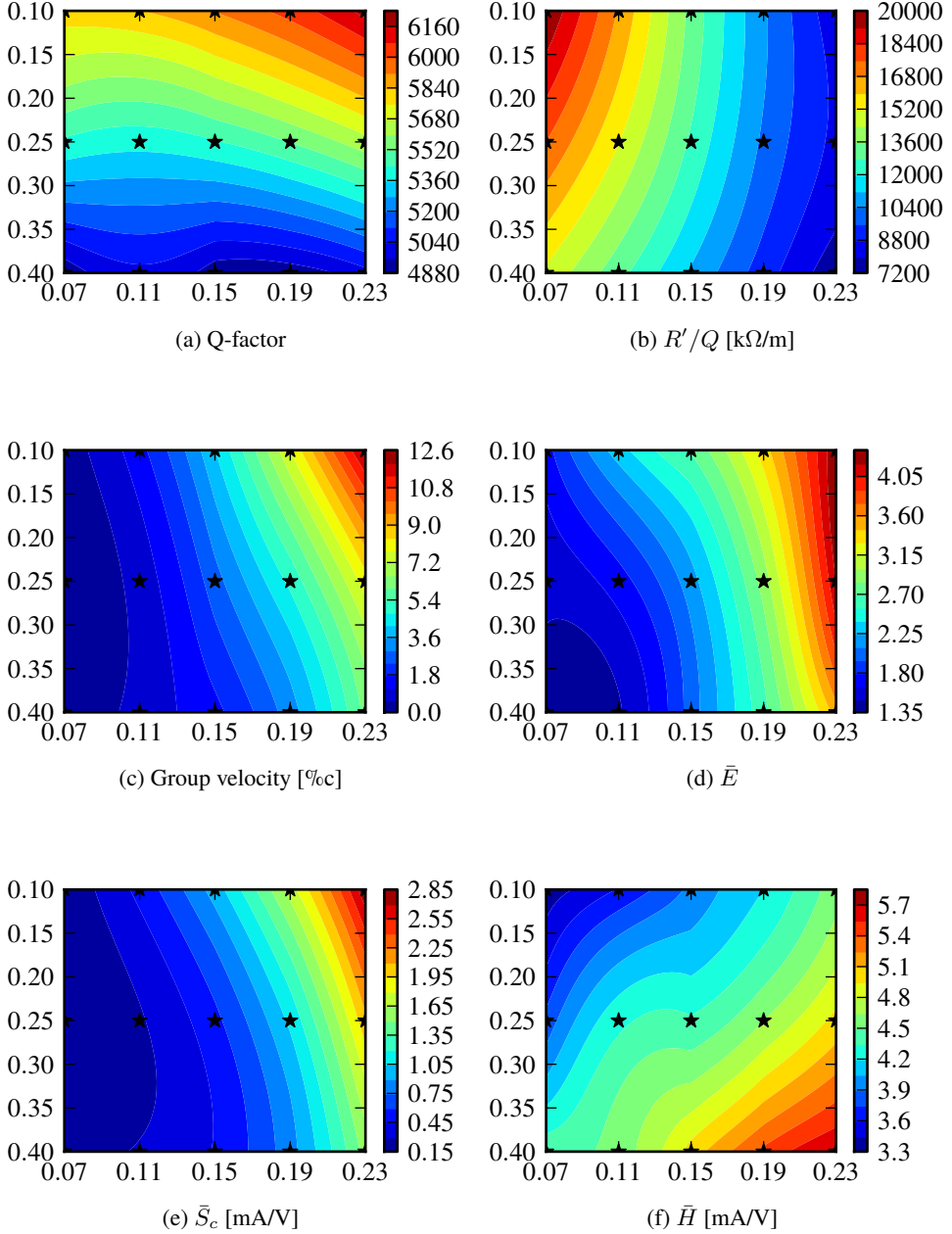
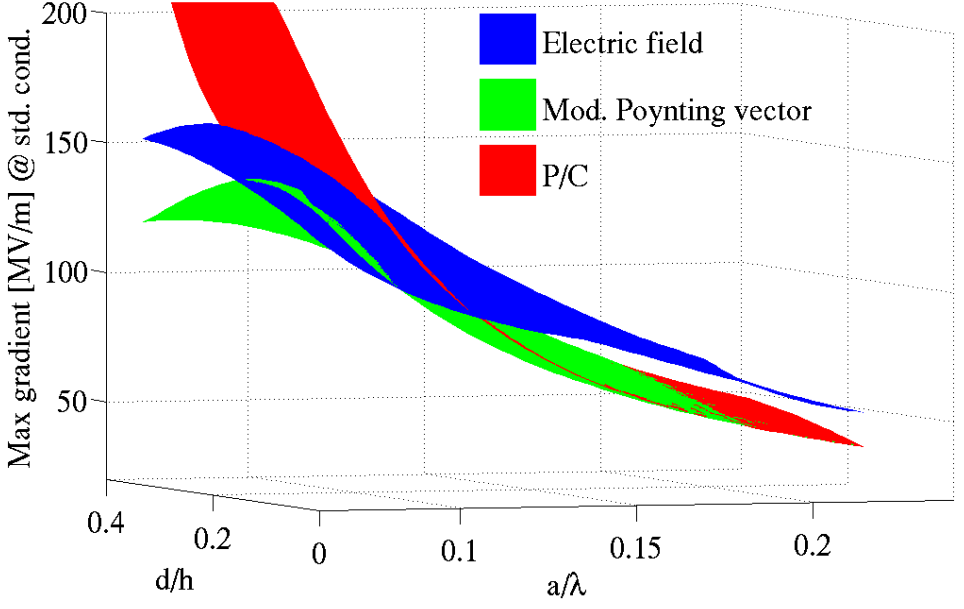
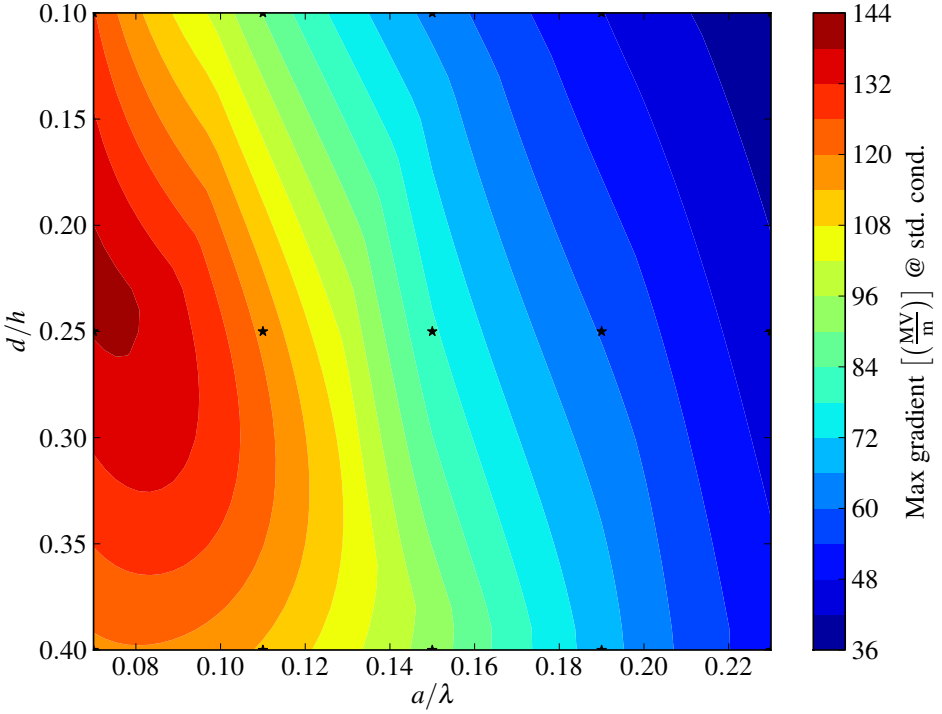


Figure 5.12.: RF parameters for database version 1 cells. The X-axes of the plots are the normalized iris aperture  $a/\lambda$ , the Y-axis the normalized iris thickness  $d/h$ . Note that the y-axis is inverted in order to match the layout of the tables.



(a) Gradient limits from  $\vec{E}$ ,  $\vec{S}_c$ , and  $P_+/C$  separately.

(b) Overall gradient limit.

Figure 5.13.: Gradient limits at standard conditions for database version 1 cells.

## 5. Cell geometry optimization

| $d/h \backslash a/\lambda$ | 0.07     | 0.11     | 0.15     | 0.19      | 0.23     | Variable | [unit] |
|----------------------------|----------|----------|----------|-----------|----------|----------|--------|
| 0.1                        | 0.035    | 0.01     | 0.01     | 0.25      | 0.5      | sFrac    | [-]    |
|                            | 1.75     | 1.01     | 1.01     | 1.01      | 1.01     | e        | [-]    |
|                            | 2.95     | 3.05     | 3.25     | 3.45      | 3.5      | eow      | [-]    |
|                            | 0.4      | 0.5      | 0.5      | 0.8       | 1.25     | c        | [mm]   |
|                            | 8.280743 | 8.458519 | 8.769250 | 9.194505  | 9.712798 | b        | [mm]   |
| 0.25                       | 0.1      | 0.3      | 0.4      | 0.6       | 0.8      | sFrac    | [-]    |
|                            | 5.75     | 2.8      | 1.4      | 1.1       | 1.2      | e        | [-]    |
|                            | 3.15     | 3.05     | 3.2      | 3.35      | 3.5      | eow      | [-]    |
|                            | 0.45     | 0.55     | 0.7      | 0.9       | 1.25     | c        | [mm]   |
|                            | 8.525954 | 8.580390 | 8.830901 | 9.215200  | 9.709893 | b        | [mm]   |
| 0.4                        | 0.01     | 0.01     | 0.4      | 0.65      | 0.8      | sFrac    | [-]    |
|                            | 3.4      | 3.4      | 2.9      | 1.6       | 1.4      | e        | [-]    |
|                            | 3.2      | 3.25     | 3.4      | 3.5       | 3.5      | eow      | [-]    |
|                            | 0.55     | 0.8      | 0.75     | 0.925     | 1.25     | c        | [mm]   |
|                            | 8.774644 | 9.068544 | 9.113631 | 9.36022 3 | 9.836833 | b        | [mm]   |

(a) Optimized geometry parameters.

| $d/h \backslash a/\lambda$ | 0.07       | 0.11      | 0.15      | 0.19      | 0.23      | Variable    | [unit]          |
|----------------------------|------------|-----------|-----------|-----------|-----------|-------------|-----------------|
| 0.1                        | 11.9942022 | 11.994206 | 11.994203 | 11.994216 | 11.994190 | $f$         | [GHz]           |
|                            | 5798.2     | 5837.8    | 5924.5    | 6034.7    | 6187.7    | $Q$         |                 |
|                            | 19.95081   | 16.70638  | 13.3501   | 10.53568  | 8.24821   | $R'/Q$      | [k $\Omega$ /m] |
|                            | 0.35410    | 1.60632   | 4.1830    | 7.8121    | 12.29160  | $v_g$       | [% c]           |
|                            | 1.739      | 2.33      | 2.720     | 3.38      | 4.33      | $\bar{E}$   |                 |
|                            | 0.2037     | 0.497     | 0.973     | 1.718     | 2.82      | $\bar{S}_c$ | [mA/V]          |
|                            | 3.378      | 3.613     | 3.94      | 4.20      | 4.59      | $\bar{H}$   | [mA/V]          |
| 0.25                       | 11.994208  | 11.994203 | 11.994080 | 11.994199 | 11.99415  | $f$         | [GHz]           |
|                            | 5424.9     | 5390.2    | 5433.7    | 5523.1    | 5648.3    | $Q$         |                 |
|                            | 17.5921    | 15.2292   | 12.65032  | 10.237662 | 8.14536   | $R'/Q$      | [k $\Omega$ /m] |
|                            | 0.21623    | 0.84906   | 2.37597   | 4.97111   | 8.6015    | $v_g$       | [% c]           |
|                            | 1.54       | 1.734     | 2.19      | 2.92      | 4.2       | $\bar{E}$   |                 |
|                            | 0.20903    | 0.2855    | 0.56      | 1.088     | 2.06      | $\bar{S}_c$ | [mA/V]          |
|                            | 3.798      | 4.3       | 4.37      | 4.650     | 5.00      | $\bar{H}$   | [mA/V]          |
| 0.4                        | 11.99419   | 11.994206 | 11.994205 | 11.994192 | 11.994216 | $f$         | [GHz]           |
|                            | 4895.0     | 5018.2    | 4909.52   | 4913.4    | 5013.5    | $Q$         |                 |
|                            | 15.043     | 13.0868   | 11.0804   | 9.18009   | 7.457969  | $R'/Q$      | [k $\Omega$ /m] |
|                            | 0.117536   | 0.80406   | 1.6344    | 3.3208    | 6.1877    | $v_g$       | [% c]           |
|                            | 1.4555     | 1.4836    | 2.03      | 2.651     | 3.52      | $\bar{E}$   |                 |
|                            | 0.2836     | 0.3124    | 0.46      | 0.843     | 1.56      | $\bar{S}_c$ | [mA/V]          |
|                            | 4.452      | 4.5750    | 5.0153    | 5.44      | 5.7031    | $\bar{H}$   | [mA/V]          |

(b) Optimized RF parameters.

Table 5.2.: Parameters of the accelerating cells in cell database version 1.

also achieve much higher group velocities. The iris thickness also has some effect, mainly on the  $Q$ -factor and the peak surface magnetic field  $\vec{H}$ . It is also interesting to observe that from Figure 5.13a, the peak surface electric field is important for low-aperture cells which have little power flow, while the power flow quantities  $S_c$  and  $P_+/C$  dominate the larger aperture cells.

Part of the reason for the very high peak fields in the high-aperture cells is that the  $P_+/C$  breakdown criteria favors lower group velocities. This is most important for the large apertures, pushing sFrac to high values and thus yielding very “square” iris profiles. A second version of the database [23, Section 4.2] was therefore created, where the  $P_+/C$  criteria was ignored in the iris optimization and only  $\min(\hat{G}_E, \hat{G}_{S_c})$  was maximized. This version of the database may be a safer choice to use for doing structure optimization, as it contains more “traditional” cell designs, which are closer to those found in the structures on which the high gradient limits are based.

## 5.8. Summary and conclusions

As shown in this chapter, a method was developed for optimizing the geometry of an traveling wave accelerating cell. This method took into account the best known high gradient limitations, discussed in Chapter 3, weighed them against each other, and used this to find an optimal cell geometry. The method was then applied to 15 different sets of iris parameters  $(a/\lambda, d/h)$ , producing the cell database which was shown in Section 5.7.



## 6. Wake fields

As the beam is composed of charged particles, it creates an electromagnetic field which surrounds it. If a charged particle is traveling at a constant and highly relativistic velocity in a completely empty space, this field becomes a “pancake” field when observed in the lab frame. This means that the field is almost only present in the space directly to the side of the particle, relative to the direction of motion. The field behind or in front of the particle is therefore very weak. However, when the particle or a bunch of particles are traveling in a particle accelerator, the field from the particles interacts with charges in the materials of the machine. These charges react, shift positions, and make that the overall field is something different than the vacuum pancake. This leads to the presence of a non-zero electromagnetic field behind the bunch, which can create a force which affects the trajectory of any particles trailing it via the Lorentz force.

This chapter first discusses the basic physics of wake fields and some useful relations describing how they interact with the beam. Then, practical considerations for simulating wake fields in waveguide damped structures using ACE3P [22] are presented. Finally, the parameters of the first wake field dipole modes for the cells in the cell database first presented in Section 5.7 are shown and discussed.

### 6.1. Wake field modes

Just like the accelerating modes discussed in Chapter 2, wake fields can often also be described by eigenmodes. The difference is that instead of the primary excitation being an external RF generator such as a klystron or PETS structure, wake fields are only excited by the beam. Further, usually multiple modes are excited. Wake field modes can therefore also be described by an oscillation frequency  $f$  and a quality factor  $Q$ , just like the accelerating mode. The scaling of wake field mode parameters with cavity size (and thus the main mode frequency) will be described in Section 7.2.

In order for the beam to interchange energy with an electromagnetic field, there must be an electric field component parallel to the beam velocity, presenting an accelerating or decelerating voltage to the beam. In this way, the beam can either be accelerated while draining energy from the RF field, or the beam can be decelerated while the RF field gains energy and field amplitude. Beam loading of accelerating structures (as will be discussed in Chapter 7) are therefore at the fundamental level a beam excitation (i.e. a wakefield) of the accelerating mode, generated  $180^\circ$  out of phase and thus interfering destructively with the externally driven field.

## 6.2. Wake functions, bunch potentials, and impedance

When discussing wake fields, two very useful concepts are wake functions and wake impedance. These are usually split into two categories – longitudinal and transverse – however they are described using the same framework.

The wake functions are in this work called  $W_z(s)$  and  $\vec{W}_\perp(s)$ . They are Greens functions describing the kick on a trailing particle due to the shock response of the field to a bunch with a  $\delta$ -function charge distribution, observed at the position of a witness particle traveling with the same velocity and in the same direction as the driving bunch at a distance  $s$  after the driving bunch [148, 149]. The wake functions are normalized to the charge  $Q$  of the driving bunch, and sometimes (as in the case for a periodic structure) it is convenient to also normalize them to the period  $L$ . In all cases, the beam is assumed to travel on a straight line at the speed of light and parallel to the  $z$ -axis.

The longitudinal wake function can be calculated as

$$W_z(s) = \frac{-1}{qQL} \int_0^L F_{z,\delta} \left( z, t = \frac{z+s}{c} \right) dz = \frac{-1}{QL} \int_0^L E_{z,\delta} \left( z, t = \frac{z+s}{c} \right) dz, \quad (6.1)$$

where the negative sign is used so that  $\lim_{s \rightarrow 0^+} W_z(0) > 0$  even though the field is decelerating at this point (see Section 6.3). Similarly, the transverse can be calculated as

$$\begin{aligned} \vec{W}_\perp(s) &= \frac{1}{qQL} \int_0^L \vec{F}_{\perp,\delta} \left( z, t = \frac{z+s}{c} \right) dz \\ &= \frac{1}{QL} \int_0^L \vec{E}_{\perp,\delta}(z, t) + c\hat{z} \times \vec{B}_{\perp,\delta}(z, t) dz. \end{aligned} \quad (6.2)$$

In both cases

$$\vec{F} = q \left( \vec{E} + \vec{v} \times \vec{B} \right) \quad (6.3)$$

is the Lorentz force acting on a test charge  $q$ , and  $\vec{E}_\delta$  and  $\vec{B}_\delta$  are the fields generated by a  $\delta$ -function bunch at  $s = 0$ . The notation  $\vec{D}_\perp$  represents a vector given by only the  $x$ - and  $y$ -component of the 3-vector  $\vec{D}$ , leaving out the  $z$  component  $D_z$ .

The bunch potential  $\vec{V}$  is the wake created by a non- $\delta$ -function beam. This is defined the same way for both longitudinal- and transverse directions. It is calculated as the convolution of the wake function and the longitudinal bunch charge distribution  $\lambda(s')$ , i.e.

$$\vec{V}(s) = \int_{-\infty}^{\infty} \lambda(s') \vec{W}(s - s') ds'. \quad (6.4)$$

This what is actually obtained when calculating the wake using numerical methods, as discussed below in Section 6.7.

The dimensions of the wake functions are voltage per charge and distance, while for the bunch potential it is voltage per distance. There is also another quantity called the wake potential, which is equal to the bunch potential except that it is also normalized to the charge of the driving bunch  $Q$ , and thus has the same units as the wake function. When reporting the transverse dipole bunch or wake potential, which is often the most interesting part of the transverse wake, it is commonly further normalized to the transverse offset  $\Delta_x$  (or  $\Delta_y$ ) of the driving bunch. This is done because the strength of the excitation is proportional to the

offset of the driving beam, as discussed below in Section 6.6. The normalization therefore removes this factor.

The beam impedance  $Z$  describes the wake potential for a sinusoidal current with the linear charge density  $\tilde{\lambda}(s; k) = \lambda_0 \exp(iks)$ , where the real part is physically meaningful. Using Equation (6.4), the complex bunch potential is given as

$$\begin{aligned}
 \mathbf{V}(s; k) &= \int_{-\infty}^{\infty} \lambda_0 \exp(iks') \vec{W}(s - s') ds' \\
 &= \int_{-\infty}^{\infty} \lambda_0 \exp(ik(s - s'')) \vec{W}(s'') ds'' \\
 &= \lambda_0 \exp(iks) \int_{-\infty}^{\infty} \exp(-iks'') \vec{W}(s'') ds'' \\
 &= \lambda(s; k) \mathcal{F}\{\vec{W}(s)\}(k) = \frac{I}{c} \exp(iks') \mathcal{F}\{\vec{W}(s)\}(k) \\
 &\equiv I(s; k) \mathbf{Z}(k),
 \end{aligned} \tag{6.5}$$

where the first transformation was done by a change of variable, and the last used the relationship between the beam current  $I = c\lambda$  and the linear charge density of the beam. Here, the impedance  $\mathbf{Z}(k)$ , which is a Fourier transformation of the wake function, is the relation between the bunch potential  $\mathbf{V}(s)$  and the current  $I$  when the wake is excited by a monochromatic current  $I(s; k)$  with wavenumber (spatial angular frequency)  $k$ . This is a complex quantity, reflecting the fact that there may be a phase shift between the exciting current and the voltage. The dimensions of the impedance is here voltage / (charge  $\times$  speed), and may thus be given in units of Ohm/m. Again, for the transverse dipole wake, the impedance is often normalized by the beam offset  $\Delta_x$  or  $\Delta_y$ , giving the units an extra “per mm”.

