

Modeling and Simulation of Microwave Ablation of Liver Tumors

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Abstract

The goal of this research is to study, understand, and robustly model and simulate microwave ablation of liver tumors. This is one of the possible treatments for cancerous tumors that appear in the liver, and there is room for a better understanding and prediction of how such interventions develop, from a mathematical point of view. The areas that could benefit from a more rigorous quantification range from planning of the invasive aspect of the procedure, influence of the vascular system, all the way to predicting the resulting damage in biological tissue. This would ultimately also benefit clinicians, that have much to gain from such results, as it would allow them to plan microwave ablation procedures on a patient-to-patient basis, thus obtaining a better outcome.

This research has been done under the supervision of Prof. Dr. Tobias Preußer, Head of Modeling and Simulation at Fraunhofer MEVIS, and Professor of Mathematics at Jacobs University Bremen, as well as Prof. Dr. Marcel Oliver, Professor of Mathematics at Jacobs University Bremen. I have also been supervised by Dr. Hanne Ballhausen and Dr. Torben Pätz, from Fraunhofer MEVIS, throughout various phases of my research.

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Chapter 1

Introduction and Motivation

Cancer is a disease which manifests through abnormal cell growth, that has the potential to spread throughout the body. In 2012, liver cancer was the second most common cause of death from cancer worldwide, accounting for approximately 9.1% of all cancer related deaths [9]. Considering that the mortality rate of those diagnosed with cancer varies wildly, from 10% into the upper 90%, depending on the type and position of the cancerous cells, there is a real interest to always find better treatment methods, which fit a wider range of situations, and that provide increasingly better outcomes.

Thermal ablation is one of the medical techniques used to treat cancerous tumors without excision. This is done by heating and destroying the cancer cells, through various methods. Other ablation techniques might involve freezing the cancer cells, or ablation by alcohol injection into the cancerous tumor.

Perhaps the most widespread thermal ablation method, radio frequency ablation (RFA), requires the use of alternating electric current in the radio frequency range. Another technique involves the use of high intensity focused ultrasound (often abbreviated HIFU), which has the advantage of being noninvasive [40]. Finally, the method which will be discussed in the research at hand, is microwave ablation (MWA). This relies on using electromagnetic waves, as in RFA, but of higher frequency. The differences between RFA and MWA shall be elaborated on in the following section. Both techniques emanate the energy into the human body through an antenna placed inside a catheter, visualized schematically in Figure [1].

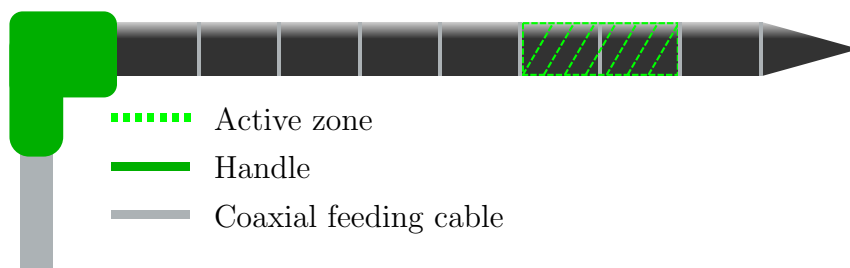


Figure 1: Sketch of sample catheter used in RFA and MWA procedures.

The tip of the catheter is inserted into the body, the energy emanates from the hashed area, called the *active zone*, and the energy is fed into the shaft through a coaxial cable.

The research at hand will focus on mathematically modeling, simulating, and optimizing, from a mathematical standpoint, scenarios where microwave-frequency electromagnetic waves are interacting with tissues that share the same properties as the human liver. The first part of the work will be focused on accurately reproducing such an interaction numerically, by implementing the physical laws and equations that dictate how electromagnetic waves behave. Secondly, the heat that is generated by such an interaction will be studied, and its influence on the electromagnetic simulation will be analyzed.

Aside from gaining a better scientific understanding of the process, one of the main reasons for conducting this research is to provide better tools for clinicians to perform ablation interventions. The present research is part of a larger project, entitled MICROPLAN, which has been funded by the Deutsche Forschungsgemeinschaft, and has taken place jointly at Fraunhofer MEVIS and Jacobs University Bremen, with clinical partners in Charité - Universitätsmedizin Berlin and Medizinische Hochschule Hannover. This project aimed to provide a complete patient-specific treatment planning tool, aided by modeling and simulation, and image processing techniques. Deeper knowledge in this area would aid in prediction and planning of patient-individual procedures. Normally, medical personnel rely on generic predictions offered by hardware manufacturers, and have to account themselves for various factors that might lead to a different result. Some examples of these factors are: position of blood vessels, position of insertion of the antenna into the body, pre-existing additional conditions, etc. However, as we shall soon highlight, MWA can overcome some of these hindering factors to a larger extent than RFA.