The complex function  $\mathbf{Z}(k)$  can also be interpreted as an impedance spectrum, i.e. the beam impedance as a function of the wavenumber  $k$ . In order to convert  $k$  to the more commonly used variable  $\omega$ , the oscillation frequency in dimensions of radians per unit time, the relationship  $\frac{\omega}{k} = c$  can be used to substitute. Further, the oscillation frequency is usually reported as number of full oscillations per time, which is related to  $\omega$  through  $\omega = 2\pi f$ .

Since the bunch potential is given by convoluting the wake function with the bunch charge distribution (Equation (6.4)), the relation between the Fourier transform of the bunch potential and the Fourier transform of  $\lambda(s)$  is simply

$$\mathcal{F}\{\mathbf{V}(s)\}(k) = \mathcal{F}\{\vec{W}(s)\}(k) \mathcal{F}\{\lambda(s)\}(k). \tag{6.6}$$

This can be used to find the impedance spectrum

$$\mathbf{Z}(k) = \frac{\mathcal{F}\{\vec{W}(s)\}(k)}{\mathcal{F}\{I(s)\}(k)} = \frac{\mathcal{F}\{\vec{W}(s)\}(k)}{c \mathcal{F}\{\lambda(s)\}(k)} \tag{6.7}$$

from simulation data, since the excitation  $\lambda(s)$  is a known input to the simulation.

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### 6.2.1. The impedance spectrum of a damped resonance

One of the most commonly used models for an impedance is that of a damped harmonic oscillator. As a function of  $s$  and assuming that  $Q > 1/2$  (i.e. not critically damped or overdamped) and that the undamped resonance angular frequency  $k_0 > 0$ , the excitation is given as

$$g(s) = \begin{cases} A \exp\left(-\frac{k_0 s}{2Q}\right) \sin\left(k_0 s \sqrt{1 - \frac{1}{4Q^2}} + \phi\right) & s \geq 0 \\ 0 & s < 0 \end{cases}. \quad (6.8)$$

Following the convention of Equation (6.5), the Fourier transform of this is

$$G(k) = \mathcal{F}\{g(s)\}(k) = A \frac{k_0 \sqrt{4Q^2 - 1} \cos(\phi) + (k_0 + 2ikQ) \sin(\phi)}{2ik k_0 - 2k^2 Q + 2k_0 Q}. \quad (6.9)$$

As will be discussed in Section 6.5, transverse wakes (which is what we eventually want to model) are “sine-like”, so we may take  $\phi = 0$ . This model was used to estimate the wanted parameters of the wakefield modes from the fitted impedance spectra.

### 6.3. The fundamental theorem of beam loading

The relationship between the induced field in the cavity and the energy loss of the particles that are exciting the field is given by the fundamental theorem of beam loading. Following [149], a bunch with a longitudinal charge profile  $\lambda(s)$  such that  $\int_{-\infty}^{\infty} \lambda(s) ds = q$  is assumed. Further, every particle in this bunch generates a longitudinal wake field  $E_{z,\delta}(s)$ , which is observed at a distance  $s$  after the driving particle. This field has the property that  $E_{z,\delta}(s < 0) = 0$ , i.e. no field is generated in front of the generating particle, as is required by causality for a highly relativistic beam. The field at position  $s'$  is thus given as

$$E_z(s') = \int_{-\infty}^{s'} \lambda(s) E_{z,\delta}(s' - s) ds. \quad (6.10)$$

Using this, the work performed by the field on the bunch, i.e. the change in energy  $dE$  per unit distance traveled  $dz$  is (in analogy to Equation (6.4))

$$\frac{dE}{dz} = \int_{-\infty}^{\infty} \lambda(s') E_z(s') ds' = \int_{-\infty}^{\infty} \lambda(s') \left[ \int_{-\infty}^{s'} \lambda(s) E_{z,\delta}(s' - s) ds \right] ds'. \quad (6.11)$$

If assuming that the bunch length is short relative to the wave length of the induced wake, then the field inside the bunch can approximately be written as

$$E_{z,\delta}(s) \approx \begin{cases} -E_{z,\delta}(0^+) & s \geq 0 \\ 0 & s < 0 \end{cases} \quad (6.12)$$

The integral in Equation (6.11) can then be solved as

$$\frac{dE}{dz} \approx -E_{z,\delta}(0^+) \int_{-\infty}^{\infty} \lambda(s') \left[ \int_{s'}^{\infty} \lambda(s) ds \right] ds' = -\frac{1}{2} q^2 E_{z,\delta}(0^+). \quad (6.13)$$



Thus, a short bunch that is not creating a field “ahead of itself” (due to causality for a highly relativistic electron beam) sees an effective decelerating field amplitude which is half of what it generates.

Following [72], it can be shown that this is a consequence of energy conservation. Considering two identical short bunches which pass through an initially unexcited cavity, the first one sees a retarding voltage  $V_1 = -fV_c$ , where  $V_c$  is the accelerating voltage which would be seen by a witness particle passing through the cavity immediately after the bunch, and  $f$  is a positive real number. If now the second bunch passes the assumed loss-less cavity one oscillation period later, it sees an accelerating voltage  $+V_c$  and also the retarding “self-voltage”  $-fV_c$ , such that  $V_2 = (1 - f)V_c$ . In the case of maximum energy transfer, the cavity is completely field-free after the second bunch has left the cavity due to the two wakes interfering destructively, and all the energy lost by the first bunch is gained by the second. Thus  $V_1 + V_2 = 0 = (1 - 2f)V_c$ , implying that  $f = 1/2$ . This is the same result as seen in Equation (6.13).

A closely related result is that the *transformer ratio*, which is the ratio between the energy/particle gained by the second bunch  $\Delta E_2$  and the energy/particle lost by the leading bunch  $-\Delta E_1$  [149], cannot exceed 2. This assumes that the bunches are short relative to the wake wavelength, that the bunches are traveling on the same path, and that they are composed of particles with the same charge magnitude. Further assumed is that the position of the 2<sup>nd</sup> bunch relative to the 1<sup>st</sup> is “optimal”, such that the wake function  $W(s)$  generated by the first bunch at the position of both bunches are the same but with opposite signs. Note that since the self-wake is decelerating,  $W(0^+) > 0$  as defined in Equation (6.1). The energy change per particle of each bunch after they have traversed the same region of length  $L$  is then given as

$$\Delta E_1 = -\frac{1}{2}N_1q_1^2W_z(0^+)L \quad (6.14)$$

$$\begin{aligned} \Delta E_2 &= -\frac{1}{2}N_2q_2^2W_z(0^+)L - q_2N_1q_1W_z(s_{\text{opt}})L \\ &= W_z(0^+)Lq_2\left(q_1N_1 - \frac{1}{2}N_2q_2\right). \end{aligned} \quad (6.15)$$

Here  $q_1$  and  $q_2$  are the particle charges of the 1<sup>st</sup> and 2<sup>nd</sup> bunch,  $N_1$  and  $N_2$  the number of particles per bunch. The ratio of the energy changes per particle, i.e. the transformer ratio, is thus given as

$$\frac{\Delta E_2}{-\Delta E_1} = 2\left(\frac{q_2}{q_1}\right)^2\left[\frac{q_1}{q_2} - \frac{1}{2}\frac{N_2}{N_1}\right]. \quad (6.16)$$

If  $q_1 = q_2$ ,  $N_1 \gg N_2$ , and the 1<sup>st</sup> beam is allowed to spend all its energy ( $\Delta E_1 = E_1$ ), this implies that the maximum possible energy gain by the 2<sup>nd</sup> beam is  $\Delta E_2 = 2E_1$ .

The fundamental theorem of beam loading thus implies that accelerating one beam by decelerating another within a single structure is not very efficient, requiring a large number of low-energy drive beams to be used for accelerating one high-energy beam. However, it is possible to bypass this problem by violating the assumptions of the theorem: Pointlike bunches traveling at  $v = c$ , following the same path. For the first violated assumption, one may get a transformer ratio larger than 2 by using a “ramped” drive bunch where the charge density is increasing linearly with  $s$  [149]. The second is used in CLIC, which uses two different structures for the drive beam and accelerated beam, as was described in Section 1.2.

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This works so that the drive beam is decelerated in a set of structures which has a lower field for the same stored energy<sup>1</sup>, and the extracted energy then transferred to a structure which produces a stronger field for the same energy. Another example of this two-structure acceleration is in a klystron-powered accelerator. Here, a high-current energy electron beam which is electrostatically accelerated to around 100 keV and then decelerated in a set of output cavities. This again produces a wake field, which is extracted as RF power and can be used to power accelerating structures. These structure may achieve a higher accelerating gradient than the klystron.

### 6.4. Transverse kicks

In order to kick the beam transversely, there must be a transverse component of the Lorentz force (Equation (6.3)). When working with highly relativistic and thus stiff electron beams, one may define a vector quantity

$$\vec{V}'_{\perp} = \int_0^L \frac{\vec{F}_{\perp}}{q} dz = \int_0^L \vec{E}_{\perp} + c\hat{z} \times \vec{B} dz, \quad (6.17)$$

which has the dimension of voltage. Here  $q$  is the electron charge and  $\vec{v} \approx \hat{z}c$ , where  $c$  is the speed of light. This is mathematically related to the transverse bunch potential  $\vec{V}_{\perp}$  by not including the “per length” normalization, such that  $\vec{V}'_{\perp} = L\vec{V}_{\perp}$ . Another difference is that the transverse voltage  $\vec{V}'_{\perp}$  makes no reference to how the field was excited; it may for example be excited by a RF generator. Making a change in coordinates from length to time using the relationship  $z = ct$ , it is clear that

$$q\vec{V}'_{\perp} = \int_0^L \vec{F}_{\perp} dz = c \int_0^{L/c} \vec{F}_{\perp} dt = c \int_0^t \frac{dp_{\perp}}{dt} dt = c\Delta p_{\perp}. \quad (6.18)$$

The change in angle is therefore

$$\Delta x' = \frac{\Delta p_x}{p_s} = \frac{qV'_x}{cp_s}, \quad (6.19)$$

where  $x$  may also be replaced by the other transverse coordinate  $y$ .

### 6.5. The Panofsky-Wenzel theorem

The Panofsky-Wenzel theorem [150] (PWT) relates the transverse and longitudinal wake functions and wake/bunch potentials to each other. It is extremely useful when analyzing the transverse kick provided from electromagnetic fields, including wake fields.

To construct the PWT, one may start by building an expression for the Lorentz force. Following the derivation in [151], the first piece needed can be derived by looking at the curl of the “magnetic force field”  $\vec{v} \times \vec{B}$ , assuming that the velocity vector  $\vec{v}$  is constant:

$$\nabla \times (\vec{v} \times \vec{B}) = \vec{v}(\nabla \cdot \vec{B}) - \vec{B}(\nabla \cdot \vec{v}) + (\vec{B} \cdot \nabla)\vec{v} - (\vec{v} \cdot \nabla)\vec{B} = -(\vec{v} \cdot \nabla)\vec{B} \quad (6.20)$$

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<sup>1</sup>The relationship between stored energy and accelerating voltage is given by Equation (2.7), and the effects from that the energy has to travel through the structures and losses along the structures etc. will be treated in detail in Section 7.4.

Here the first term of the expansion is zero because there are no free magnetic charges, and the two next terms are also zero because  $\vec{v}$  is constant. This implies that

$$\nabla \times (\vec{v} \times \vec{B}) + (\vec{v} \cdot \nabla) \vec{B} = 0, \quad (6.21)$$

which is then inserted on the right hand side of the induction law

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} = -\frac{\partial \vec{B}}{\partial t} - \nabla \times (\vec{v} \times \vec{B}) - (\vec{v} \cdot \nabla) \vec{B}. \quad (6.22)$$

This can be expressed using the Lorentz force (Equation (6.3))

$$\nabla \times (\vec{E} + \vec{v} \times \vec{B}) = \frac{\nabla \times \vec{F}}{q} = -\frac{\partial \vec{B}}{\partial t} - (\vec{v} \cdot \nabla) \vec{B} = -\frac{d\vec{B}}{dt}. \quad (6.23)$$

Here, the last transformation is due to that

$$d\vec{B} = \frac{\partial \vec{B}}{\partial t} dt + \frac{\partial \vec{B}}{\partial x} dx + \frac{\partial \vec{B}}{\partial y} dy + \frac{\partial \vec{B}}{\partial z} dz = \frac{\partial \vec{B}}{\partial t} dt + (d\vec{r} \cdot \nabla) \vec{B}, \quad (6.24)$$

where  $d\vec{r}$  is an infinitesimal translation in space. The field of interest is that seen by a witness particle with a constant velocity vector  $\vec{v}$ , so that  $d\vec{r} = \vec{v} dt$  and thus

$$d\vec{B} = \frac{\partial \vec{B}}{\partial t} dt + (d\vec{r} \cdot \nabla) \vec{B} = \frac{\partial \vec{B}}{\partial t} dt + (\vec{v} \cdot \nabla) \vec{B} dt \Rightarrow \frac{d\vec{B}}{dt} = \frac{\partial \vec{B}}{\partial t} + (\vec{v} \cdot \nabla) \vec{B}, \quad (6.25)$$

which is the expression for  $\frac{d\vec{B}}{dt}$  used in Equation (6.23).

Integrating Equation (6.23) along the length of the structure, as when defining the wake functions in Section 6.2, yields:

$$\int_0^L \frac{\nabla \times \vec{F}}{q} dz = - \int_0^L \frac{d\vec{B}}{dt} dz \quad (6.26)$$

As the fields are assumed to be seen by a particle traveling along  $\vec{r} = \vec{v}t + \vec{r}_0 = \hat{z}(vt - s)$ , the substitution  $dz = v dt$  can again be used. This leads to

$$\int_0^L \frac{d\vec{B}}{dt} dz = v \int_{t_{\text{entry}}}^{t_{\text{exit}}} \frac{d\vec{B}}{dt} dt = v \left( \vec{B}_{\text{entry}}(s) - \vec{B}_{\text{exit}}(s) \right), \quad (6.27)$$

where  $\vec{B}_{\text{entry}}(s)$  is the magnetic field seen by a particle at position  $s$  (as defined before) when entering the cavity, and similar for  $\vec{B}_{\text{exit}}(s)$ . It is normally assumed that these terms cancel, such that

$$\int_0^L \frac{\nabla \times \vec{F}}{q} dz = \vec{0}. \quad (6.28)$$

The next step is to pull the curl outside the integral, which can be done via a change of variables from  $(x, y, z, t) \rightarrow (x, y, z, s)$ . For the curl operator, this is done by noticing that  $z = tv - s$ , and thus  $\frac{\partial}{\partial z} = -\frac{\partial}{\partial s}$ . Equation (6.28) can therefore be written as

$$\begin{aligned} \int_0^L \frac{\nabla \times \vec{F}}{q} dz &= \frac{1}{q} \left( \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} - \hat{z} \frac{\partial}{\partial s} \right) \times \int_0^L \vec{F} dz \\ &= \frac{QL}{q} \left( \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} - \hat{z} \frac{\partial}{\partial s} \right) \times (\hat{x} W_x(s) + \hat{y} W_y(s) - \hat{z} W_z(s)) \\ &= \frac{QL}{q} \nabla_s \times \vec{W}'(s) = \vec{0}, \end{aligned} \quad (6.29)$$

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where  $\nabla_s \equiv \left( \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} - \hat{z} \frac{\partial}{\partial s} \right)$  and  $\vec{W}' \equiv (\hat{x} W_x(s) + \hat{y} W_y(s) - \hat{z} W_z(s))$ . The last line of Equation (6.29), which after dropping the constant factors states that

$$\nabla_s \times \vec{W}'(s) = \vec{0}, \quad (6.30)$$

is known as the generalized Panofsky-Wenzel theorem.

Several things can be shown from the generalized PWT, including the usual form of the PWT given in Equation 6.32. This can be found by

$$\begin{aligned} \hat{z} \times (\nabla_s \times \vec{W}) &= \hat{z} \times \vec{0} = \vec{0} = \\ \hat{z} \times \left[ \hat{x} \left( -\frac{\partial W_z}{\partial y} + \frac{\partial W_y}{\partial s} \right) - \hat{y} \left( -\frac{\partial W_z}{\partial x} + \frac{\partial W_x}{\partial s} \right) + \hat{z} \left( \frac{\partial W_y}{\partial x} - \frac{\partial W_x}{\partial y} \right) \right] &= \\ \hat{x} \left( -\frac{\partial W_z}{\partial x} + \frac{\partial W_x}{\partial s} \right) + \hat{y} \left( -\frac{\partial W_z}{\partial y} + \frac{\partial W_y}{\partial s} \right) &= -\nabla_{\perp} W_z + \frac{\partial \vec{W}_{\perp}}{\partial s}, \end{aligned} \quad (6.31)$$

where  $\nabla_{\perp} \equiv \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y}$  and  $\vec{W}_{\perp} = \hat{x} W_x + \hat{y} W_y$ . The usual form of the PWT is then:

$$\nabla_{\perp} W_z = \frac{\partial \vec{W}_{\perp}}{\partial s}. \quad (6.32)$$

In constructing the PWT, the only assumptions made are Maxwell's equations, that the test particle is traveling with constant velocity along a straight line, and that the magnetic field at the entrance and exit of the structure vanish or cancel when the test charge passes through it. It may therefore be applied to any field, not exclusively to those one driven by a  $\delta$ -function bunch. Therefore the wake function  $\vec{W}(s)$  can in Equation (6.32) be replaced with the bunch potential  $\vec{V}(s)$  or by the wake potential, as they follow the same sign conventions, and the normalizations anyway cancel. The PWT can also be applied to the field pattern of an eigenmode.

One of the main implications of the Panofsky-Wenzel theorem is that TE-modes, i.e. modes where  $\vec{E} \cdot \hat{z} = 0$  everywhere, cannot apply transverse kicks on the beam. This is due to that these modes also have  $V_z = 0$ , and thus  $\frac{\partial \vec{V}_{\perp}}{\partial s} = 0$ . The only allowed nontrivial solution for the transverse bunch potential for such a mode is therefore that  $\vec{V}_{\perp} = \text{constant}$ , i.e. a constant “external” field. For the fields, this means that in a TE mode, the kick from the transverse electric field must be perfectly compensated by the magnetic field.

Another consequence of the PWT is that if longitudinal wake functions are “cosine-like”, i.e. that they are maximally decelerating at the position of the driving particle at  $s = 0$ , then transverse wake functions are “sine-like”, i.e. they are zero at the position of the particle. In other words, if  $W_z(x, y, s) = A \cos(k_0 s)$  where  $A$  is the amplitude of the longitudinal wake, then

$$\nabla_{\perp} W_z(x, y, s) = (\nabla_{\perp} A) \cos(k_0 s). \quad (6.33)$$

Equation (6.32) then yields that

$$\begin{aligned} \vec{W}_{\perp}(s) - \vec{W}_{\perp}(0) &= \int_0^s \frac{\partial \vec{W}_{\perp}(s)}{\partial s} ds = \int_0^s \nabla_{\perp} W_z ds \\ &= (\nabla_{\perp} A) \int_0^s \cos(k_0 s) ds = \frac{(\nabla_{\perp} A)}{k_0} \sin(k_0 s), \end{aligned} \quad (6.34)$$

i.e. the transverse wakes are “sine-like” and  $90^\circ$  out of phase with the longitudinal.

## 6.6. Dipole wake

Often, the most critical part of the transverse wake field are the dipole modes, such as the one shown in Figure 2.6. These modes are characterized by a field distribution that makes one full period oscillation when going once around beam axis in the azimuthal direction, as was discussed in Section 2.2.1.

Further, the transverse voltage from the dipole modes is to first order independent of the position of the beam, while the longitudinal voltage is proportional to the offset from the center of the cavity. In the case of a pillbox mode, the field components of a  $TM_{11}$  mode (one of the two polarizations) are given as [72]

$$E_z(r, \theta, t) = E_0 J_1 (rx_{1,1}/R) \cos(\theta) \exp(i\omega t) \quad (6.35)$$

$$B_r(r, \theta, t) = -i\omega \frac{R^2}{x_{1,1}^2 r c^2} E_0 J_1 (rx_{1,1}/R) \sin(\theta) \exp(i\omega t) \quad (6.36)$$

$$B_\theta(r, \theta, t) = -i\omega \frac{R}{x_{1,1} c^2} E_0 J_1' (rx_{1,1}/R) \cos(\theta) \exp(i\omega t) \quad (6.37)$$

$$E_r = E_\theta = B_z = 0, \quad (6.38)$$

where  $J_m(r')$  is the  $m^{\text{th}}$  Bessel function,  $J_m'(r') \equiv \left. \frac{dJ_m(r)}{dr} \right|_{r=r'}$ ,  $x_{1,1} \approx 3.832$  is the position of the first root of  $J_1$ ,  $R$  the cavity radius and  $E_0$  the field amplitude.

Observed at a point  $(x, y) = (\Delta_x, 0)$ , corresponding to  $(r, \theta) = (\Delta_x, 0)$ , the field is then given as

$$E_z(\Delta_x, t) = E_0 J_1 (\Delta_x x_{1,1}/R) \exp(i\omega t) \quad (6.39)$$

$$B_y(\Delta_x, t) = -i\omega \frac{R}{x_{1,1} c^2} E_0 J_1' (\Delta_x x_{1,1}/R) \exp(i\omega t) \quad (6.40)$$

$$E_x = E_y = B_x = B_z = 0. \quad (6.41)$$

Expanding the Bessel functions in  $E_z$  and  $B_y$  as a Taylor series of  $r' \equiv \Delta_x x_{1,1}/R \ll 0$  yields

$$\begin{aligned} E_z(\Delta_x, t) &= E_0 \left[ \sum_{j=0}^{\infty} \frac{(-1)^j}{j! \Gamma(j+2)} \left( \frac{r'}{2} \right)^{2m+1} \right] \exp(i\omega t) \\ &\approx E_0 \left[ \frac{\Delta_x x_{1,1}}{2R \Gamma(2)} \right] \exp(i\omega t) \propto \Delta_x, \end{aligned} \quad (6.42)$$

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$$\begin{aligned}
B_y(\Delta_x, t) &= -i\omega \frac{R}{x_{1,1}c^2} E_0 J_1'(r') \exp(i\omega t) \\
&= -i\omega \frac{R}{x_{1,1}c^2} E_0 \frac{1}{2} (J_0(r') - J_2(r')) \exp(i\omega t) \\
&= -i\omega \frac{R E_0}{2x_{1,1}c^2} \left[ \sum_{j=0}^{\infty} \frac{(-1)^j}{j! \Gamma(j+1)} \left(\frac{r'}{2}\right)^{2m} \right. \\
&\quad \left. - \sum_{j=0}^{\infty} \frac{(-1)^j}{j! \Gamma(j+3)} \left(\frac{r'}{2}\right)^{2m+2} \right] \exp(i\omega t) \\
&\approx -i\omega \frac{R E_0}{x_{1,1}c^2 \Gamma(1)} \exp(i\omega t) \propto 1.
\end{aligned} \tag{6.43}$$

The Lorentz-force acting on a test particle traveling with  $v = c$  on a trajectory parallel to the  $z$ -axis and intersecting the  $(x, y)$  plane at  $(\Delta_x, 0)$  is then  $\vec{F} = q(E_z \hat{z} + cB_y \hat{x})$ . Here, the longitudinal component is thus (to the leading order) proportional to  $\Delta_x$ , while the transverse component is not a function of the offset. Because of this, the amplitude of the dipole wake induced by a particle traveling at an offset  $\Delta_x$  is proportional to the offset. This is why dipole wakes and impedances typically are normalized to the offset  $\Delta_x$  of the exciting beam, as was discussed in Section 6.2. While this was just demonstrated for a pillbox mode, the result also holds for more complicated geometries.

This proportionality is also consistent with the PWT, as can be understood by assuming the longitudinal wake to be proportional to the  $x$ -coordinate. Inserting  $A = \mathcal{C}x$  in Equation (6.34), where  $\mathcal{C}$  is some constant, yields

$$\vec{W}_\perp(s) - \vec{W}_\perp(0) = \frac{\nabla_\perp(\mathcal{C}x)}{k_0} \sin(k_0 s) = \frac{\mathcal{C}\hat{x}}{k_0} \sin(k_0 s). \tag{6.44}$$

This is the same result as was explicitly demonstrated for the pillbox TM<sub>11</sub> field.

## 6.7. Calculating wake fields using ACE3P

In the work presented in this thesis, the transverse dipole wake fields from the cell designs presented in Chapter 5 were calculated using the transient solver T3P. This solver is part of the ACE3P package [22]. The procedure is very similar to when calculating the fields for the accelerating mode, i.e. first setting up the geometry and mesh with CUBIT and `acdtool`, and then running the simulation in time domain with T3P on the remote high performance computing facility `hopper.nersc.gov`. This yields the longitudinal bunch potential  $V(s)$ , which was then used for further analysis, such as calculating the transverse wake field and impedance. These calculations were based on the theory described earlier in the chapter, and the implementation will be described below.

As the calculation was done in time domain and the goal was to investigate the coupling between the beam current and the field, the fields were excited by a simulated beam. This beam had a Gaussian charge distribution  $\lambda(s)$  and a total charge of 1 pC. Further, the cell under study was repeated along the  $z$ -axis between 5 and 50 times, in order to approximate an infinite periodic structure. This enabled simultaneous study of multiple modes, some of which travel through the structure fast and couple weakly to the beam. Finally, “beam

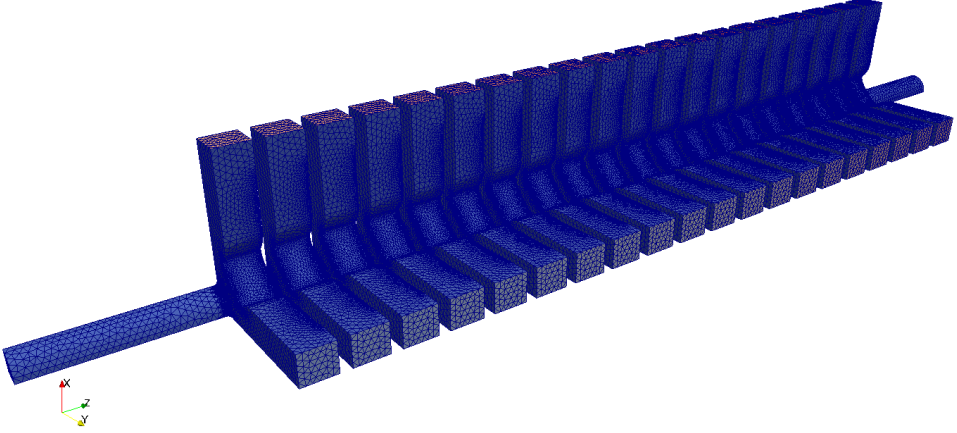


Figure 6.1.: Typical quarter-cell geometry used for simulating the geometrical transverse dipole wakefield in CLIC cells. The single cell, which was described in Section 5.6, is here repeated 20 times, and beam pipes attached to the ends.

pipes” were added to the entry and exit aperture of the structure. This was done in order to minimize the fields on the entry and exit apertures, which leads to reflections that creates unwanted standing waves [152]. The beam pipes used have an opening equal to the iris aperture of the structure, and a typical length of 30 mm. A detailed convergence study finding the appropriate mesh, finite element order, wake length, and damping waveguide boundary conditions is presented in [23].

As was discussed in Section 6.6, the primary modes of interest are dipole modes. A quarter-cell symmetry was therefore used, as it yields the smallest possible mesh. The symmetry planes used electric wall boundary condition on the  $y$ -axis and magnetic wall boundary condition on the  $x$ -axis, such as shown in Figure 2.6 and discussed in Section 2.4.2. To excite these modes, the beam enters the structure with a small offset  $\Delta_x$  from the geometrical centerline. One example of a simulation geometry is shown in Figure 6.1.

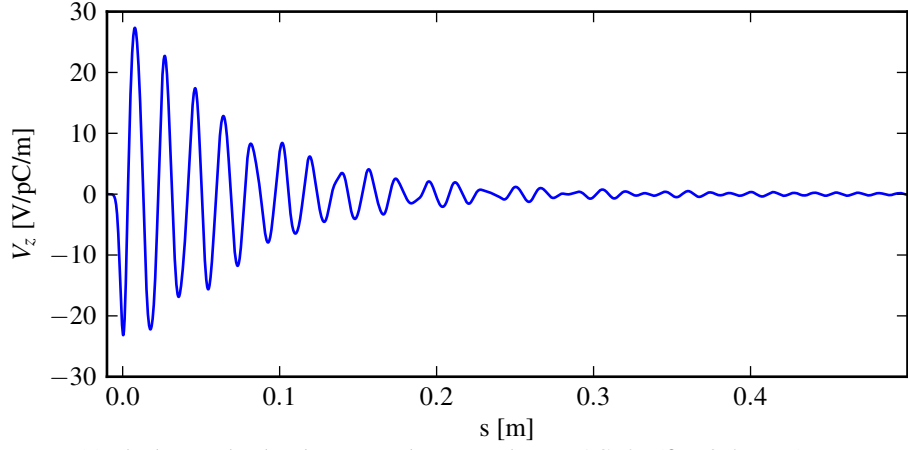
The primary output from the simulation is the longitudinal bunch potential<sup>2</sup>  $V_z(s)$ , as shown in Figure 6.2a. This can be converted to the transverse bunch potential  $V_x(s)$  using the Panofsky-Wenzel theorem as shown in Equation (6.32), taking only the  $x$ -component. This is done by finding the derivative  $\partial V_z(s)/\partial x$  and integrating over  $s$ , i.e.

$$\int_0^s \frac{\partial V_z(s')}{\partial x} ds' = \int_0^s \frac{\partial V_x(s')}{\partial s'} ds' = V_x(s) - V_x(0). \quad (6.45)$$

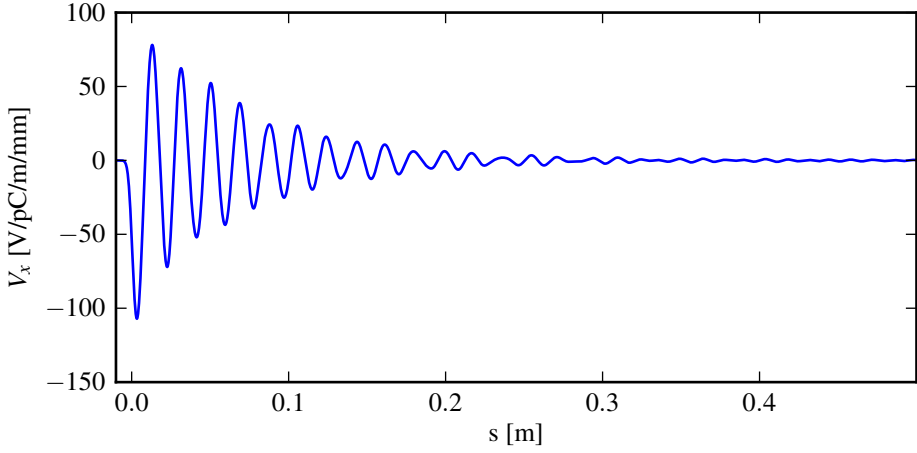
For calculating the partial derivative  $\partial V_z(s)/\partial x$ , the longitudinal wake is extracted along a line displaced by  $\Delta_x$ , and normally the same offset was used here as for the exciting beam. Further, since quarter-symmetry is used,  $V_z(s)|_{x=\Delta_x} = -V_z(s)|_{x=-\Delta_x}$ . The numerical

<sup>2</sup>In this case, the distinction between the bunch and wake potential does not matter, since the bunch potential is calculated for a bunch with unit charge (1 pC).

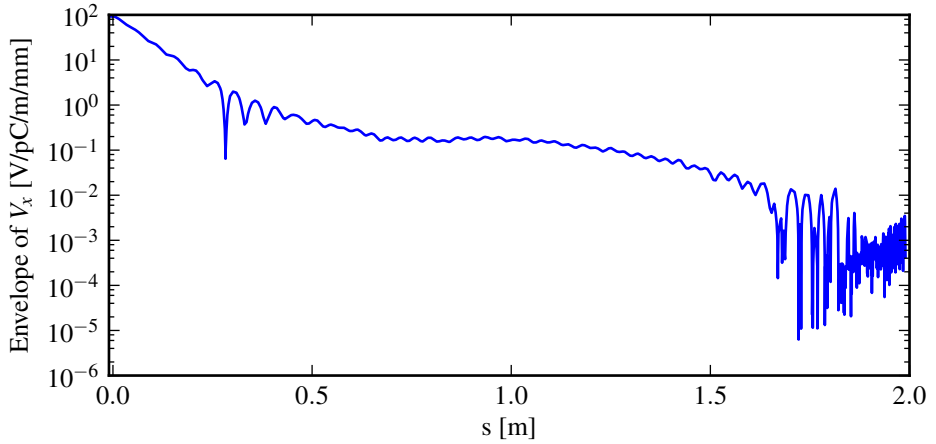
## 6. Wake fields



(a) The longitudinal wake potential computed using ACE3P (first 0.5 meter).



(b) Transverse wake potential calculated using the PWT (first 0.5 meter).



(c) Double peak-to-peak envelope of the transverse wake potential.

Figure 6.2.: Wake potential from the typical cell design presented in Section 5.6, i.e.  $a/\lambda = 0.15$ ,  $d/h = 0.25$ , version 1.



midpoint derivative is thus given as

$$\left. \frac{\partial V_z(s)}{\partial x} \right|_{x=0} \approx \frac{V_z(s)|_{x=\Delta_x} - V_z(s)|_{x=-\Delta_x}}{2\Delta_x} = \frac{V_z(s)|_{x=\Delta_x}}{\Delta_x}. \quad (6.46)$$

This is then integrated using Simpson method, which was chosen because it can be used with predetermined evaluation points  $s_i$ , and as it is easily adapted to quickly calculating the integral over all the domains  $[0, s_i] \forall i$ . This produces a transverse wake such as the one shown in Figure 6.2b.

The envelope, as shown in Figure 6.2c is found using a “double peak-jumper” algorithm. The algorithm is similar to the one which will be described in Section 7.9, except that in this case the wake is only defined at discrete points, and the peaks are simply defined as points which are larger or smaller than both its two neighbors. This finds the local maxima and minima of the oscillating function, and two piece-wise linear functions passing through these (one for the maxima and one for the minima) are then constructed. The envelope is then computed as half the difference between these two interpolating functions. This method avoids the problem that an accumulation of errors in the Simpson integration sometimes makes the transverse bunch potential “drift” off-center, making it impossible to track the decay of the oscillating functions down to very small values, as is required for the semi-logarithmic envelope plots.

### 6.7.1. Treatment of the impedance spectra

When the transverse bunch potential  $V_z(s)$  is computed, the impedance spectrum can be calculated using a Fourier transform. A typical impedance spectrum is shown in Figure 6.3a.

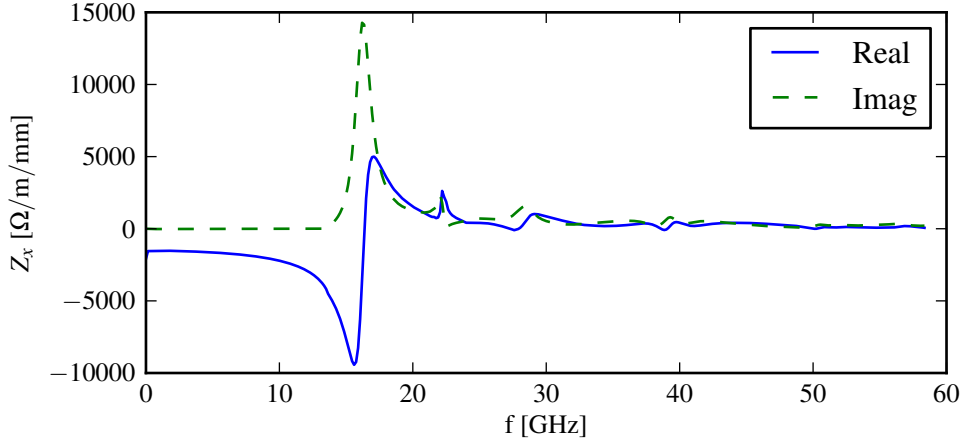
When calculating this, it is important to take into account that the available signal  $V_x(s)$  is the bunch potential excited by a Gaussian bunch  $\lambda(s)$ , and not the wake function  $W_x(s)$ , for which the impedance is defined. This means that higher frequencies are excited less strongly than the lower frequencies, as the Fourier transform of a Gaussian is another Gaussian, and their widths are inversely related. It is therefore necessary to deconvolute the signal in order to obtain the impedance spectrum  $\mathbf{Z}(f)$ , as shown in Equation (6.6). Further, this means that for high frequencies the excitation is close to zero, and the noise is thus dramatically amplified. This is remedied by removing all frequencies above

$$f_c = \frac{c\sqrt{3/2}}{\pi\sigma_z}, \quad (6.47)$$

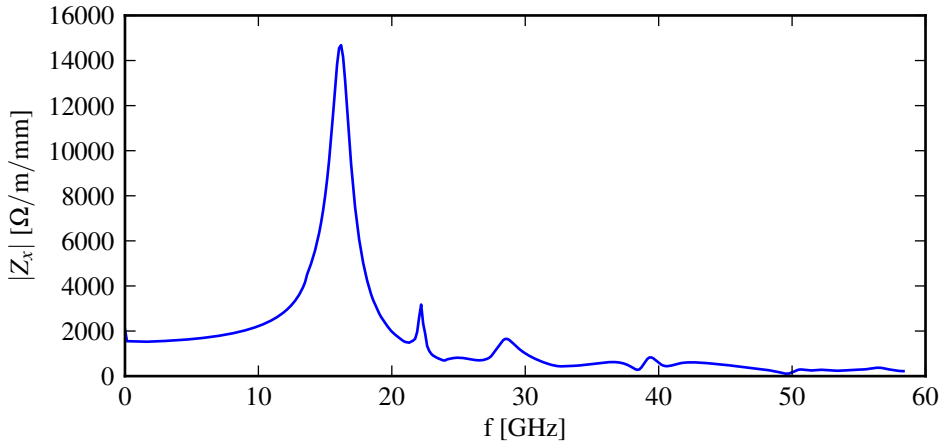
from the computed impedance spectra, where  $\sigma_z$  is the bunch length which was normally equal to 2.0 mm, corresponding to 58 GHz. This cutoff is chosen so that it happens when the current spectrum has fallen a factor  $\exp(-3)$  from the peak intensity (at  $f = 0$ ).

After obtaining the impedance spectrum, the absolute value  $|\tilde{Z}_x(f)|$  is taken and used for fitting the model impedance spectrum which was presented in Section 6.2.1. The details of how the model was fitted to  $|\tilde{Z}_x(f)|$  and the accuracy of the obtained data is explained in [23]<sup>3</sup>. This procedure produced usable estimates for the parameters of the dipole modes.

<sup>3</sup>Note that in [23], the convention for  $k$  is number full oscillations per unit length, not radians per unit length as in this document.



(a) Impedance, both real and complex part.



(b) Absolute value of the impedance function, used for fitting.

Figure 6.3.: Transverse impedance from the typical cell design presented in Section 5.6, with  $a/\lambda = 0.15$ ,  $d/h = 0.25$ , version 1.

### 6.7.2. Wake field damping waveguides

As was discussed in Section 5.1, each cell in the CLIC RF structures are equipped with four damping waveguides. These allow the energy stored in the higher order modes to radiate out from the central chamber of the cell (where the beam is), greatly lowering their Q-factor. At the same time, the cutoff of the damping waveguides being above the 12 GHz of the accelerating mode means that this mode does not leak into it, keeping its Q-factor high.

In the actual CLIC RF structures, the damping waveguides are terminated by a Silicon Carbide (SiC) loads [153, 154]. These absorb the energy radiated out of the cells, with very small reflections. In the simulations presented here, these loads are approximated as an infinitely long waveguide. This was done using a waveguide boundary condition [155], which works by decomposing as much as possible of the incident wave into a sum of known waveguide modes, which may then be absorbed. This is done separately for each of the waveguide modes propagating through the damping waveguides. As a test and comparison, a 1.0 m long wake was also computed using 500 mm long damping waveguides [23], ensuring that the reflection from the end of the waveguides were not able to reach any of the “test particles” that are used for calculating the wake field. This test showed that the waveguide boundary condition does successfully emulate an infinitely long wave guide.

In the actual CLIC structures, the damping waveguides have an almost rectangular cross-section, with a small rounding in two corners along the same long edge, as shown in Figure 5.1. This rounding means that the waveguide modes are not exactly the same as usually found in a rectangular waveguide, and must thus be found numerically. While this is supported by ACE3P, the very large number of such waveguides needed proved to be problematic, making the simulations very heavy and crash-prone. The problem was therefore avoided by making a gradual transition to a rectangular waveguide, where an analytical solution for the guided waves could be used. The scattering parameters of these transitions were computed for many modes and frequencies, and compared to the those for a constant cross-section waveguide piece [23]. This showed that the error introduced by this transition was negligible.

A set of rectangular waveguide modes are shown in Figures 6.4 and 6.5. These plots were made by solving the modes in a very thin, rectangular geometry, with the end-wall being electric walls (for TM modes) or magnetic walls (for TE modes). In the quarter-cell geometry shown in Figure 6.1, each of the waveguides are divided by an electric- or magnetic wall boundary which halves the length of the long edges. For this, it was found (as also seen in the plots) that if the first mode index is divisible by two, the mode is permitted by electric wall symmetry, while the other modes are permitted by magnetic wall symmetry.

Each of the modes have a cutoff frequency [156]

$$f_c = \frac{c}{2} \sqrt{\left(\frac{n}{A}\right)^2 + \left(\frac{m}{B}\right)^2}, \quad (6.48)$$

which is the lowest frequency that can be effectively transmitted through a long waveguide. In this equation,  $A$  is the length of the long side of the waveguide, and  $B$  the short side. For the simulations, enough modes were included at each waveguide port so that that the first mode not included was the first mode where the cutoff frequency was higher than the bunch cutoff from Equation (6.47). This means that typically, for each waveguide port the lowest 10 modes obeying the boundary conditions were used.