It is also of great interest to gain insight into the interaction of electromagnetic waves, specifically in the microwave frequency range, with healthy and unhealthy tissue in the human body. This has become a popular topic especially in the context of interaction of microwave and electromagnetic wave emitters with the human body, for example with the increase in popularity of cellular phones [30], and household appliances such as microwave ovens, or wireless communication such as WiFi. A good understanding of their effect on humans is necessary in order to allow safe manufacturing and usage guidelines.

The ideal scenario of a tumor ablation procedure, or any cancer treatment for that matter, would consist of 100% of cancerous cells being destroyed, and as little as possible of the surrounding healthy tissue. Normally, there is a so-called safety margin, of tissue surrounding the cancerous tumor, which is also ablated as a precaution, as it is not easy to determine the exact boundary between healthy and cancerous cells. The planning tool that will incorporate this research would be of interest to clinicians, as it would allow them to more accurately plan such an intervention. Instead of relying on generic predictions provided by the ablation hardware manufacturers, clinicians could tailor the medical procedure based on the individual patient's needs. For instance, relying on predictions about the shape of the ablated tissue zone might lead to suboptimal results, either in the form of remaining non-ablated cancer tissue (for example due to cooling done by blood vessels), too much destroyed healthy tissue, or damage done to so-called *risk tissue*, such as blood vessels.

The way in which electromagnetic waves behave and propagate in a medium is dictated by Maxwell's equations, which are a set of partial differential equations that lay out the foundations of classical electromagnetism. Thus, any research conducted into microwave ablation procedures would have these equations as a starting point for investigations.

Both RFA and MWA rely on ablating tissue through heating produced by electromagnetic waves. In short, this works by converting some of the electromagnetic energy into heating energy, where the proportion depends on a material parameter called electrical conductivity.

One could say that RFA and MWA are competing techniques that have the same goal. Let us present some of the differences. Specifically in the context of liver tumors ablation, where there are numerous blood vessels, there is a high chance of a heat sink effect appearing. This means that the flow of blood absorbs the heat generated by the ablation procedure, functioning as a cooling system. Electromagnetic waves in the microwave frequency seem more able to overcome this effect [26], partly due to their ability to deliver more energy, creating large zones of ablation even in the vicinity of blood vessels of 10 mm diameter. In contrast, RFA is less effective around vessels larger than 3 mm in diameter. The higher success rate of MWA can be also observed in the local recurrence rate, for example for liver cancer, where the rate is between 1% and 33% [23], whereas for RFA it can be as high as 82% [24].

Furthermore, RFA heavily relies on the tissue having a high enough conductivity in order to propagate, and this is dictated mostly by the water content. In radiofrequency applications, when the temperature rises above the boiling point of water, the conductivity lowers significantly, making RFA become significantly less effective. Microwave ablation on the other hand is not as reliant on this aspect. A qualitative plot of temperature versus application time is presented in Figure [2], based on the data presented in [26], to further illustrate this difference. The oscillation due to boiling and condensation of the water in the RFA can be observed.

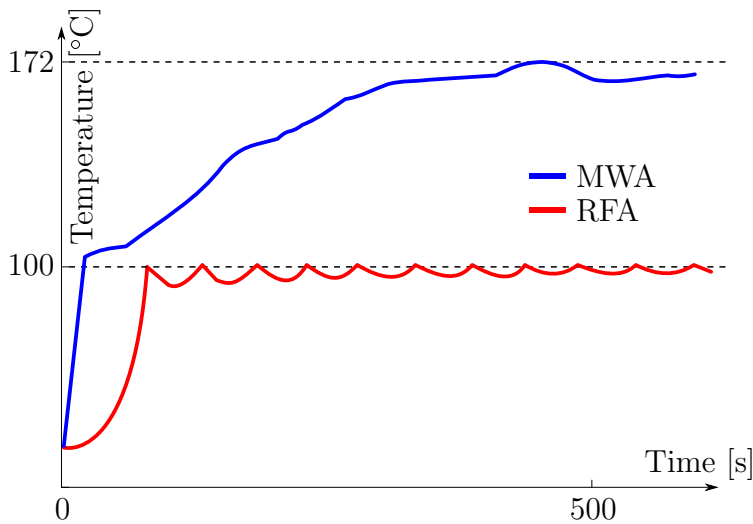


Figure 2: MWA vs. RFA temperatures in in-vivo porcine kidneys, based on [26].

One of the disadvantages of both RFA and MWA is the heating taking place in the applicator which is introduced into the organ, due to the generated signal that is transmitted through the shaft. This effect is illustrated in Figure [3]. One way to solve this would be to additionally cool down the applicator shaft. This would restrict the cause of ablation to the electromagnetic influence, and not the direct thermal contact with the shaft. Thus, the ablation pattern inside the organ would remain close to the desirable shape, and would not become elongated, or *tear-shaped*.