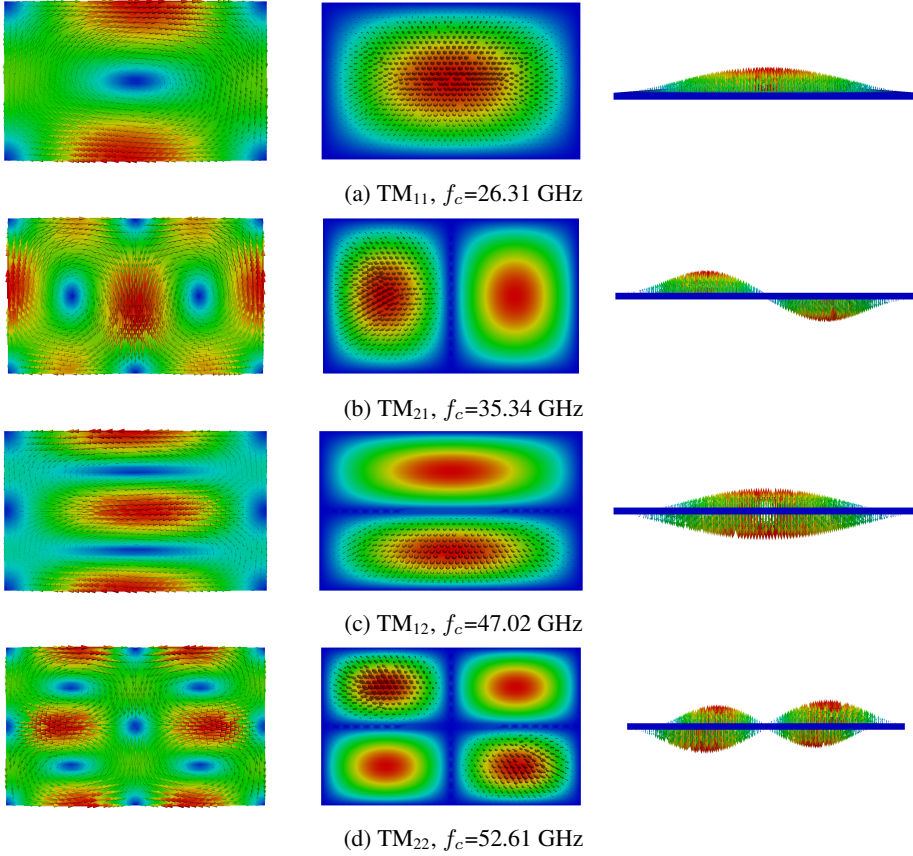


Figure 6.4.: Some examples of TM-type waveguide modes in a rectangular crosssection with long edge length  $A=11$  mm and short edge  $B=6.6617$  mm. From left to right: B-field (cross section), E-field (cross section) and E-field (side view).

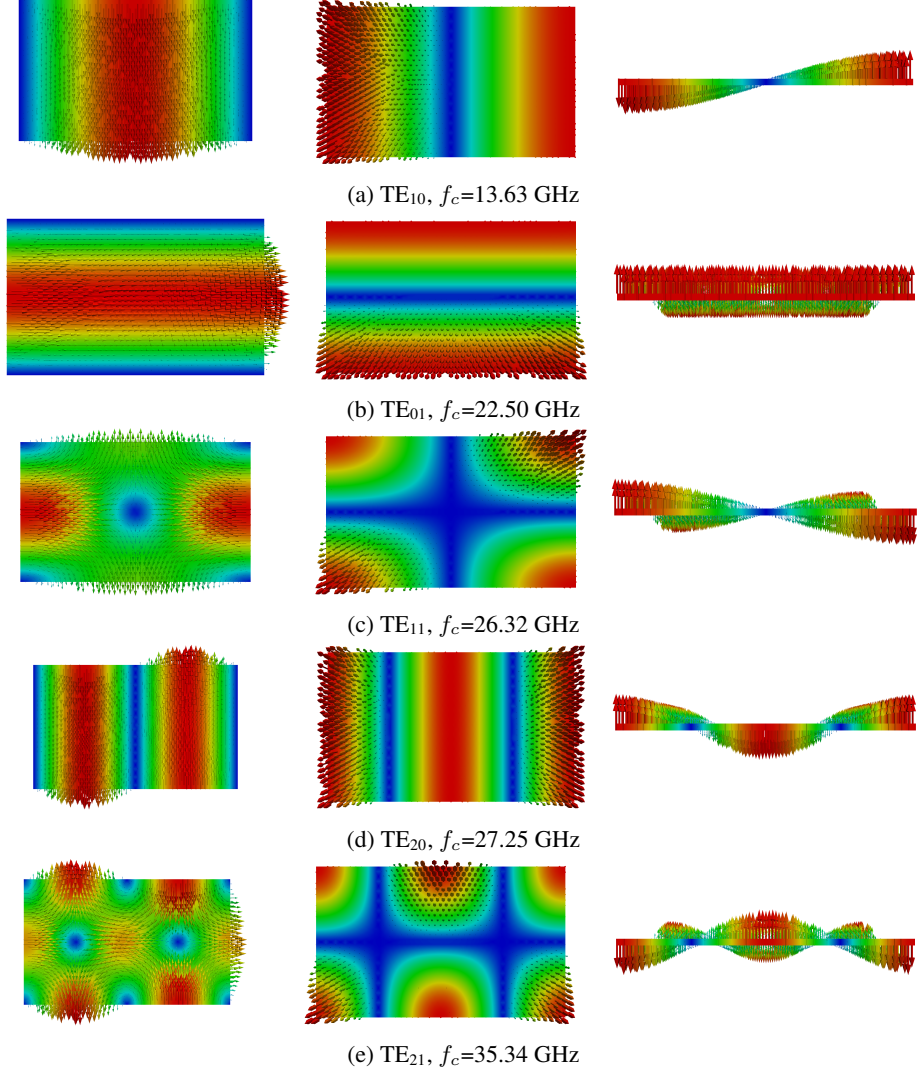


Figure 6.5.: Some examples of TE-type waveguide modes in a rectangular crosssection with long edge length  $A=11$  mm and short edge  $B=6.6617$  mm. From left to right: E-field (cross section), B-field (cross section) and B-field (side view).

## 6. Wake fields

| $\frac{a/\lambda}{d/h}$ | 0.07  | 0.11   | 0.15   | 0.19   | 0.23   | Variable  | [unit]      |
|-------------------------|-------|--------|--------|--------|--------|-----------|-------------|
| 0.1                     | 17.79 | 17.17  | 16.09  | 15.107 | 14.38  | Frequency | [GHz]       |
|                         | 6.22  | 8.03   | 12.1   | 16.6   | 21.6   | Q-factor  |             |
|                         | 264   | 189    | 119    | 75.6   | 51.2   | Amplitude | [V/pC/mm/m] |
| 0.25                    | 17.38 | 17.041 | 16.180 | 15.254 | 14.486 | Frequency | [GHz]       |
|                         | 6.76  | 8.6    | 11.713 | 17.6   | 28.33  | Q-factor  |             |
|                         | 245   | 184.5  | 127.74 | 79.6   | 33.89  | Amplitude | [V/pC/mm/m] |
| 0.4                     | 16.90 | 16.37  | 15.883 | 15.182 | 14.456 | Frequency | [GHz]       |
|                         | 7.74  | 10.38  | 12.93  | 17.52  | 25.7   | Q-factor  |             |
|                         | 214.3 | 146.07 | 114.22 | 79.23  | 51.6   | Amplitude | [V/pC/mm/m] |

Table 6.1.: Wake parameters for the 1<sup>st</sup> dipole mode, cell database version 1.

### 6.7.3. Wake fields from typical cell design and the cell database

The wake field from a typical cell is shown in Figure 6.2, and the corresponding impedance in Figure 6.3. This cell comes from the cell database version 1 and has the parameters  $a/\lambda = 0.15$  and  $d/h = 0.25$ . The cell database is discussed in detail in [23], and as will be described in Chapter 7 and in [24], the purpose of the cell database is to quickly estimate the parameters of a full RF structure, including the wakefield. This is necessary for when doing an overall optimization of the full machine, comparing energy reach, luminosity potential, power requirements, costs etc. The details of the how these structure parameters are estimated are discussed in Chapter 7 and in [24]. Further, parameters of the first dipole mode in the cells from database version 1 are listed in Table 6.1 and plotted in Figure 6.6.

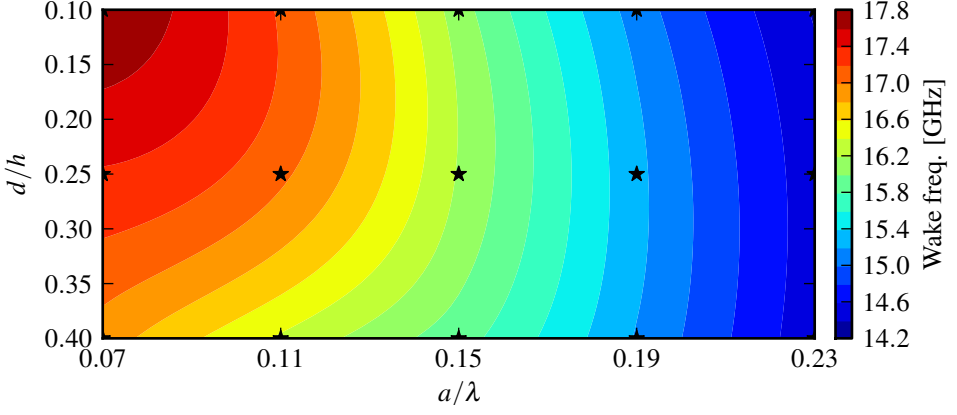
The impedance spectrum for the selected cell is rather typical for the cells moderate to large opening  $a/\lambda$ . It shows a large peak around 16 GHz, followed by several smaller peaks, the second one (around 22 GHz) being rather narrow and sometimes difficult to find.

If in the cell database one is looking at cells with very small  $a/\lambda$ , the peaks at higher frequencies becomes much more prominent, and many resonances appear which are not seen for the more open cells. Conversely, the more open cells have much fewer significant resonances, and as seen in Figure 6.6c, the main dipole mode is weaker as well – however the Q-factor is significantly higher. This is likely a consequence of the frequency being lower, shifting it closer to the first cutoff frequency of the damping waveguides at 13.6 GHz for TE<sub>10</sub>.

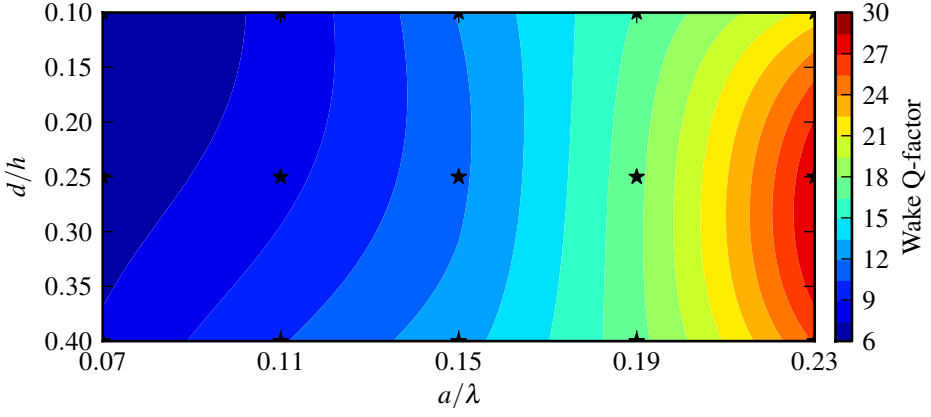
The geometry parameter  $d/h$  is seen to have a smaller effect than  $a/\lambda$ , at least for the larger openings. For the smaller openings, the main effect of increasing the iris thickness is to decrease the main dipole mode frequency. Further, higher modes becomes relatively weaker, and between  $d/h = 0.1$  and  $d/h = 0.25$ , there is a strong and sharp resonance which shifts down in frequency from  $\approx 38$  GHz to  $\approx 22$  GHz.

The two database versions are most different for large  $a/\lambda$  and large  $d/h$ , while for small  $a/\lambda$  no differences exists as the cells are identical. The main difference seen is that the version 1 cells, which have more “square” irises, have fewer and weaker higher modes.

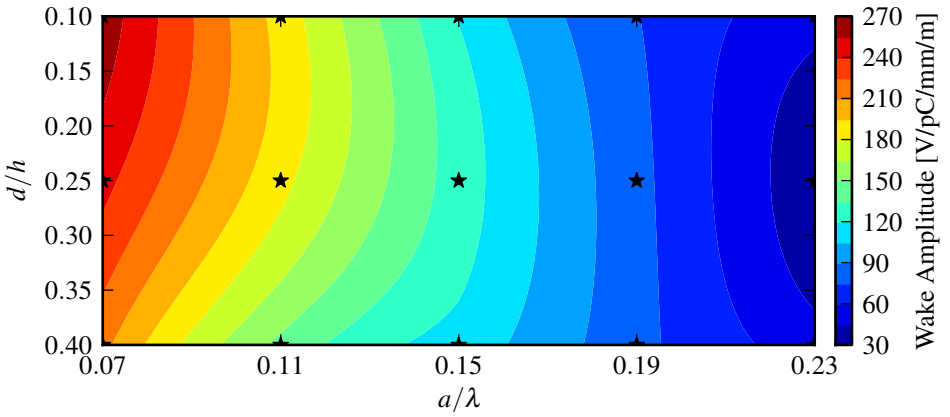
When creating the cell database, only the first mode was used, since it is strong and is present in all the designs. Further, the higher modes are sometimes difficult to find, and since their parameters are much more variable, the type of interpolation which is used difficult.



(a) Wake frequency [GHz]



(b) Wake Q-factor



(c) Wake amplitude [V/pC/mm/m]

Figure 6.6.: Wakefield parameters for the 1<sup>st</sup> dipole mode, cell database version 1. Note that the  $y$ -axis is inverted in order to match the layout of the tables.

## 6.8. Summary and conclusions

As shown in this chapter, a robust method was developed for calculating the transverse wake field in the waveguide damped structures using ACE3P. This is done by calculating the wake with T3P, taking the damping waveguides into account, and then extracting the impedance spectrum. The method was then applied to the accelerating cell geometries described in Chapter 5, yielding the parameters of the first transverse wakefield mode. As was discussed in Section 6.7.3, these mainly show a clear dependency on the iris aperture  $a/\lambda$ , with the frequency dropping while Q-factor increases with increasing aperture. Further, when comparing the smallest to the largest iris aperture, the wake amplitude decreases by almost an order of magnitude. This table is incorporated into the cell database, used to quickly estimate the parameters of a whole RF structure, as described in Chapter 7.



## 7. Structure parameter calculation

This chapter describes a model for predicting the performance of a traveling wave accelerating structure based on its length, iris aperture, tapering etc., using the cell designs described in Chapter 5 and 6. This is implemented in the C++ library “CLICopti”, which is described in detail in [24]. The purpose of CLICopti is to be used as the RF structure performance model inside the larger framework used for the overall optimization of the CLIC machine [157].

At the base of CLICopti is an analytic method [158] for calculating the steady state gradient profile  $G(z)$  from the structure geometry, the input power  $P_0$  and the beam loading current  $I$ . In the gradient profile calculation, the structure geometry is described via its length  $L$  and the structure RF parameters  $v_g(z)$ ,  $R'(z)$  and  $Q(z)$  as a function of the coordinate  $z$  along the length of the structure. Knowing the gradient profile  $G(z)$ , the peak fields  $\hat{E}$ ,  $\hat{S}_c$  and  $\hat{H}$  as well as  $P_+/C$  can be calculated. Together with the breakdown and pulsed surface heating limits that were discussed in Section 3.3.1, these are used to estimate the maximum allowable pulse length. Finally, knowing the structure geometry, also the long range dipole wake can be estimated by summing over the single-cell wakes.

Sections 7.1, 7.2 and 7.3 will present the method for converting the overall structure parameters used in the machine optimization, such as the length, aperture and tapering, into the RF parameters ( $v_g(z)$  etc.) used by the steady state field profile calculation. Then, the steady-state field profile calculation and the relationship between the input power, beam current and accelerating voltage will be presented in Section 7.4 and 7.5. Further, the pulse shape, RF-to-beam energy efficiency, and the estimation of maximum pulse length will be discussed in Section 7.6, 7.7 and 7.8. At last, the transverse wake estimation will be presented in Section 7.9, and the validation of the method presented in this chapter and its implementation (CLICopti) will be presented in Section 7.10.

### 7.1. Converting cell geometry parameters to cell RF parameters: the cell database

While the structure RF parameters as a function of  $z$  are needed in order to calculate the field profile, the user (i.e. the machine optimization program) will typically provide geometry parameters such as the iris aperture  $a$  and thickness  $d$  for the first and last cell. These geometry parameters are used to look up the cell RF parameters for from the cell database, which was presented in Section 5.7 and 6.7.3. For this to work, it must be possible to look up the RF parameters of any point in the  $(a, d)$  parameter space, not just at the few exact points where specific cell designs are available. Some kind of interpolation is therefore needed. This interpolation is usually done using a 2<sup>nd</sup> order spline surface for each of the RF parameters under consideration, such that the sub-surfaces are constructed from the 9 nearest  $(a, d)$ -points. The resulting interpolating surfaces are continuous and pass through all the points in the database. Examples of such interpolated surfaces are shown in Figures 5.12

## 7. Structure parameter calculation

and 6.6. In CLICopti, this interpolation is done by the “cell database interface” code [24, Chapter 3].

### 7.2. Frequency scaling

It is often necessary to scale the design of an accelerating structure or cell, moving the frequency  $f$  of the main mode to a new frequency  $f'$ . This is done by changing the size of the cavity, such that the geometrical length scale  $\ell$  scales proportionally to the accelerating mode free space wavelength  $\lambda$ , which again is proportional to  $1/f$ . A further assumption is that the configuration of the field patterns do not change, only their spatial extension and oscillation frequency.

#### 7.2.1. Accelerating mode parameters

The parameters used for describing an accelerating mode is the Q-factor, the normalized shunt impedance  $R'$  and the normalized peak fields  $\bar{E}$ ,  $\bar{H}$  and  $\bar{S}_c$ . In a traveling wave structure the group velocity  $v_g$  is also needed.

Assuming that only the spatial extension and frequency of the field patterns changes when rescaling the cell size implies that the normalized peak fields  $\bar{E}$ ,  $\bar{H}$  and  $\bar{S}_c$  are invariant under frequency scaling. Also invariant is the phase advance per cell  $\psi$  of a traveling wave structure, as  $\psi = hf2\pi/v_p \propto \ell f/v_p \propto 1$  where the phase velocity  $v_p$  is constant and fixed by the particle velocity.

Several of the other quantities can be expressed using the stored energy per cell  $U$ , the surface power dissipation  $P$  averaged across one cycle, and the shunt impedance per length  $R'$ .

The stored energy is given by Equation (2.41), and the stored energy in steady state is constant for a given field level  $F$ , to which both the electric- and magnetic field is everywhere proportional. Further, the volume is proportional to  $\ell^3$ . The stored energy thus has the following scaling:

$$U \propto F^2 \ell^3 \propto F^2 \lambda^3. \quad (7.1)$$

Similarly, the power dissipation  $P$  averaged over one cycle is given by Equation (2.40). As the surface area is proportional to  $\ell^2$ ,  $\mathbf{H} \propto F$  and the RF surface resistance  $R_s \propto \sqrt{f}$ , this implies that  $P$  scales as

$$P \propto F^2 \lambda^{3/2}. \quad (7.2)$$

For the shunt impedance per unit length  $R'$ , using Equation (2.6) and that the average gradient  $G = V/L \propto F$  (where  $L$  is the length of the cavity), this can be expressed as

$$R' = R/L = \frac{V^2/P}{L} = \frac{F^2 L}{P}. \quad (7.3)$$

Combined with Equation (7.2), this leads to the scaling

$$R' \propto \frac{F^2 \lambda}{F^2 \lambda^{3/2}} = \lambda^{-1/2}. \quad (7.4)$$

Using the scaling relations shown in Equations (7.1) and (7.2), the accelerating mode quality factor scales as

$$Q = \frac{\omega \cdot U}{P} \propto \frac{\lambda^{-1} \cdot \lambda^3 F^2}{F^2 \lambda^{3/2}} = \sqrt{\lambda} \propto \frac{1}{\sqrt{f}}. \quad (7.5)$$

Combining this with Equation (7.4),  $R'/Q$  scales as

$$\frac{R'}{Q} \propto \frac{\lambda^{-1/2}}{\lambda^{1/2}} = \lambda^{-1} \propto f. \quad (7.6)$$

The group velocity  $v_g$  of a cell in a traveling wave structure is given by Equation (2.15), where  $P_+$  is given by Equations (2.44), such that  $P_+ \propto F^2/f^2$ . Combining this with Equations (2.15), (7.1) and the scaling of geometrical lengths  $\ell \propto \lambda$ , the scaling behavior of the group velocity is given as

$$v_g \frac{P_+}{U/h} \propto \frac{\lambda^2 F^2}{F^2 \lambda^3 / \lambda} = 1. \quad (7.7)$$

The group velocity is therefore constant with frequency and gradient.

### 7.2.2. Transverse wakefield mode parameters with waveguide damping

In addition to the accelerating mode, the cavity may have one or more *wakefield* modes. These are modes with a different field pattern and frequency than the main mode, such as the  $\text{TM}_{1,1,0}$  mode shown in Figure 2.6. Some of these modes can be excited by the beam when it passes through the cavity, creating the wakefield which is the sum of these modes. The primary discussion of wakefields is found in Chapter 6. The discussion in this subsection is specific to structures or cells where the waveguide modes are primarily damped by radiation through damping waveguides, as is the case for CLIC waveguide damped structures.

For the wakefield frequency  $f_w$ , it may simply be assumed that  $f_w \propto 1/\lambda_w$  where  $\lambda_w$  is the wakefield wavelength. As all the modes are scaled together with the cells,  $\lambda_w \propto \ell \propto \lambda \propto 1/f$ , and thus  $f_w \propto f$ .

The wakefield quality factor  $Q_w$  is given by Equation (2.5) in the same way as for the main mode. As the loss through the damping waveguides dwarfs the loss from surface resistance, the total power loss can be found by integrating the power flow through the waveguides

$$P_w = \int_{\Gamma_{\text{WG}}} \vec{S} \cdot d\vec{\Gamma}, \quad (7.8)$$

where  $\vec{S}$  is the Poynting vector and  $\Gamma_{\text{WG}}$  is a (discontinuous) surface which covers all the damping waveguides. Knowing that  $\vec{S} = \vec{E} \times \vec{B}/\mu_0 \propto F^2$ , where  $F$  represents the field level of the wake mode, the power loss scales as  $P_w \propto F^2 \ell^2 \propto F^2/f^2$ , since  $\Gamma_{\text{WG}} \propto \ell^2$ . The stored energy  $U_w$  scales the same way as for the accelerating mode (Equation (7.1)). Combining these relations, the quality factor of the wakefield mode can be written as

$$Q_w = \frac{\omega_w U_w}{P_w} \propto \frac{f \cdot F^2 f^{-3}}{F^2 f^{-2}} \propto 1, \quad (7.9)$$

which shows that the wakefield quality factor does not scale with the main mode frequency.