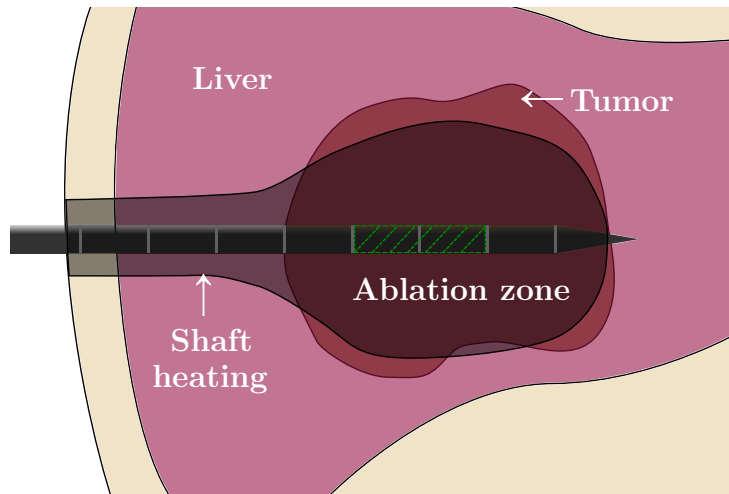


Figure 3: Schematic of MWA procedure, highlighting shaft heating.

Due to its advantages over RFA, more and more clinicians are choosing MWA as their procedure of choice for thermal ablation interventions. This furthermore justifies the research at hand in the context of the MICROPLAN project.

A multitude of publications related to MWA refer first of all to 2D axis-symmetric simulations as a model of organs, which assume a homogeneous medium in which the procedure takes place [1, 2, 4]. This reduces the problem from a 3D to essentially a 2D one, where the 2D model is rotated around an axis to emulate a 3D model. This is quite far from the clinical reality, as the organs are highly heterogeneous, for example due to the vascular system, which does not fit such axis symmetry assumptions.

Fully 3D models that make no homogeneity assumptions, and furthermore couple with such heat equations, are scarce at best. For example Deshan Yang's *Measurements, Antenna Design and Advanced Computer Modeling for Microwave Tissue Ablation* [45], which analyzes the influence of the heat, uses a fully 3D approach, but assumes homogeneity of the organ. Models which also assume that the tissue parameters vary with temperature are even harder to come by, for example Punit Prakash's *Theoretical Modeling for Hepatic Microwave Ablation* [32], which does all of the above except assume heterogeneity.

1.1 Goals

The main goal of this research is to study, within the framework of the Finite Difference Time Domain method (FDTD), a model and simulation of MWA of the human liver. The model shall consist of the following:

1. A simulation of Maxwell's equations
2. A simulation of the bioheat equation
3. A tissue damage model
4. A tissue parameter model

From this list, we shall focus on the simulation of Maxwell's equations. The equations governing items 1-4 above form a set of partial differential equations, which are coupled through the temperature dependent parameters, and through the fact that the output of item 1 provides the input for item 2. The emphasis of the present research shall be on the following:

Time scales. One problem that arises in the setting of coupled electromagnetic and thermal effects is the following: electromagnetic simulations of microwave applications take place in the frequency range of 915 to 2400 MHz. Therefore they require a very fine spatial and temporal discretization, whereas the heat equation does not develop significantly on such a fine temporal level. Thus, one would want to reduce the complexity of the electromagnetic simulation, in order to produce some sort of averaged quantity that can be more rarely plugged into the heat equation. One could do this by taking advantage of the lossy nature of the medium, and realizing that the simulation stabilizes after some relatively short time period. The exact mathematical way to determine when the simulation should be considered stable is yet to be determined. For instance, some averaged quantification of the electric field could be used as a reference. One could then cut off the electromagnetic simulation after a certain number of time steps, and plug that state into the heat equation.

Antenna model. An important point of this process shall be accurately modeling the antenna that delivers the electromagnetic signal. Since antennas are usually mechanically and geometrically complex, and the simulation relies on having accurate electromagnetic material properties, one would either have to obtain the exact specifications of such an antenna, or reverse engineer its properties mathematically. The reverse engineering could be done by varying the parameters until a similar (or ideally identical) ablation pattern or heat distribution is obtained. One would need to know the current and charge density distribution within the antenna, which act as source terms in Maxwell's equations, and the electromagnetic properties of all the components, such as the electric permittivity, the magnetic permeability, and electric resistivity. If such information is not available, one would have to infer them from some averaged quantities, such as the delivered power in Watts. As these parameters might change as the temperature changes, temperature-dependent information in this regard would be of great help in increasing the reliability of the antenna model.