In order to find the scaling relation for the wakefield amplitude  $A_w$ , a useful starting point is the loss factor  $k_w$  [159, Equation (3.257)] of the mode, which is given as

$$k_w = \frac{\omega_w R'_w L}{4Q_w} \quad (7.10)$$

## 7. Structure parameter calculation

where  $\omega_w = 2\pi f_w$ ,  $R'_w$  is the wakefield longitudinal shunt impedance per unit length of the wakefield mode and  $L$  is the cavity length. Further, the longitudinal voltage left behind in the cavity by a  $\delta$ -function bunch of charge  $q$  is given as

$$V_w = 2k_w q, \quad (7.11)$$

where  $V_w \propto FL \propto F\ell \propto F/f$  such that  $F \propto fV_w = f2k_w q$ . Further, the loss factor scales as  $k_w \propto fR'_w L/Q_w \propto R'_w/Q_w$ . Combining these leads to the scaling relation  $F \propto fR'_w/Q_w$ . As discussed above, in the case of waveguide damped accelerating structures, the wakefield modes are primarily damped by radiation through the damping waveguides, and not through surface losses. Thus to find the scaling relation for the wakefield amplitude, the scaling of  $R'_w/Q_w$  with radiation losses must be found. It is already known that  $Q_w \propto 1$ , and the shunt impedance per unit length is given as

$$R'_w = \frac{V_w^2/P_w}{L} \propto \frac{F^2 L^2}{F^2/f^2} f \propto \frac{F^2/f^2}{F^2/f^2} f \propto f. \quad (7.12)$$

This means that  $R'_w/Q_w \propto f$ , and  $F \propto f^2$ . Knowing how the wake field level scales with main mode frequency  $f$ , the wake amplitude  $A_w$  can be found by noting that it is normalized to the beam offset  $\Delta x$ . In order for the beam to see the same field patterns (and not intersect the cavity walls), this offset must be scaled as well, such that  $\Delta x \propto \ell \propto f^{-1}$ . The scaling relation for the wakefield amplitude is therefore given as

$$A_w \propto \frac{F}{\Delta x} \propto \frac{f^2}{f^{-1}} = f^3. \quad (7.13)$$

### 7.3. Parameter interpolation along the RF structure

While the cell database can be used to find the RF parameters of a cell with arbitrary iris aperture  $a$  and thickness  $d$  (Section 7.1), the field profile calculation needs the RF parameters as continuous functions of  $z$ . This is done using a quadratic interpolation of each of the parameters along the length of the structure, with interpolation points at  $z_0 = 0$ ,  $z_1 = L/2$  and  $z_2 = L$ , where  $L$  is the length of the structure. These interpolation points are found by using the cell database to look up the RF parameters of the first, last, and middle cell, as shown in Figure 7.1. For this, the structures are assumed to have a linear tapering, such that the iris parameters of the middle cell is the average of the first- and last-cell iris parameters, which are directly specified by the user. The parameters are then interpolated along the structure as a Lagrange polynomial

$$\begin{aligned} F(z) = & F_0 \frac{(z - z_1)(z - z_2)}{(z_0 - z_1)(z_0 - z_2)} \\ & + F_1 \frac{(z - z_0)(z - z_2)}{(z_1 - z_0)(z_1 - z_2)} \\ & + F_2 \frac{(z - z_0)(z - z_1)}{(z_2 - z_0)(z_2 - z_1)}, \end{aligned} \quad (7.14)$$

where the interpolation points  $F_0, F_1, F_2$  are the values of the interpolated function  $F$  (i.e. the RF parameter) evaluated at the interpolation points  $z_0, z_1$  and  $z_2$ .

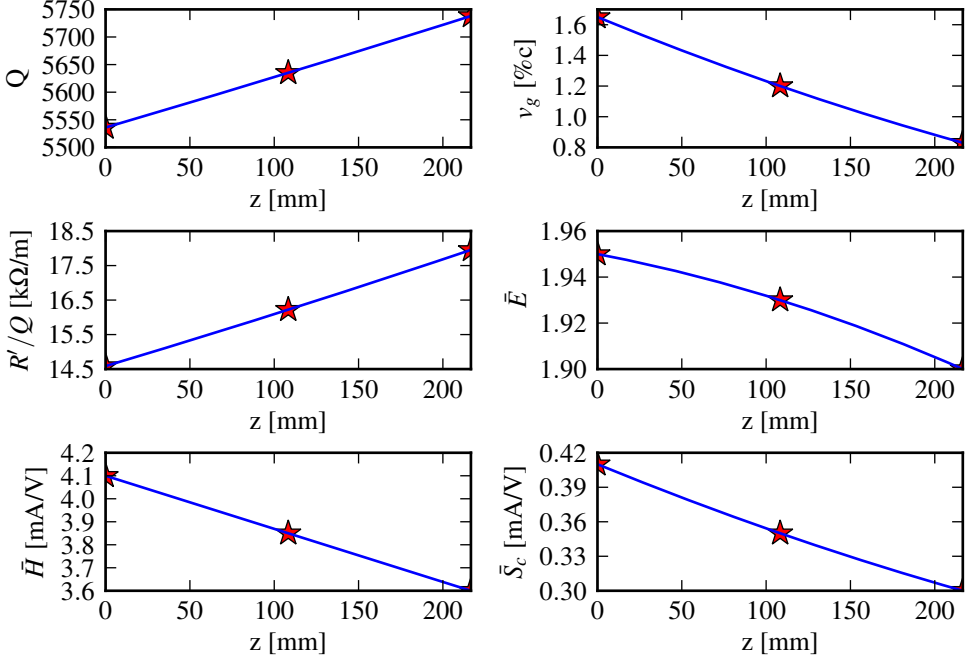


Figure 7.1.: Main RF parameters for CLIC\_G R05 [160] with 26 cells, plotted along the length of the structure. Interpolation points located at  $z = 0$ ,  $z = L$  and  $z = L/2$ , where  $L$  is the length of the structure, are indicated with red stars.

## 7.4. Field profile

The field profile is calculated using the analytical method derived in [158]. It is based on the power flow through a traveling wave structure at steady state, and is valid under the assumptions that the structure is perfectly matched at both ends and that the time of separation between each bunch is much less than the filling time of the structure.

The basic relation is that of instantaneous energy conservation, and is given as

$$\frac{\partial U'}{\partial t} = -\frac{dP_+}{dz} - \frac{U'\omega}{Q} - GI, \quad (7.15)$$

where  $U'$  is the stored energy per unit length,  $P_+$  the power flowing through the structure (as defined in Section 2.4.3),  $\omega = 2\pi f$  where  $f$  is the oscillation frequency,  $Q$  the quality factor,  $G$  the accelerating gradient and  $I$  the beam current. All of these, with the exception of  $\omega$  and  $I$ , are functions of the position  $z$  along the structure. Further,  $G$  and  $I$  can also be functions of the time  $t$ , where  $t = 0$  when the power is first switched on.

In order to find the steady state solution,  $\frac{\partial U'}{\partial t} = 0$  is assumed. Further, a useful slight rearrangement of Equation (2.15) is

$$P_+ = U'v_g, \quad (7.16)$$

## 7. Structure parameter calculation

and Equations (2.5) and (2.6) can be combined to yield the relation

$$U' = \frac{G^2}{\omega \frac{R'}{Q}}, \quad (7.17)$$

where  $R'$  is the shunt impedance per unit length. Combining Equations (7.16) and (7.17) and taking the derivative with respect to  $z$  yields

$$\begin{aligned} \frac{dP_+}{dz} &= \frac{d}{dz} \left( \frac{G^2(z) v_g(z)}{\omega \frac{R'}{Q}(z)} \right) \\ &= \frac{G^2}{\omega \frac{R'}{Q}} \frac{dv_g}{dz} + \frac{v_g}{\omega} \left( \frac{2G}{\frac{R'}{Q}} \frac{dG}{dz} - \frac{G^2}{(\frac{R'}{Q})^2} \frac{d(\frac{R'}{Q})}{dz} \right). \end{aligned} \quad (7.18)$$

Similarly, solving Equation (7.15) with  $\frac{\partial U'}{\partial t} = 0$  for  $\frac{dP_+}{dz}$ , removing  $U'$  by using Equation (7.17) and combining with Equation (7.18) results in the first order nonhomogenous differential equation with variable coefficients

$$\frac{dG}{dz} = -G(z) \alpha(z) - \beta(z), \quad (7.19)$$

where the coefficients are given as

$$\alpha(z) = \frac{1}{2} \left( \frac{1}{v_g} \frac{dv_g}{dz} - \frac{1}{\frac{R'}{Q}} \frac{d(\frac{R'}{Q})}{dz} + \frac{\omega}{Q v_g} \right) \text{ and} \quad (7.20)$$

$$\beta(z) = I \frac{\omega \frac{R'}{Q}}{2v_g}. \quad (7.21)$$

The general solution of Equation (7.19) can be written as

$$G(z) = G_0 g(z) - I g_L(z), \quad (7.22)$$

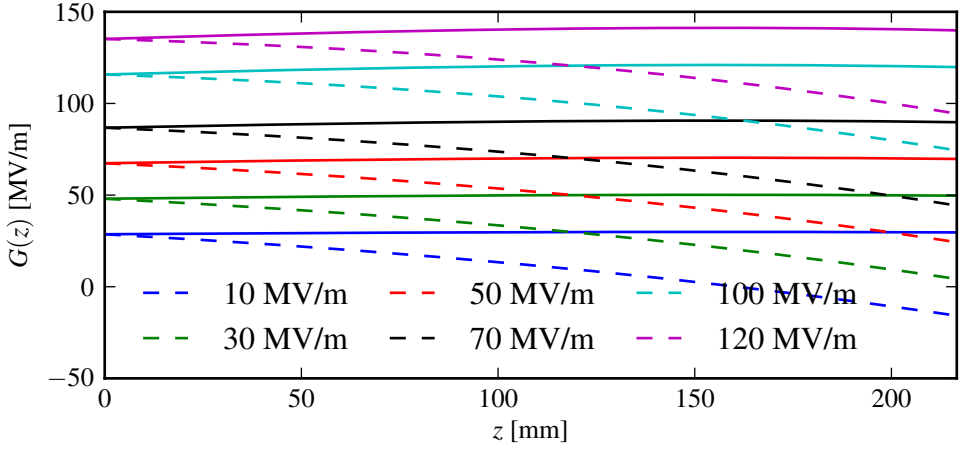
where

$$g(z) = \sqrt{\frac{v_g(0) \frac{R'}{Q}(z)}{v_g(z) \frac{R'}{Q}(0)}} \exp \left[ -\frac{1}{2} \int_0^z \frac{\omega}{v_g(z') Q(z')} dz' \right], \quad (7.23)$$

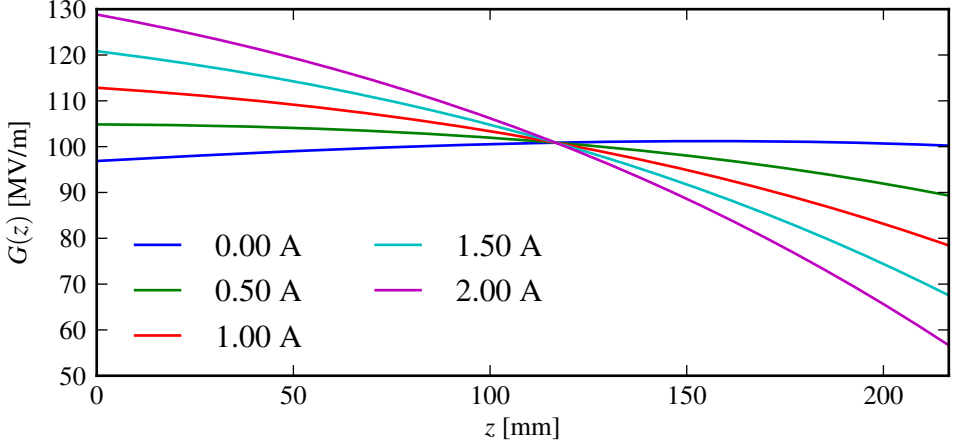
$$g_L(z) = g(z) \int_0^z \frac{\omega \frac{R'}{Q}(z')}{g(z') 2v_g(z')} dz', \quad (7.24)$$

$$G_0 = \sqrt{\frac{\omega \frac{R'}{Q}(0) P_0}{v_g(0)}}, \quad (7.25)$$

and  $P_0$  is the input power of the structure. Equation (7.22) is used by CLICopti for calculating the gradient profile, which is the basis for calculating the required input power to reach a given accelerating voltage at a given beam loading, and for estimating the pulse length limits.



(a) Loaded and unloaded gradient profiles  $G(z)$  for input powers corresponding to the listed average loaded gradients at beam current  $I = 1.19$  A.



(b) Gradient profiles  $G(z)$  with average gradient  $\langle G \rangle = V/L = 100$  MV/m and different beam currents.

Figure 7.2.: Gradient profiles for CLIC\_G R05 [160] with 26 cells and different input powers and beam loading currents.

## 7. Structure parameter calculation

### 7.5. Power and voltage

Knowing the field profile from Equation (7.22), the accelerating voltage  $V$  at a given  $G_0(P_0)$  and  $I$  is given as

$$V = \int_0^L G(z) dz = G_0 \int_0^L g(z) dz - I \int_0^L g_L(z) dz, \quad (7.26)$$

where  $L$  is the length of the structure. The input power  $P_0$  required to reach a certain loaded voltage  $V$  can then be calculated as

$$P_0 = \frac{v_g(0)}{\omega \frac{R'}{Q}(0)} \left( \frac{V + I \int_0^L g_L(z) dz}{\int_0^L g(z) dz} \right)^2. \quad (7.27)$$

As an example, Figure 7.2 shows a number of gradient profiles as calculated using Equation (7.22) in the same structure. For this, the input powers  $P_0$  (and thus the input gradient  $G_0$ ) required for the given gradients and beam currents were found using Equation (7.27).

### 7.6. Pulse shape

The pulse shape used for the RF-to-beam efficiency and max pulse length calculations presented in Sections 7.7 and 7.8 is a simplified version of a typical CLIC pulse. As seen in Figure 7.3, this pulse is described by five segments – a linear ramp in power from  $P = 0$  to  $P_{\text{start}}$  in the time  $t_r$  (as rapid as allowed by dispersion effects), followed by a linear ramp from  $P_{\text{start}}$  to  $P_0$  in the time  $t_f$  to compensate for the transient beam loading during beam injection. The power is then constant for a time  $t_b$ , powering the structure for as long as a beam is present in the structure. Finally, the power drops off such that  $P(t) = P_0 - P(t - t_r - t_f - t_B)$  (mirroring the rising edge), as the pulse shape is generated by offsetting bunches in a drive beam [18, 161].

The rise time of the structure  $t_r$  is estimated by scaling the parameters of the CLIC\_G structure [18], using the scaling relation

$$t_r = t_{r0} \frac{\psi}{\psi_0} \frac{v_{g0}}{\check{v}_g}, \quad (7.28)$$

where  $t_{r0} = 21.0$  ns,  $v_{g0} = 0.83c$  and  $\psi_0 = 120^\circ$  are the CLIC\_G parameters. The parameters from the current structure are the phase advance per cell<sup>1</sup>  $\psi = \omega h$  and the minimum group velocity  $\check{v}_g = \min \{v_g^{(0)}, v_g^{(1)}, v_g^{(2)}\}$ .

This scaling relation comes from the proportionality  $t_r \propto Q_E$ , where  $Q_E$  is the external quality factor of the cell with the largest  $Q_E$ . The external quality factor is used as it dominates the quality factor  $Q_0$  from resistive losses, and the cell with smallest group velocity is used as this has the smallest bandwidth and thus largest risetime. The external quality factor is as usual defined as  $Q_E = \omega U / P$ , where the power  $P$  here is equal to the power through the iris  $P_+$ , and  $U$  the stored energy of the cell. This is again related to the group velocity, as  $v_g = P_+ / (U/h)$ . Combining these yields  $Q_E = \frac{\omega h}{v_g}$ , and assuming that the phase velocity is synchronous with the beam means that  $\omega h = c\psi$ . Further, combining these yields  $t_r \propto Q_E = \frac{c\psi}{v_g}$ , which is equivalent to the scaling relation in Equation (7.28).

<sup>1</sup>Whenever  $\psi$  appears in an equation, is given in units of radians/cell.



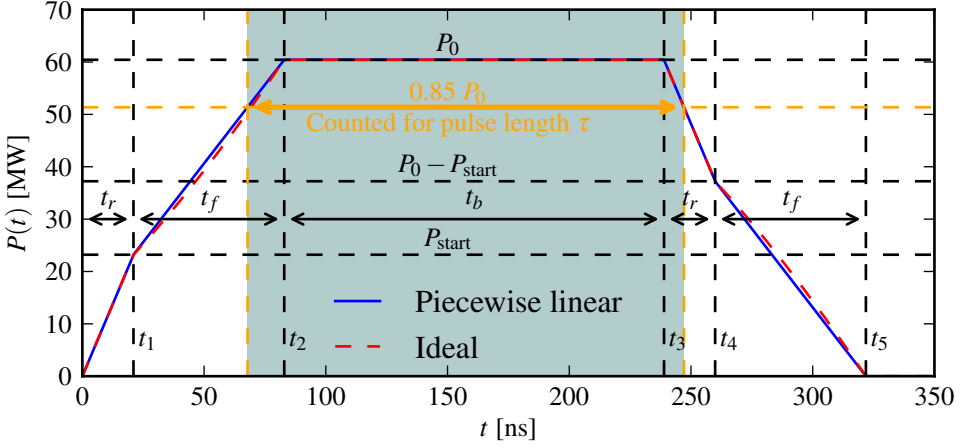


Figure 7.3.: Pulse shape for CLIC\_G R05 [160] with 26 cells, with  $P_0 = 60.4$  MW,  $P_{\text{start}} = 22.3$  MW,  $t_b = 156$  ns. This produces an average gradient  $\langle G \rangle = 100$  MV/m with a beam loading current  $I = 1.19$  A.

The 2<sup>nd</sup> ramp over time  $t_f$  is there to compensate for the transient beam loading when injecting the beam. If this ramp is omitted and the structure instead just filled with an input power  $P_0$  for a time  $t_f$  before injecting the beam, the first bunches in the train would see the unloaded gradient profile (see Figure 7.2) and thus a greater voltage than the bunches later in the train, which would see the loaded profile. This would lead to a spread in accelerating voltage, creating a spread in energy along the bunch train. In order for all bunches to see the same total voltage in the cavity, the input power is modulated such that the first bunches see an unloaded cavity powered with a smaller input power, while the later bunches see a heavier loaded cavity but with higher input power. This compensates for the transient beam loading, such that the cavity voltage stays constant for all bunches, avoiding an energy spread along a multibunch train.

To understand how this works, consider that if neglecting dispersion effects which limits how quickly the field can change, the field takes a time

$$t(z) = \int_0^z \frac{dz'}{v_g(z')} \quad (7.29)$$

to propagate from the input of the structure to the point  $z$ . Similarly, the time for the field to propagate from a point  $z'$  to  $z$  is  $t(z) - t(z')$ . Further assuming  $G(z, t = 0) = 0$  and that the input gradient  $G(0, t) = G_0(t)$ , the time-dependent gradient profile  $G(z, t)$  may be written as [158]

$$G(z, t) = G_0(t - t(z)) g(z) H(t - t(z)) - g(z) \int_0^z \frac{I(t - t(z) + t(z'))}{g(z')} \frac{H(t - t(z) + t(z'))}{2v_g(z')} \frac{\omega \frac{R'}{Q}(z')}{2v_g(z')} dz', \quad (7.30)$$

where  $G_0(t)$  is defined as in Equation (7.25) but with time dependent input power, replacing  $P_0 \rightarrow P(t)$ . The function  $g(z)$  is defined as in Equation (7.23) and  $H(t)$  is the Heaviside

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step function. This means that the gradient at the point  $z$  is given by the input power  $P(t)$  at a time  $t(z)$  earlier, and the beam loading at all points  $z'$  upstream of  $z$  at the time  $t(z) - t(z')$ .

The exact pulse shape can be found by requiring all bunches to see the same gradient profile  $G(z)$  as in the steady state. This can be achieved by requiring that the first bunch in the train, which is injected at the time  $t_2$  as defined in Figure 7.3, sees the same gradient profile as in the steady state. This can be achieved with the input power pulse shape found by equating Equation (7.30) (with  $I = 0$ ) and (7.22) (including the beam loading), yielding

$$G_0(t_2 - t(z)) g(z) = G_0 g(z) - I \cdot g_L(z), \quad (7.31)$$

where  $H(t - t(z)) = 1$ . The function  $G_0$  is as defined in Equation (7.25), with input power  $P_0$  in the time-independent case and  $P(t)$  in the time-dependent case. Further, the time  $t(z)$  and position  $z$  are dependent variables, and the variable of interest is the time

$$t'(z) \equiv t_2 - t(z) = t_1 + t_f - t(z) = \int_z^L \frac{dz'}{v_g(z')} + t_1, \quad (7.32)$$

where  $t_f \equiv t(L)$ . Thus Equation (7.31) may be rewritten as

$$G_0(t') = G_0 - I \frac{g_L(z(t'))}{g(z(t'))}, \quad (7.33)$$

where  $z(t')$  is the solution to the inverse problem of Equation (7.32). The pulse shape can be found by inserting  $G_0$  and solving for  $P(t)$ , which yields

$$P(t') = P_0 \left[ 1 - \sqrt{\frac{v_g(0)}{\omega (R'/Q)(0) P_0}} I \frac{g_L(z(t'))}{g(z(t'))} \right]^2. \quad (7.34)$$

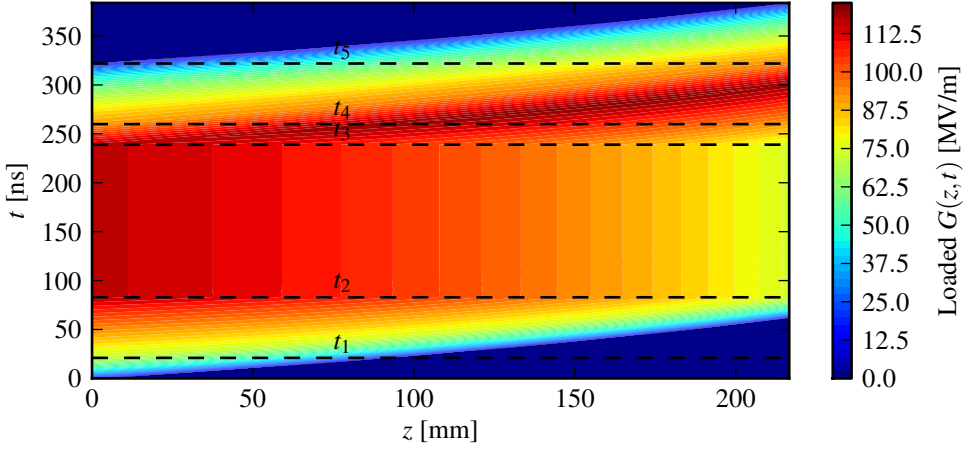
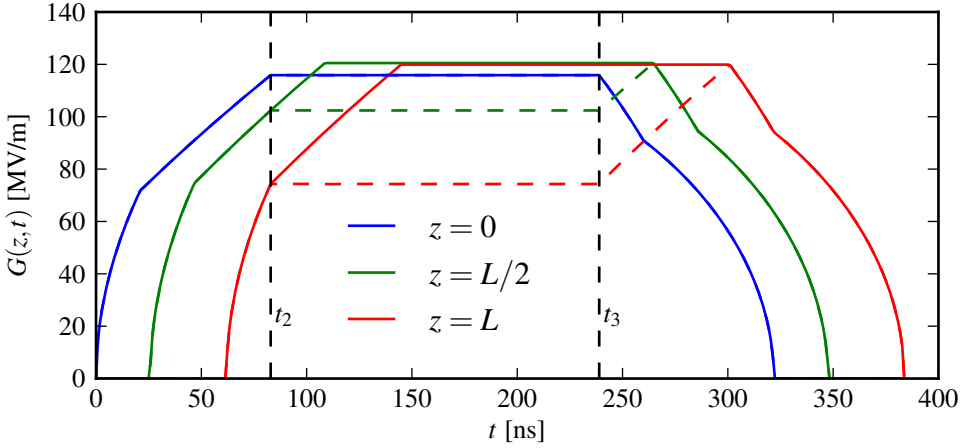
The resulting pulse profile is shown as the “Ideal” line in Figure 7.3, assuming a linear ramp from  $t = 0$  to  $t_1$ , and that  $P(t) = P_0 - P(t - t_3)$  for  $t \geq t_3$ . The time-dependent gradient profile is shown in Figure 7.4. Figure 7.5 shows the resulting voltages as function of time, which are found by integrating the gradient profiles at each time point. These figures show that the beam loading compensation ramp described by Equation (7.34) provides a constant voltage for all bunches, not just the first bunch as was the criterion when deriving the ramp.

To understand why Equation (7.31) works, consider that if not assuming  $\frac{\partial U'}{\partial t} = 0$ , Equation (7.15) can be written as [158]

$$\begin{aligned} \frac{\partial G(z, t)}{\partial t} &= -\frac{G}{2} \frac{dv_g}{dz} - v_g \frac{dG}{dz} + \frac{v_g G}{2R'/Q} \frac{d(R'/Q)}{dz} - \frac{\omega G}{2Q} - I(t) \frac{\omega R'/Q}{2} \\ &= v_g \left[ -G(z, t) \alpha(z) - \beta(z, t) - \frac{dG(z, t)}{dz} \right]. \end{aligned} \quad (7.35)$$

As the gradient profile  $G(z, t_2)$  equals the steady-state gradient profile and  $I(t)$  is constant,  $G(z, t_2)$  is a solution to Equation (7.19). This makes the right-hand side of Equation (7.35) zero, which is a sufficient condition for  $\frac{\partial G}{\partial t} = 0$ . The structure is thus in a steady state for all  $t_1 < t < t_3$ .

As mentioned in the beginning of this section, the pulse shape  $P(t)$  is for the calculation of RF-to-beam efficiency and maximum pulse lengths assumed to be composed of linear

(a) Local loaded gradient  $G(z, t)$  as a function of time and position.(b) Local gradient  $G(z, t)$  as a function of time at  $z = 0$ ,  $z = L/2$  and  $z = L$ . Both unloaded (solid) and loaded (dashed) gradients are shown. Time of beam injection and end of beam injection showed as dashed lines.Figure 7.4.: The local gradient  $G(z, t)$  as function of time and position in CLIC\_G R05 [160] with 26 cells, average gradient  $\langle G \rangle = 100$  MV/m with  $I = 1.19$  A. The input power pulse shape  $P(t)$  is the “Ideal” pulse from Fig. 7.3.

## 7. Structure parameter calculation

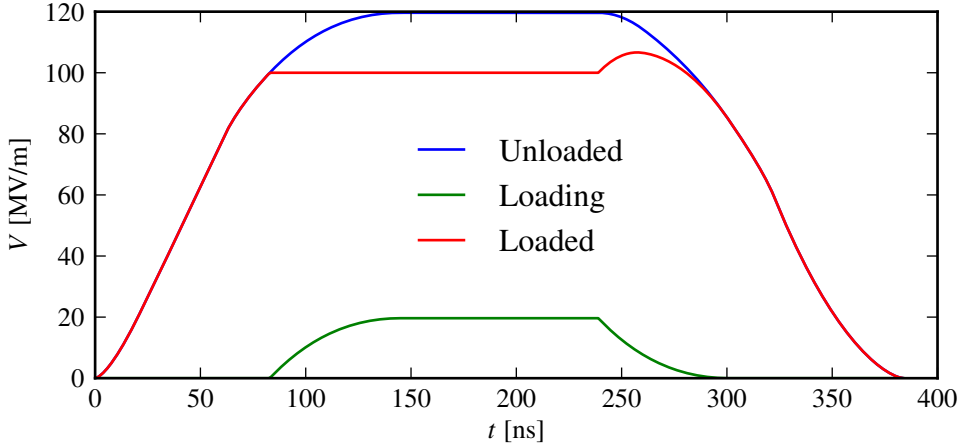


Figure 7.5.: The accelerating voltage (loaded, unloaded and the loading) as function of time for CLIC\_G R05 [160] with 26 cells. The average loaded gradient is  $\langle G \rangle = 100$  MV/m with beam loading current  $I = 1.19$  A.

segments. As seen in Figure 7.3, the difference between the pulse shape described by a linear ramp between  $(t_1, P_{\text{start}})$  and  $(t_2, P_0)$ , and the pulse shape from the exact power ramp described by Equation (7.34), is very small. Thus, the quantity of interest from Equation (7.34) is the power at  $P_{\text{start}} = P(t_1)$ , which through Equation (7.32) corresponds to  $z(t') = L$ . The power  $P_{\text{start}}$  is thus given as

$$P_{\text{start}} = P(t_1) = P_0 \left[ 1 - \sqrt{\frac{v_g(0)}{\omega (R'/Q)(0) P_0} I \frac{g_L(L)}{g(L)}} \right]^2. \quad (7.36)$$

The power levels of in the pulse are thus described by Equations (7.27) and (7.36), and the power at  $t_4$  is given as  $P_0 - P_{\text{start}}$ .

The falling edge of the pulse is also an approximation, as the power is actually produced by a drive-beam in a Power Extraction and Transfer Structure (PETS) [18]. Assuming that the drive-beam current changes slowly compared to the filling time of a PETS<sup>2</sup>, the gradient at the output end of the PETS is roughly given as  $G(L_{\text{PETS}}, t) = -I_{\text{DB}}(t)g_L(L_{\text{PETS}})$ . This yields a PETS output power

$$P_{\text{out}}(t) = \frac{G^2(t) v_g}{\omega R'/Q} \Big|_{z=L_{\text{PETS}}} \propto I_{\text{DB}}^2(t). \quad (7.37)$$

If assuming no dispersion effects or losses in the wave guide network, the PETS output power  $P_{\text{out}}(t)$  is equal to the accelerating structure input power  $P(t)$ . Further, the pulse shape is created by shifting bunches in the drive beam pulse, effectively removing some bunches at the beginning of the pulse to lower the produced power here, and then adding these bunches to the end of the pulse. Thus for  $t \in (t_3, t_5)$ ,  $I_{\text{DB}}(t) = I_0 - I_{\text{DB}}(t - t_3)$ , where  $I_0$  is

<sup>2</sup>This implies that the steady-state approximation of Equation (7.22) can be used. This is a reasonable assumption, as the group velocity in the PETS are 43% of  $c$  and they have a length of 213 mm, resulting in a filling time of 1.57 ns [18], which is much smaller than the time constants in the accelerating structures.

the current needed to produce  $P_0$ . Assuming the linear-segment pulse shape  $P(t)$  for the leading edge, the trailing edge takes the form shown in Figure 7.6a, having a much faster falloff than the piecewise linear pulse shape. The consequence of this for the pulse length limits is discussed in Section 7.8. It is also seen that the total energy in the drive beam RF pulse is much lower than for the linear power pulse, and the consequence of this is discussed in Section 7.7.

## 7.7. RF-to-beam efficiency

The RF-to-beam efficiency  $\eta$  is simply calculated as the ratio of the energy absorbed by the beam to the input energy. When only considering the time between  $t_2$  and  $t_3$ , the structure is always accelerating a beam, and the so-called steady-state efficiency is given as

$$\eta_{\text{flattop}} = \frac{IG \cdot V}{P_0}, \quad (7.38)$$

where  $V$  is the loaded voltage defined in Equation (7.26).

Taking the rising edge of the power pulse into account, the total efficiency is

$$\eta_{\text{total}} = \eta_{\text{flattop}} \frac{t_b}{t_r + t_f + t_b}. \quad (7.39)$$

This is obviously true for the pulses where the power at the trailing edge is described as  $P(t) = P_0 - P(t - t_3)$  for  $t \in (t_3, t_5)$ . It is also true for drive-beam pulses when counting the power needed to create the drive beam, which is proportional to the drive beam current. In this case, the “missing” energy ends up as a energy spread in the drive beam, as the energy extracted from each drive beam electron varies with the drive beam current.

## 7.8. Peak fields and pulse length limits

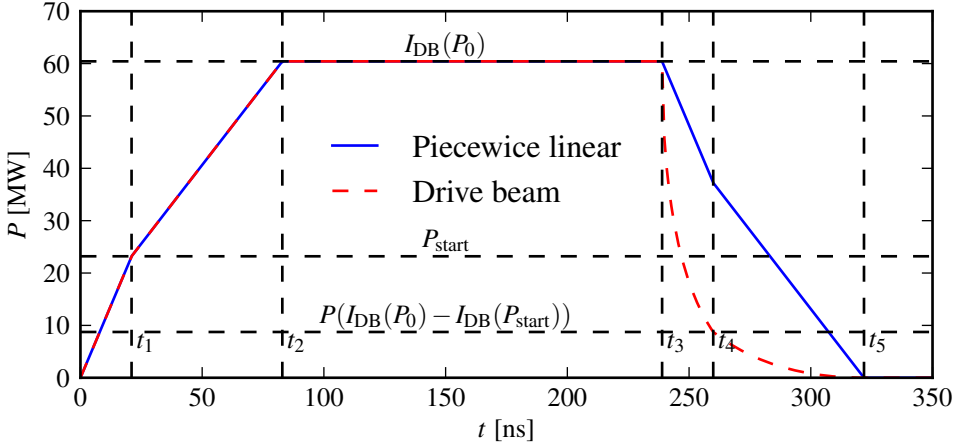
As discussed in Section 3.3, the peak fields and the pulse length determine the breakdown rate and maximum pulsed surface heating. Having calculated the accelerating gradient profile  $G(z)$  using Equation (7.22), the local peak fields  $\hat{E}(z)$ ,  $\hat{S}_c(z)$ ,  $\hat{H}(z)$  can be found using the normalized peak fields  $\bar{E}(z)$ ,  $\bar{S}_c(z)$  and  $\bar{H}(z)$ , which were defined in Section 3.3.1. For  $P_+/C(z)$ , the power flow can be found using Equation (3.24) and the circumference as  $C = 2\pi \cdot a(z)$ , where the iris aperture  $a(z)$  is found by interpolation along the structure in the same manner as the other parameters. Typical peak surface field and  $P_+/C$  profiles are shown in Figure 7.7.

The maximum of these quantities are used to find the maximum beam time  $t_b$ , as defined in Figure 7.3. The maximum beam time estimation assumes a piecewise linear pulse shape  $P(t)$ . Assuming that the gradient's dependence on the time  $t$  and position  $z$  can be factorized and written as

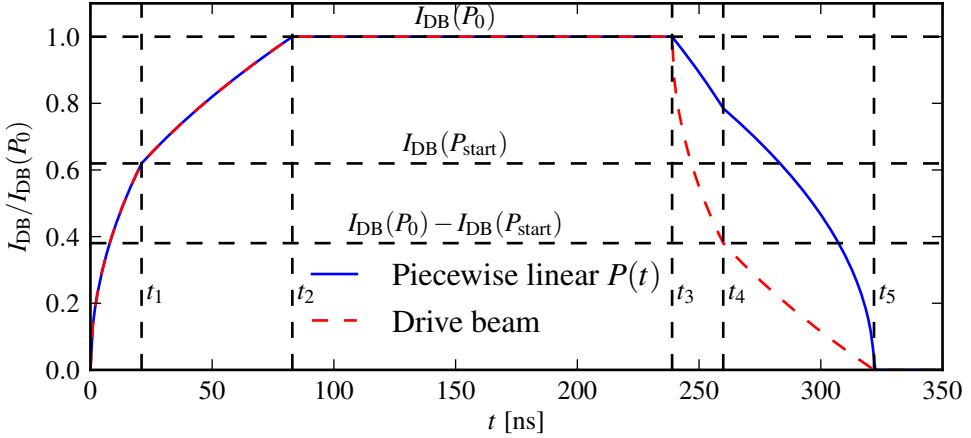
$$G(z, t) = \frac{G_0(t - t(z))}{G_0} G(z) \equiv \frac{G_0(t_z)}{G_0} G(z), \quad (7.40)$$

the same pulse shape is seen everywhere along the structure, shifted by a time  $t(z)$ . However, as seen from Figure 7.4, in the loaded case the gradient at the end of the structure has a rapid increase just after switching off the beam. This means that the assumption of Equation (7.40)

## 7. Structure parameter calculation



(a) RF power produced from piecewise linear  $P(t)$  and from shifting drive beam bunches.



(b) Drive beam current producing the two pulse shapes.

Figure 7.6.: Drive beam current and produced RF power as a function of time, for CLIC\_G R05 [160] with 26 cells. Average loaded gradient  $\langle G \rangle = 100$  MV/m and beam loading  $I = 1.19$  A. Both plots show both the linear power pulse shape and the pulse shape from shifting bunches in a drive beam. For both pulse shapes, the leading edges are identical.

is not exactly correct when in loaded condition. But, as can be seen from Equation (7.30), the assumption is correct in the unloaded case, and the loaded gradient almost<sup>3</sup> never exceeds the unloaded, given that the input power is the same in both cases. Thus, using the unloaded gradient profile together with the pulse shape that includes the beam loading compensation yield a conservative estimate of the maximum pulse length. Assuming a pulse shape  $P(t)$  composed of linear segments also tends to overestimate the input power at the end of the pulse compared to the drive beam pulse, as shown in Figure 7.6.

### 7.8.1. Pulse length limits from scaling laws

The overall peak fields  $\hat{E}$ ,  $\hat{S}_c$  and  $\max(P/C)$  are then used to find an estimate for the maximum pulse length  $\tau$ , defined as the length of the interval where  $P(t) > 0.85 \cdot P_0$  [162], as shown in Figure 7.3. This is done though the high gradient limits which were presented in Section 3.3.1, connecting the pulse length  $\tau$  and breakdown rate BDR to the peak fields. From Equations (3.26), (3.27) and (3.28), the maximally allowed pulse lengths are given as

$$\tau_E \leq \frac{\hat{E}_0^6 \tau_0}{\hat{E}} \left( \frac{\text{BDR}}{\text{BDR}_0} \right)^{1/5}, \quad (7.41)$$

$$\tau_{S_c} \leq \frac{\hat{S}_{c0}^3 \tau_0}{\hat{S}_c} \left( \frac{\text{BDR}}{\text{BDR}_0} \right)^{1/5} \text{ and} \quad (7.42)$$

$$\tau_{P/C} \leq \frac{(P/C)_0 \tau_0}{\max(P/C)} \left( \frac{\text{BDR}}{\text{BDR}_0} \right)^{1/5}. \quad (7.43)$$

The maximally allowed pulse length  $\tau$ , defined as shown in Figure 7.3, is thus found by taking the smallest of the three scaling law pulse length estimates

$$\tau \leq \min(\tau_E, \tau_{S_c}, \tau_{P/C}). \quad (7.44)$$

The maximum beam time  $t_b$  may then be found by subtracting the “wasted time”  $t_w$  when  $P(t) > 0.85 \cdot P_0$  and also no beam is present. The actual maximum beam time estimate from  $\hat{E}$ ,  $\hat{S}_c$  and  $\max(P/C)$  is thus  $t_b = \tau - t_w$ , which must then be compared to the estimate from pulsed surface heating.

### 7.8.2. Pulse length limits from pulsed surface heating

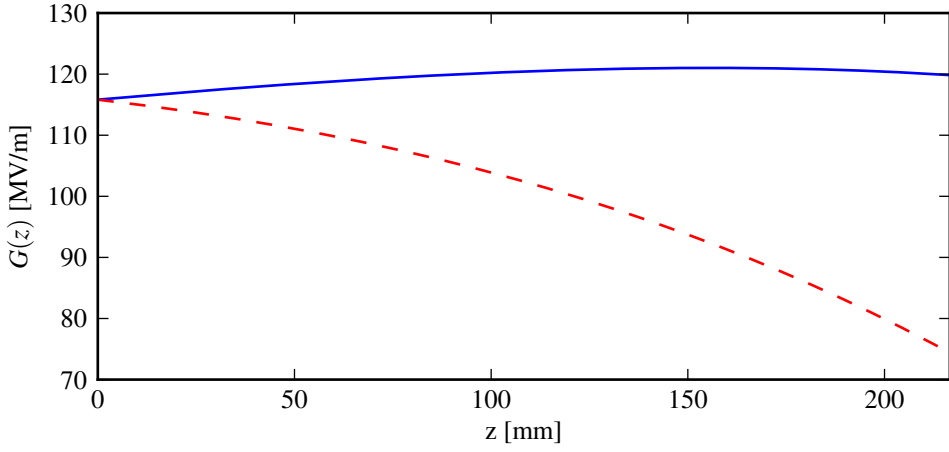
As was discussed in Section 3.4, the surface magnetic field causes pulsed heating of the metal surface. This repeated heating causes roughening and cracking of the surface, degrading the performance of the accelerating structure. In order to prevent or delay this degradation, the maximum temperature rise  $\Delta T$  should be limited, and the chosen limit is  $\Delta T \leq 50 \text{ K}$ .

The pulsed temperature rise can be calculated using Equation (3.38), and including the dependence on  $z$  yields the expression

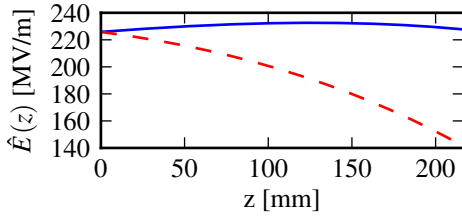
$$\Delta T(z, t) = \frac{\sqrt{\mu_0 \omega}}{2\sqrt{\rho c_\epsilon \pi k} 2\sigma} \bar{H}^2(z) \int_0^t \frac{G^2(z, t') dt'}{\sqrt{t - t'}}, \quad (7.45)$$

<sup>3</sup>The absolute value of the loaded gradient may exceed the unloaded in cases of extreme overloading of the structure.

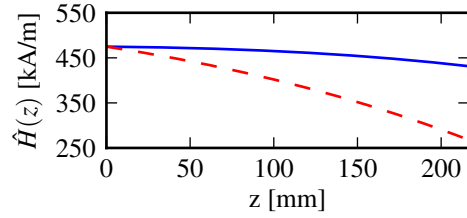
## 7. Structure parameter calculation



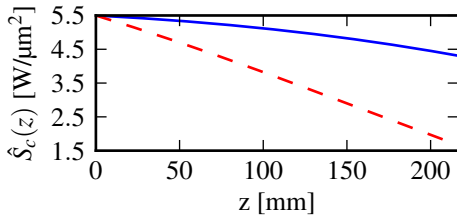
(a) Accelerating gradient profile.



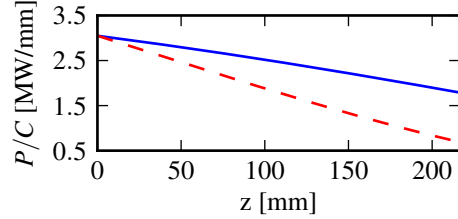
(b) Peak surface electric field profile.



(c) Peak surface magnetic field profile.



(d) Peak modified Poynting vector profile.



(e)  $P_+/C$  profile.

Figure 7.7.: Peak field profiles in CLIC\_G R05 [160] with 26 cells, with input power such that the average gradient is  $\langle G \rangle = 100$  MV/m at beam loading  $I = 1.19$  A. The unloaded steady-state profiles are showed in blue/solid, and the loaded profiles in red/dashed.



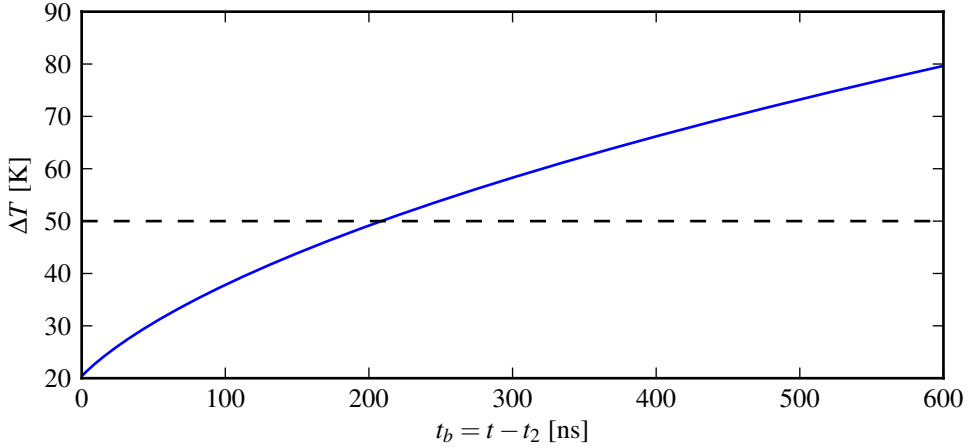


Figure 7.8.: Pulsed surface heating as function of  $t_b$  in CLIC\_G R05 [160] with 26 cells, with average gradient  $\langle G \rangle = 100$  MV/m, pulse including beam loading compensation for  $I = 1.19$  A. For this structure the highest point of  $\hat{H}^2$  is at  $z = 0$ , such that loaded/unloaded doesn't matter (see Figure 7.7), unless the structure is overloaded to such a degree that  $G(z) < 0$  at the end of the structure, and  $G^2 \bar{H}^2$  is greater here than at  $z = 0$ .

The gradient  $G$  must then be found as a function of time and position, which is done through the assumption of Equation (7.40). This means that  $G^2(z, t) \propto G^2(z)P(t_z)$ . Ignoring the time shift  $t(z)$ , the integral for  $\Delta T(z, t)$  may thus be written as

$$\Delta T(z, t) = \frac{\sqrt{\mu_0 \omega}}{2\sqrt{\rho c_\epsilon \pi k 2\sigma}} \bar{H}^2(z) \frac{G^2(z)}{P_0} \int_0^t \frac{P(t') dt'}{\sqrt{t - t'}}. \quad (7.46)$$

This integral can be solved analytically [24], yielding a closed form expression for  $\Delta T(t, \hat{H}(z))$  when  $t_2 < t < t_3$ . As an example, Figure 7.8 shows  $\Delta T$  as a function of  $t_b$  at the point of the peak surface magnetic field of a typical structure.

The closed form of Equation (7.46) is then used to find the maximum  $t_b$  allowed for the structure from the  $\Delta T$ . For this, the maximum of  $\hat{H}(z)$  is used, and the estimate has a precision of one RF cycle. This estimate for  $t_b$  is then combined with the estimates from  $\hat{E}$ ,  $\hat{S}_c$  and  $\max(P/C)$  which were discussed in Section 7.8.1, and the smallest of all four estimates is used for determining the maximum acceptable pulse length in the structure for the given gradient and beam loading.

## 7.9. Transverse wakefields

The long range transverse wakefields in the structure are estimated as

$$W_{\perp}(s) = \frac{1}{N_{\text{cells}}} \sum_{i=0}^{i < N_{\text{cells}}} W_i(s), \quad (7.47)$$

where the sum runs over all the cells in the structure, and the single-cell modes are written as

$$W_i(s) = -A_i \exp\left(\frac{-\omega_i s/c}{2Q_i}\right) \sin\left(\omega_i s/c \sqrt{1 - \frac{1}{4Q_i^2}}\right). \quad (7.48)$$

Here  $s$  is a coordinate measuring the distance behind the driving bunch, which is taken to be of  $\delta$ -function length. The other main assumption of the model is that only the first dipole mode in each cell is taken into account, and that there are no coupling between the cells. The parameters  $A_i$ ,  $\omega_i$  and  $Q_i$  are taken from the interpolation along the structure as for the other parameters, where the continuously interpolated functions are evaluated at the points

$$z_i = \frac{iL}{N_{\text{cells}} - 1}, \quad i \in 0, 1, \dots, N_{\text{cells}} - 1. \quad (7.49)$$

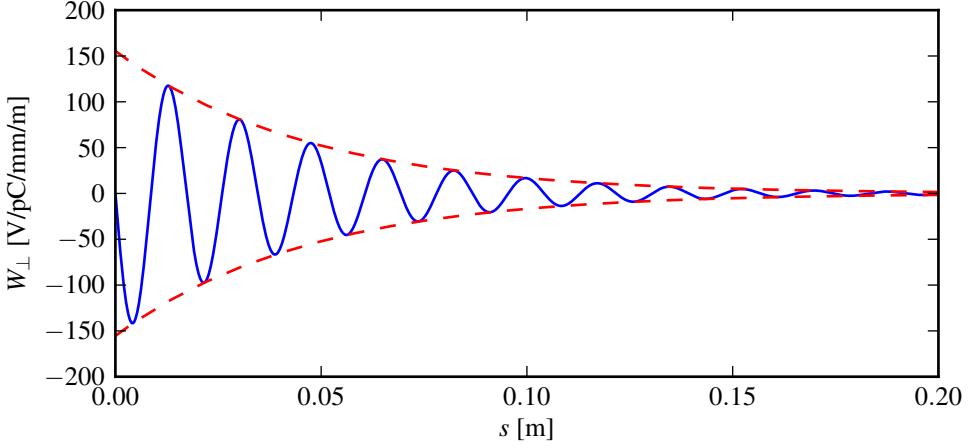
The envelope is found by first finding the maxima and minima of  $W_{\perp}(s)$  using a numerical method. This is used to build an array of coordinates  $(s_i, |W_{\perp}(s_i)|)$  of the extrema locations, where the first coordinate is found by searching backwards from  $s = 0$ . The value of the wake envelope at any given  $s$  can then be found by linear interpolation between the extrema values in the array.

The numerical method is a combination of a fixed-step bracketing and a golden search [163]. The step size for the bracketing was set to  $\frac{2}{11} \frac{\tilde{\lambda}}{2}$ , where  $\tilde{\lambda}$  is the smallest transverse wavelength

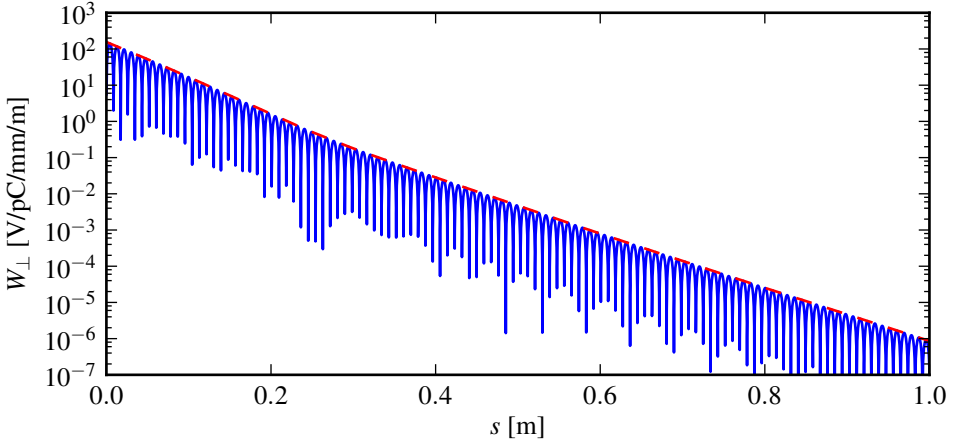
$$\frac{c}{\frac{\omega^{(j)}}{2\pi} \sqrt{1 - \frac{1}{4(Q^{(j)})^2}}} \quad (7.50)$$

seen in any of the three interpolation points  $j \in \{0, 1, 2\}$ . The factor  $1/2$  in the bracketing is used as the search is for peaks in the absolute value of  $W_{\perp}(s)$  (halving the period of  $W_{\perp}(s)$ ), while the factor  $2/11$  is set to make it less likely that one edge of a bracket happens to be exactly on the searched-for maxima (more likely in structures with no detuning), leading to missing that maxima.

As an example, a wakefield and its envelope is plotted in Figure 7.9. Using the envelope, the minimum number of RF cycles between bunches can easily be found, given a limit for the maximum  $\text{env}(W_{\perp})$ , where  $\text{env}(W)$  means finding the envelope of  $W$  as described above. This is done simply by checking  $\text{env}(W_{\perp}(s_i))$  for  $s_i = c \frac{2\pi}{\omega} i$  for  $i = 1, 2, \dots$  until  $\text{env}(W_{\perp}(s_i))$  is below the limit.



(a) Linear scale. Both positive and negative envelopes are shown.



(b) Logarithmic scale. Absolute value and envelope of wake plotted.

Figure 7.9.: Estimated transverse wakefield (first dipole mode only) in CLIC\_G R05 [160, 153] with 26 cells. The wakefield is plotted in blue/solid, and the estimated envelope in red/dashed. The two plots show the same data. Note that the x-axis ranges are different.

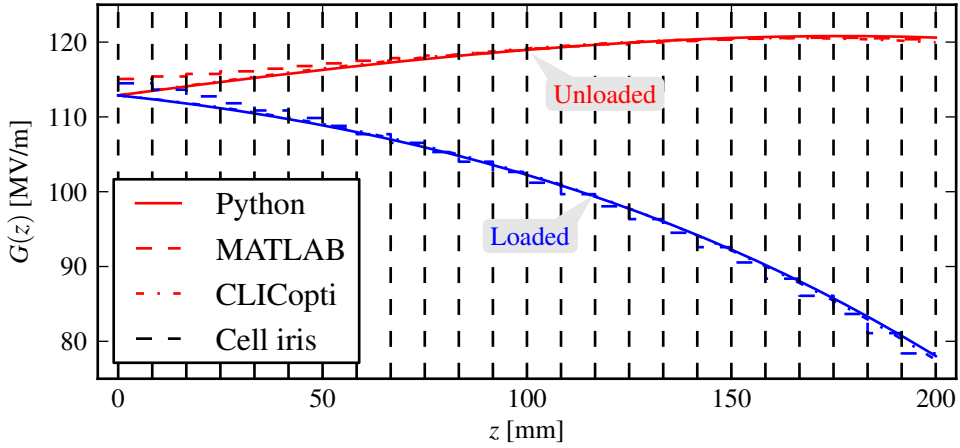


Figure 7.10.: Loaded and unloaded gradient profiles along the length of a CLIC\_G [164] structure with 24 cells using CLICopti, the Python code and the old MATLAB code.

## 7.10. Validation of the model and the CLICopti library

As this model for the structure performance is an important part of the re-optimization of the CLIC machine [157], it is important that the results produced from it can be trusted. The model was therefore tested both by comparison to other models, and by comparison to experimental results.

### 7.10.1. Gradient profile $G(z)$ calculation

The field profile calculation was tested by comparing the results from CLICopti to the results from a Python code implementing the same method, and also to a MATLAB code implementing a similar method. The MATLAB code was used in the design effort which led to CLIC\_G, and calculates the gradient in one point per cell, unlike CLICopti and the Python equivalent<sup>4</sup> which uses the continuous approximation described in Section 7.4. The choice of interpolation points are also slightly different, with CLICopti and the Python equivalent using  $z = \{0, L/2, L\}$  and the MATLAB code using  $z = \{h/2, h(\text{int}(N/2) - 0.5), L - h/2\}$ . The calculated loaded and unloaded gradient profiles from all three codes are shown in Figure 7.10.

These plots show that there are no significant differences in the gradient profiles between the two implementations of the continuous approximation (CLICopti and the Python code). Further, while there are some differences between the two types of approximations, they are relatively small.

<sup>4</sup>The Python equivalent of CLICopti was developed when optimizing the CLIC\_502 design [165].

| Design level    | Input power $P_0$ [MW]<br>to reach $\langle G \rangle = 100$ MV/m | Structure filling time $t_f$ [ns] |
|-----------------|-------------------------------------------------------------------|-----------------------------------|
| 1 <sup>st</sup> | 42.82                                                             | 51.38                             |
| 2 <sup>nd</sup> | 41.07                                                             | 58.64                             |
| 3 <sup>rd</sup> | 42.2                                                              | 64.55                             |

Table 7.1.: Input power and filling time as predicted from CLICopti (stage 1 and 2) and HFSS for CLIC\_G. Here the database is the old 30 GHz database scaled to 11.9942 GHz [95], using the scaling relations given in Section 7.2. The filling time of the full RF design is calculated for the whole structure, including the matching cells and parts of the power couplers. Data for 2<sup>nd</sup> and 3<sup>rd</sup> design level from [164].

### 7.10.2. Accuracy of power requirement predictions

When designing a new accelerating structure, the RF design is typically done in three stages. The goal of the first stage is to determine the required structure length, aperture and tapering etc., in order to fit with the machine for which it is designed. This is done by extracting cells from a database, in order to estimate the performance of a possible RF structure design during machine optimization. The optimization is done by varying several parameters of the machine, including the parameters of the RF structures. Once the overall structure parameters are decided, the second stage is typically to optimize the cells at the picked points, instead of extracting and interpolating them from a cell data-base. For an example of this, see the optimization of the CLIC\_502 design [165]. Having obtained these “tweaked” cells, the third stage is to create and optimize the full 3D model of the complete structure, including the couplers etc.

A fast analytical method, such as presented in this chapter, is typically used to calculate the structure power requirements in stage 1 and 2, while a finite element S-parameter solver such as S3P or HFSS must be used for the third stage. The goal is that the predicted performance from the first stage should be as similar as possible to that of the final design. This depends both on the accuracy of the method for calculating the field profile, and also on the quality of the cell database, which should contain cells that are well optimized such that the interpolated single-cell RF parameters are close to those found in stage 2.

To check the quality of prediction, a comparison between the three levels was made for the CLIC\_G structure with 24 cells<sup>5</sup> [164]. As shown in Table 7.1, the results are relatively consistent, even as the geometry is slightly changed between the design levels. Especially important is that the change from 2<sup>nd</sup> to 3<sup>rd</sup> stage is very small, indicating that the method for calculating the gradient profile works well. This table also uses data from the old 30 GHz database [95], which is not as highly optimized as the new 12 GHz database. Thus the new database (presented in Chapters 5 and 6) should therefore need less geometry changes between the 1<sup>st</sup> and 2<sup>nd</sup> stages, leading to greater accuracy in the predictions from CLICopti as used in the machine re-optimization.

<sup>5</sup>This is not the R05 structure, and it does not have compact couplers.

## 7. Structure parameter calculation

### 7.10.3. Pulse length and breakdown rate

One of the main functions of CLICopti is to estimate the maximum pulse length which a structure can hold without exceeding the acceptable breakdown rate, as discussed in Section 7.8.1. This was tested with the design of the KEK TD24R05#4 structure at 11.424 GHz, by scaling the interpolation points from a normal CLIC\_G to this frequency using the scaling relations given in Section 7.2. The estimated maximum pulse length from CLICopti at  $1.0 \cdot 10^{-6}$  breakdowns/pulse was 242 ns. In testing, this structure achieved 100 MV/m at  $1.1 \cdot 10^{-6}$  breakdowns/pulse and 252 ns pulse length [97, 98]. Using Equation (3.20) to scale the estimated pulse length from CLICopti to  $1.0 \cdot 10^{-6}$  breakdowns per pulse, this is equivalent to  $\tau = 257$  ns, which is in agreement with what was achieved in the experiment.

### 7.10.4. Wakefield

As discussed in Section 7.9, CLICopti estimates the long range transverse wakefield in order to find the required minimum bunch spacing  $s_{\min}$ . This bunch spacing is determined such that  $W_{\perp}(s_{\min}) < \hat{W}_{\perp}$ .

For CLIC, the wake limit is  $\hat{W}_{\perp} = 6.6$  V/pC/m/mm [21, 18]. Using this limit, CLICopti predicts a minimum bunch spacing of 6 RF cycles for CLIC\_G R05 [160, 153] with 26 cells. Using cells extracted from the 30 GHz database yields the same minimum bunch spacing. This is the same limit as is expected from GdfidL simulations of the whole structure [18].

## 7.11. Summary and conclusions

This chapter described the methods implemented in the C++ library CLICopti, which is used for re-optimizing the CLIC design. The library uses the cell database, which was described in Sections 5.7 and 6.7.3, to quickly predict the performance of an RF structure based on a few overall parameters such as its length and the radius and thickness of the first and last aperture. It can be used to predict both the fundamental structure performance such as the voltage-power relation, effect of beam loading etc., and can also estimate the transverse wakefield. Further, it is able to predict the high gradient performance of the structure based on the high gradient limits presented in Chapter 3, taking both the peak electric field,  $S_c$ ,  $P/C$ , and peak pulsed surface heating from the magnetic field into account. These limits yield a maximally allowable pulse length for the given structure, gradient, and beam loading.

## 8. Summary, conclusions, and outlook

In the work presented in this thesis, several aspects of vacuum arcs and their causes in normal-conducting RF accelerating structures have been explored. A model capable of predicting the probability of a breakdown in such structures as a function of their field pattern, voltage, and pulse length was used and expanded upon (Chapter 3 and [99]). The expansion enabled direct comparison of different breakdown criteria, in terms of an accelerating gradient limit. This model was then used to create a program for automatically predicting the performance of an RF structure designed according to certain criteria such as length, aperture, and tapering ([24] and Chapter 7). This tool was essential in the re-baselining of the CLIC accelerator complex [25], and has also been used for the a proposed FEL design [54, 166].

The structures generated by the above mentioned program are based on a table of highly optimized accelerating cells (Chapter 5 and [23]). These cells were optimized using the ACE3P [22] solvers, driven by a program that semi-automatically varied the geometry and analyzed the solutions in order to look for the optimum geometry (Section 5.5 and [29]). Again, the same model as mentioned above was used to compare the different breakdown criteria, in order to find an overall optimum.

In addition to the work done with the CLIC machine optimization, the fundamental physics of vacuum arc ignition was explored using the 2D ArcPIC particle-in-cell code (Chapter 4 and [112, 31]). This yielded some new insights, especially it was clearly demonstrated that the energy of the ions hitting the surface during the ion bombardment is on the order of the sheath potential, and that there must be some mechanism enhancing the neutral emission (sputtering or evaporation) in this stage of the arc. The results from 2D ArcPIC was in good agreement with experimental results from the CERN DC spark experiment and other literature. It would still be interesting to continue the development of this code and improve its physics modules as outlined in Section 4.4, in order to study for example the effect of temperature and changed work functions, and to improve the code's performance and be able to do more and more detailed parameter scans.

For the future, both of these directions open many interesting possibilities. To improve the accuracy of the predictions from the breakdown limits, a dedicated experimental program testing these limits would be highly valuable. Some work in this direction is taking place at SLAC [100, 101], in a simple structure where the power flow through the structure is varied while the electric field on a test surface is kept constant by adjusting the geometry to compensate. This allows comparison of the effects of the electric field and power-flow break on the break down rates. More such dedicated tests could improve the understanding of the causes of breakdown in RF structures, isolating and varying one of the factors at a time, including both field pattern characteristics and materials/surface treatments. Especially, such tests may provide more information on the interplay between the formation and exposure of emitters through mechanical strain on the surface, and power flow “feeding” a newly created emitter. The recent addition of XBox-3, which greatly increases the high-power X-band testing capability by providing 4 simultaneous testing slots [167], could

## 8. *Summary, conclusions, and outlook*

make such a test program possible alongside the testing of new accelerating structures.

At the same time, a deeper theoretical understanding of the initial stages of vacuum arcs would also be very useful, especially regarding the formation of the initial field emitter, the evaporation of material from the surface to create a gas that can be ionized, and the sputtering under the arc during its initial stages. Better knowledge of this would be useful both when selecting materials and their treatment for building breakdown-resistant normal-conducting accelerator structures, and for improving the understanding of the breakdown limits. Lately there has been a rapid progress in the theoretical understanding of this, as discussed in Sections 4.1.1 and 4.1.3.

Also of interest is the study of the relationship between breakdowns in DC and RF fields. It has been observed that the break down rates scales in the same way with the field strength, and that it is distributed in the same way within the pulses. This indicates that there may be common underlying factors, most likely due to the appearance of emission sites. In addition to doing dedicated “single parameter” RF experiments, complimentary DC experiments exploring for example the effect of the voltage pulse length and shape, or the effect of the energy flow by varying the gap capacitance and external circuit. Regarding the pulse length, the CERN DC spark experiment has recently been upgraded to have a much better controlled pulse length by the addition of a Marx generator high-voltage power supply [168], which should produce interesting data for comparison with RF.

On the simulation side, 2D ArcPIC already contains an RF “circuit”, which can be used to apply an external sinusoidally time-varying electric potential. This could be used to study the behavior of vacuum arcs in RF, in order to compare with the DC simulations. Furthermore, while it has been studied in the past [120] it may also be interesting to revisit the effect of RF fields on field evaporation using a more modern code such as HELMOD [121, 122]. Since this newer code tracks both the change in geometry and the ion charges ion in self-consistent way, it may yield some new insights.

Using the knowledge gained through the work on this thesis and in other studies of vacuum arc physics and high-gradient normal conducting RF structures, we will be able to design and build high-performing accelerator studies with even greater confidence. This will further increase the achievable performance while reducing the cost of both CLIC and other accelerator projects.



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## A. Finite element calculation of electromagnetic eigenmodes

This Appendix describes in further detail how to solve Equation (2.27) in order to find the field patterns  $\mathbf{E}$  of the electromagnetic eigenmodes. For this discussion, the E-formulation is used. The method described is the general Galerkin method, which includes the Finite Element Method (FEM) as implemented by e.g. ACE3P. This yields a solution that is described as a weighted linear combination of a set of basis functions (Equation (A.7)). When using the Finite Element Method, these basis functions are only non-zero in a finite subdomain, typically within one mesh cell which in this case is a tetrahedon.

In order to find the solutions  $\mathbf{E}$ , a weak formulation [169, Section 2.3] can be defined by multiplying with a test function  $\mathbf{v}$  and integrating over the simulation domain  $\Omega$ , thus taking the inner product

$$(\mathbf{F}, \mathbf{v}) = \int_{\Omega} \mathbf{F} \cdot \mathbf{v}^* d\Omega \quad (\text{A.1})$$

with  $\mathbf{v}$  on both sides of Equation (2.27), where  $\mathbf{v}^*$  is the complex conjugate of  $\mathbf{v}$ . In this case, both the test function  $\mathbf{v}$  and trial function  $\mathbf{E}$  should be in the function space  $V$ , such that

$$\mathbf{v} \in V = \{\mathbf{v} \in H_{\text{curl}}(\Omega) : \vec{n} \times \mathbf{v} = 0 \text{ on } \Gamma_E\}, \quad (\text{A.2})$$

where  $\Gamma_E$  is a domain border with a perfect conductor or *electric wall* boundary condition, and  $H_{\text{curl}}(\Omega)$  is the space of all functions  $\mathbf{v}$  such that  $\mathbf{v} \in [L_2(\Omega)]^3$  and  $\nabla \times \mathbf{v} \in [L_2(\Omega)]^3$ .

This inner product yields

$$\int_{\Omega} (\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E})) \cdot \mathbf{v}^* d\Omega = \int_{\Omega} \epsilon_r k^2 \mathbf{E} \cdot \mathbf{v}^* d\Omega \quad \forall \mathbf{v} \in V, \quad (\text{A.3})$$

where the left-hand integral may be rewritten as [169]

$$\int_{\Omega} \mu_r^{-1} \nabla \times \mathbf{E} \cdot \nabla \times \mathbf{v}^* d\Omega - \int_{\partial\Omega} [(\mu_r^{-1} \nabla \times \mathbf{E}) \times \vec{n}] \cdot \mathbf{v}^* d\Gamma, \quad (\text{A.4})$$

where  $\partial\Omega$  is the boundary of the domain  $\Omega$ , and  $\vec{n}$  is a normal vector to this boundary.

The boundary term is zero on  $\Gamma_E$ , because

$$\int_{\partial\Omega} [(\mu_r^{-1} \nabla \times \mathbf{E}) \times \vec{n}] \cdot \mathbf{v}^* d\Gamma = - \int_{\partial\Omega} (\mu_r^{-1} \nabla \times \mathbf{E}) \cdot (\mathbf{v}^* \times \vec{n}) d\Gamma, \quad (\text{A.5})$$

and  $\mathbf{v}^* \times \vec{n} = 0$  per the definition of the function space  $V$ , as  $\Gamma_E$  is an essential boundary condition.

In addition to the part of  $\partial\Omega$  which is in  $\Gamma_E$ , a perfect magnetic conductor or *magnetic wall* boundary condition may also be applied. This part of  $\partial\Omega$  is called  $\Gamma_H$ , and has the boundary

### A. Finite element calculation of electromagnetic eigenmodes

condition  $\mathbf{H} \times \vec{n} = 0$ . Applying Equation (2.24) to the boundary term of Equation (A.4) thus yields

$$\int_{\partial\Omega} [(\mu_r^{-1} \nabla \times \mathbf{E}) \times \vec{n}] \cdot \mathbf{v}^* d\Gamma = \int_{\partial\Omega} [-i\omega \mathbf{H} \times \vec{n}] \cdot \mathbf{v}^* d\Gamma = 0. \quad (\text{A.6})$$

This means that for the boundary conditions discussed above, the boundary term of Equation (A.4) is always zero.

In order to find a numerical solution, the infinite-dimensional space  $V$  must be reduced to a finite-dimensional space  $V_h \subseteq V$ , for which it is possible to find a finite basis. One such basis is Nedelec elements on a tetrahedral mesh [170, 171]. This means dividing  $\Omega$  into a large number of tetrahedons, each tetrahedon being the support of a number of basis functions. How many basis functions are used per tetrahedon is determined by the basis function order. Together, these basis functions in all of the tetrahedons span  $V_h$ , such that the trial function  $\mathbf{E}$  can be written as a linear combination

$$\mathbf{E} = \sum_i \alpha_i \mathbf{N}_i, \quad (\text{A.7})$$

where  $\mathbf{N}_i$  is one of the basis functions in the set spanning  $V$ ,  $\alpha_i$  is a complex scalar, and the sum runs over all basis functions. The weak formulation can thus be written as

$$\sum_i \alpha_i \int_{\Omega} \mu_r^{-1} \nabla \times \mathbf{N}_i \cdot \nabla \times \mathbf{N}_j^* d\Omega = k^2 \sum_i \alpha_i \int_{\Omega} \epsilon_r \mathbf{N}_i \cdot \mathbf{N}_j^* d\Omega \quad \forall \mathbf{N}_j \in V_h, \quad (\text{A.8})$$

where the trial function  $\mathbf{N}_j$  is one of the basis functions of  $V_h$ . This can then be written as a generalized eigenvalue problem

$$(\mathbb{K} - k^2 \mathbb{M}) \vec{\alpha} = 0, \quad (\text{A.9})$$

where the matrix elements are given as

$$\mathbb{K}_{i,j} = \int_{\Omega} \mu_r^{-1} \nabla \times \vec{N}_i \cdot \nabla \times \vec{N}_j d\Omega \quad (\text{A.10})$$

$$\mathbb{M}_{i,j} = \int_{\Omega} \epsilon_r \vec{N}_i \cdot \vec{N}_j d\Omega. \quad (\text{A.11})$$

Solving this eigenvalue problem yields an approximation to the complex vector field  $\mathbf{E}$ , which represents the electric field in the cavity through Equation (2.22). The magnetic field can then be calculated using Equation (2.24).



# Publications: Papers and reports



## B. Design of an accelerating structure for a 500 GeV CLIC using ACE3P

Title DESIGN OF AN ACCELERATING STRUCTURE FOR A 500 GeV CLIC USING ACE3P

Abstract An optimized design of the main linac accelerating structure for a 500 GeV first stage of CLIC is presented. A similar long-range wakefield suppression scheme as for 3 TeV CLIC based on heavy waveguide damping is adopted. The accelerating gradient for the lower energy machine is 80 MV/m. The 500 GeV design has larger aperture radius in order to increase the maximum bunch charge and length which is limited by the short-range wakefields. The cell geometries have been optimized using a new parametric optimizer for Ace3P and details of the RF cell design are described. Field parameters for the full structure are calculated using a power flow equation.

Where IPAC'12, New Orleans, USA

When May 20<sup>th</sup> – 25<sup>th</sup>, 2012

Contribution Kyrre wrote the text and made the plots and figures in this article. He also wrote the AcdOpti software, which was used to manage the Omega3P runs, and ran the Omega3P and T3P simulations presented in the paper. He also presented it at the poster session of the conference.

Main author Kyrre Sjøbæk

Co-authors Erik Adli, Alexej Grudiev and Walter Wuensch

Bibliography entry [165]

Location on-line

<http://accelconf.web.cern.ch/accelconf/IPAC2012/papers/thppc011.pdf>



## C. Surface field optimization of accelerating structures for CLIC using ACE3P on remote computing facility

Title SURFACE FIELD OPTIMIZATION OF ACCELERATING STRUCTURES FOR CLIC USING ACE3P ON REMOTE COMPUTING FACILITY

Abstract This paper presents a computer program for searching for the optimum shape of an accelerating structure cell by scanning a multidimensional geometry parameter space. For each geometry, RF parameters and peak surface fields are calculated using ACE3P on a remote high-performance computational system. Parameter point selection, mesh generation, result storage and post-analysis are handled by a GUI program running on the user's workstation. This paper describes the program, AcdOptiGui. AcdOptiGui also includes some capability for automatically selecting scan points based on results from earlier simulations, which enables rapid optimization of a given parameterized geometry. The software has previously been used as a part of the design process for accelerating structures for a 500 GeV CLIC.

Where IPAC'13, Shanghai, China

When May 12<sup>th</sup> – 17<sup>th</sup>, 2013

Contribution Kyrre was the main author of this article, and also wrote the poster which was presented by co-author and supervisor Alexej Grudiev in the poster session of the conference. Kyrre also wrote the AcdOpti software described in this paper, and ran all of the ACE3P simulations, analyzed the data and made the plots and figures in this article.

Main author Kyrre Sjøbæk

Co-authors Alexej Grudiev and Erik Adli

Bibliography entry [29]

Location on-line

<http://accelconf.web.cern.ch/AccelConf/IPAC2013/papers/mopwo011.pdf>



## D. New Criterion for Shape Optimization of Normal-Conducting Accelerator Cells for High-Gradient Applications

Title New Criterion for Shape Optimization of Normal-Conducting Accelerator Cells for High-Gradient Applications

Abstract When optimizing the shape of high-gradient accelerating cells, the goal has traditionally been to minimize the peak surface electric field / gradient, or more recently minimizing the peak modified Poynting vector / gradient squared. This paper presents a method for directly comparing these quantities, as well as the power flow per circumference / gradient squared. The method works by comparing the maximum tolerable gradient at a fixed pulse length and breakdown rate that can be expected from the different constraints. The paper also presents a set of  $120^\circ$  phase-advance cells for traveling wave structures, which were designed for the new CLIC main linac accelerating structure, and which are optimized according to these criteria.

Where LINAC'14

When August 31<sup>st</sup> – September 5<sup>th</sup> 2014

Contribution Kyrre developed the method for predicting the gradient of an accelerator cell based on the high gradient limits and eigenmode simulation of the cell, did the optimization of the presented high gradient cells, wrote the paper, and wrote the poster.

Main author Kyrre Sjøbæk

Co-authors Alexej Grudiev and Erik Adli

Bibliography entry [99]

Location on-line <http://inspirehep.net/record/1363323/files/mopp028.pdf>





## E. From Field Emission to Vacuum Arc Ignition: a New Tool for Simulating Copper Vacuum Arcs

Title From Field Emission to Vacuum Arc Ignition: a New Tool for Simulating Copper Vacuum Arcs

Abstract Understanding plasma initiation in vacuum arc discharges can help to bridge the gap between nano-scale triggering phenomena and the macroscopic surface damage caused by vacuum arcs. We present a new two-dimensional particle-in-cell tool to simulate plasma initiation in direct-current (DC) copper vacuum arc discharges starting from a single, strong field emitter at the cathode. Our simulations describe in detail how a sub-micron field emission site can evolve to a macroscopic vacuum arc discharge, and provide a possible explanation for why and how cathode spots can spread on the cathode surface. Furthermore, the model provides us with a prediction for the current and voltage characteristics, as well as for properties of the plasma like densities, fluxes and electric potentials in a simple DC discharge case, which are in agreement with the known experimental values.

Where Submitted to *Contributions to Plasma Physics*, September 15<sup>th</sup> 2014, accepted November 18<sup>th</sup> 2014.

Contribution Kyrre worked on the simulation code, restructuring, debugging and optimizing it. He also developed most of the circuit model and parts of the surface model which are presented in the paper. He also wrote large parts of the “Methods and code description” and “Simulation results and discussion” parts of the paper. Finally, he handled the simulation runs (including selecting many of the simulation parameters), wrote the analysis codes and did much of the simulation data analysis, and made the plots and figures which are presented in the article. Finally, he handled the integration of comments from co-authors and the submission of the paper to the journal.

Main author Helga Timkó

Other co-authors Lotta Mether, Sergio Calatroni, Flyura Djurabekova, Konstantin Matyash, Kai Nordlund, Ralf Schneider and Walter Wuensch

Bibliography entry [112]

Location on-line <http://onlinelibrary.wiley.com/doi/10.1002/ctpp.201400069>



## F. CLIC notes and other materials

In addition to the publications listed and reproduced above, a number of other materials are listed below. These documents were produced (or a significant contribution was made) as part of the work towards this thesis. In case the link in “Location on-line” is no longer working, please contact me at `k.n.sjobak@fys.uio.no` to obtain a copy of the PDF.

### F.1. Benchmarking of Omega3P finite element electromagnetic eigenmode solver

Title Benchmarking of Omega3P finite element electromagnetic eigenmode solver

Description This document was written while testing the Omega3P eigensolver, as a preparation for using it for cell design. This document was thus referenced from [165]. It describes testing the solver against analytic solutions and HFSS, for pillbox, undamped and damped CLIC cell geometry. Also presented are analytic solutions for Q-factors of several modes in pillbox cavities, which the author have not found in other literature. Also presented are methods for extracting RF parameters from the field patterns, which is discussed further in Section 2.4.2.

Where CERN EDMS document #116625

When October 2011

Author Kyrre Sjøbæk

Bibliography entry [90]

Location on-line <https://edms.cern.ch/document/1166750/2>

### F.2. Longitudinal space charge effects in the CLIC drive beam

Title LONGITUDINAL SPACE CHARGE EFFECTS IN THE CLIC DRIVE BEAM

Abstract The CLIC main beam is accelerated by rf power generated from a high-intensity, low-energy electron drive beam. The accelerating fields are produced in Power Extraction and Transfer Structures, and are strongly dependent on the drive beam bunch distribution, as well as other parameters. We investigate how longitudinal space charge affects the bunch distribution and the corresponding power production, and discuss how the bunch length evolution can affect the main beam. We also describe the development of a Particle-in-Cell space charge solver which was used for the study.

Where IPAC'13, Shanghai, China

When May 12<sup>th</sup> – 17<sup>th</sup>, 2013

Contribution Kyrre consulted on the implementation of the PIC solver.

Main author Reidar Lunde Lillstøl

Other co-authors Andrea Latina, Daniel Schulte and Erik Adli

Bibliography entry [172]

Location on-line

<http://inspirehep.net/record/1337195/files/tupwa045.pdf>

### F.3. Design of waveguide damped cells for 12 GHz high gradient accelerating structures

Title Design of waveguide damped cells for 12 GHz high gradient accelerating structures

Abstract This document describes the design procedure and numerical techniques used to optimize waveguide-damped traveling wave accelerating structure cells for high gradients, and characterize their wakefields. All simulations were made using ACE3P [22]. The document also contains the design data for a collection of such cells operating at accelerating mode frequency = 11.9942 GHz and 120° phase-advance. This collection of highly optimized cells are created for use with the fast RF structure parameter estimator CLICopti [24], which is used for CLIC rebaselining.

Where CLIC note 1026

When May 2014

Contribution Kyrre wrote the document, made the protocol for how to set up the simulations and analyze the data, wrote the AcdOptiGUI software, and performed the simulations.

Main author Kyrre Sjøbæk

Co-authors Alexej Grudiev and Erik Adli

Bibliography entry [23]

Errata The following errors have been found in the text:

Equation 2.2  $(G^{30}\tau^5)^{1/6}$  should be  $(G^{30}\tau^5)^{1/5}$ .

Equation 3.7  $V_x$  is used in place of  $V_z$  in the equation and in the sentence directly above.

Section 3.1 The expressions are true only for  $\phi = 0$ . See Section 6.2.1 of the thesis for further discussion.

Section 4.11 The  $Q$  prior to outer wall optimization should be 5453, not 5941.

Location on-line <https://cds.cern.ch/record/1712945>

## F.4. The CLICopti RF structure parameter estimator

Title The CLICopti RF structure parameter estimator

Abstract This document describes the CLICopti RF structure parameter estimator. This is a C++ library which makes it possible to quickly estimate the parameters of an RF structure from its length, apertures, tapering, and basic cell type. Typical estimated parameters are the input power required to reach a certain voltage with a given beam current, the maximum safe pulse length for a given input power and the minimum bunch spacing in RF cycles allowed by a given long-range wake limit.

The document describes the implemented physics, usage of the library through its Application Programming Interface (API) and the relation between the different parts of the library. Also discussed is how the library is checked for correctness, and the example programs included with the sources are described.

Where CLIC note 1031

When June 2014

Contribution

Main author Kyrre Sjøbæk

Co-authors Alexej Grudiev

Bibliography entry [24]

Errata The following errors have been found in the text:

Section 4.1.5 The power at the trailing edge should be described as  $P(t) = P_0 - P(t - t_3)$  not  $P(t) = P(t - t_3)$ . The correct form is used elsewhere.

Equation 4.29 The time  $t$  should be  $t - t(z)$ , taking the propagation time of the signal into account. The conclusion remains correct.

Location on-line <https://cds.cern.ch/record/1712948>

## F.5. Breakdown localization in the Fixed Gap System

Title Breakdown localization in the Fixed Gap System

Abstract Accurate localization of breakdowns in vacuum could help shed light on breakdown related processes that are not yet fully understood. At the DC spark lab at CERN, an instrument called the *Fixed Gap System* (FGS) has been developed partially for this purpose. Among other things, the FGS has four built-in antennas, which are intended for breakdown localization. The capability of this aspect of the FGS was explored in this report. Specifically, the feasibility of using a method similar to that which is used in cavity *Beam Position Monitors* (BPMs) was investigated. The usable frequency range of the current experimental setup was also studied.

Firstly, a modal analysis of the inner geometry of the FGS was done in HFSS. This showed that the two first modes to be expected in the spark gap quite differ from

those of the ideal pillbox – both in field pattern and in frequency ( $\approx 4$  and  $6$  GHz vs.  $0.2$  and  $3$  GHz). Secondly, S-parameters of the system were measured. These showed that the coupling between antennas is weak below  $\approx 13$  GHz, which is due to the high cut-off frequency of the waveguides in which the antennas are located. The breakdown signal was also measured using an oscilloscope connected to the antennas. However, it was determined that the detected signal was picked up from outside of the system, rendering it useless for localization purposes. It was concluded that either a new approach has to be adopted or the current system must be modified.

Where CLIC NOTE 1033

When September 2<sup>nd</sup>, 2014

Contribution Kyrre came up with the idea of treating the cavity as a BPM, provided simulation data from ArcPIC2D, and generally helped supervise Robin (who was a summer student).

Main author Robin Rajamaki

Other co-authors Walter Wuensch

Bibliography entry [173]

Location on-line <https://cds.cern.ch/record/1756445>

## F.6. 2D ArcPIC Code Description and User / Developer Manual (second edition)

Title 2D ArcPIC Code Description: Description of Methods and User / Developer Manual (second edition)

Abstract Vacuum discharges are one of the main limiting factors for future linear collider designs such as that of the Compact Linear Collider (CLIC). To optimize machine efficiency, maintaining the highest feasible accelerating gradient below a certain breakdown rate is desirable; understanding breakdowns can therefore help us to achieve this goal. As a part of ongoing theoretical research on vacuum discharges at the Helsinki Institute of Physics, the build-up of plasma can be investigated through the particle-in-cell method. For this purpose, we have developed the 2D ArcPIC code introduced here.

We present an exhaustive description of the 2D ArcPIC code in several parts. In the first chapter, we introduce the particle-in-cell method in general and detail the techniques used in the code. In the second chapter, we describe the code and provide a documentation and derivation of the key equations occurring in it. In the third chapter, we describe utilities for running the code and analyzing the results. The last chapter contains suggestions for viable and useful avenues for further work on the code.

The code and documentation are original work of the authors, written in 2010–2014, and is therefore under the copyright of the authors.

Where CLIC note 1032

When September 2014

Contribution This CLIC-note is the updated 2<sup>nd</sup> edition of a previously published document [30]. Kyrre Sjøbæk updated the document to match v3.00 of the 2D ArcPIC simulation code, and also expanded and re-organized the contents of the document.

Main author Kyrre Sjøbæk

Co-authors Helga Timkó

Bibliography entry [31]

Location on-line <https://cds.cern.ch/record/1951304>

## F.7. Updated baseline for a staged Compact Linear Collider

Title Updated baseline for a staged Compact Linear Collider

Abstract The Compact Linear Collider (CLIC) is a multi-TeV high-luminosity linear  $e^+e^-$  collider under development. For an optimal exploitation of its physics potential, CLIC is foreseen to be built and operated in a staged approach with three centre-of-mass energy stages ranging from a few hundred GeV up to 3 TeV. The first stage will focus on precision Standard Model physics, in particular Higgs and top measurements. Subsequent stages will focus on measurements of rare Higgs processes, as well as searches for new physics processes and precision measurements of new states, e.g. states previously discovered at LHC or at CLIC itself. In the 2012 CLIC Conceptual Design Report, a fully optimised 3 TeV collider was presented, while the proposed lower energy stages were not studied to the same level of detail. This report presents an updated baseline staging scenario for CLIC. The scenario is the result of a comprehensive study addressing the performance, cost and power of the CLIC accelerator complex as a function of centre-of-mass energy and it targets optimal physics output based on the current physics landscape. The optimised staging scenario foresees three main centre-of-mass energy stages at 380 GeV, 1.5 TeV and 3 TeV for a full CLIC programme spanning 22 years. For the first stage, an alternative to the CLIC drive beam scheme is presented in which the main linac power is produced using X-band klystrons.

When Document in preparation (Summer 2016)

Contribution Kyrre did parts of the research on which the RF model is based, and wrote the software for estimating RF structure parameters – see [23, 24, 99]. Also discussed the high gradient limits and the RF optimization at multiple occasions with lead authors, as well as giving extensive feedback on the text of the report.

Authors The CLIC and CLICdp collaborations

Bibliography entry [25]

Location on-line <https://edms.cern.ch/document/1690625/1>