Tissue parameters. The electromagnetic parameters of the materials that will be part of the simulation shall be considered to be temperature dependent, and they relate to several components of this research. Thus, a special emphasis shall be placed on realistically modeling their influence onto all relevant equations.

Boundary conditions. Suitable boundary conditions shall also be prescribed if necessary, both at the interface between the applicator and the organ, between different heterogeneous media inside the organ, and at the outer boundary of the computational domain. It might be the case that at some interfaces, and for some types of media, this will not be necessary, but in principle, when an electromagnetic wave traverses the interface of two media with different refractive indices, one would expect some reflected and refracted components. This should mostly be dictated by how far the electromagnetic field permeates inside each of these types of tissues.

Integration with image data. As part of the patient-specific goal of this research, the component which fulfills this aspect is the integration of the models and simulations with patient-specific image data. This shall be the cornerstone of the individual applicability of this research.

Evaluation. Furthermore, it is envisioned that this simulation will be compared to clinical data of such procedures, ideally both ex-vivo and in-vivo. The comparison will be performed firstly in order to adjust the simulation, and secondly (ideally) match the observed experimental results. The final goal is to obtain a simulation that is able to realistically predict ablation results. This whole package could then be used to plan future microwave ablation procedures.

Finally, the simulation and optimization shall be included into a software that is to be used by doctors and clinicians for planning medical interventions. To this end, the mathematical machinery should be incorporated in an intuitive way, allowing key parameters of the simulation to be specified as input, in order to obtain a user-friendly planning software.

The present thesis shall be structured as follows:

In Chapter 2, the continuous models describing the equations involved will be introduced.

In Chapter 3, the discretization of the electromagnetic equations will be presented, together with some noteworthy remarks on this discretization process.

In Chapter 4, some aspects related to putting together the building blocks of the entire simulation pipeline will be discussed.

In Chapter 5, some numerical experiments and results relevant for the discretization process will be presented.

In Chapter 6, a simulation incorporating most of the building blocks is showcased, with real patient data. This is followed by Chapter 7, comprising of the conclusions, discussion, and foreseeable future research topics.

Within these chapters, Section 3.6 (starting with p. 61), and chapters 4, 5 and 6 consist primarily of original work. The remaining chapters and sections predominantly contain results available in literature, which were adapted, expanded and aligned to the goals of the thesis at hand.

Chapter 2

Continuous Model

In this chapter we shall discuss the steps that need to be taken before the discretization process. First, we shall present the equations that govern the behavior of electromagnetic waves, or radiation. Broadly speaking, electromagnetism is the study of electromagnetic forces. Electromagnetic forces consist of the electric and the magnetic forces, which are produced by electric charges, and moving electric charges, respectively. The electromagnetic field is defined locally as the electromagnetic force.

Electrostatics and magnetostatics refer to the study of electromagnetic fields that are (approximately or exactly) constant in time, while electrodynamics is the study of time-varying electromagnetic fields. The reason why we use the word *waves* in the context of electromagnetism shall become apparent in the discussion of electrodynamics, when we shall reach some wave-like equations. These waves explain and quantify several physical phenomena, including light, X-rays, microwaves, and many other.

Let us first spend some time describing the developments that preceded electrodynamics. In the context of electrostatics, the equations can be built from the ground up in some sense, starting with the fundamentals of charges and forces, but the process is of little relevance for the work at hand. Therefore we will simply state these electrostatic equations. The manner in which they are obtained from the more general electrodynamic equations shall be clear once the latter are showcased in Section 2.1. Hereon we shall denote vector quantities with bold symbols for readability. Furthermore, we also denote by $\oint$ a closed line integral, by $\oiint$ a closed surface integral, and by $\cdot$ the dot product.

$$\nabla \times \mathbf{H} = \mathbf{J}, \quad \nabla \cdot \mathbf{B} = 0 \quad (1)$$

$$\nabla \times \mathbf{E} = 0, \quad \nabla \cdot \mathbf{D} = \rho$$

In the above, $\mathbf{E}$ is the electric field, $\mathbf{E} : \Omega \times [0, t_{\text{final}}] \rightarrow \mathbb{R}^3$ for some given time interval, with units $[\mathbf{E}]_{\text{SI}} = \frac{\text{V}}{\text{m}}$. $\mathbf{D}$ is the electric flux (or displacement), with units $[\mathbf{D}]_{\text{SI}} = \frac{\text{C}}{\text{m}^2}$. $\mathbf{H}, \mathbf{B} : \Omega \times [0, t_{\text{final}}] \rightarrow \mathbb{R}^3$ are the magnetic field, and magnetic flux, respectively, with units $[\mathbf{H}]_{\text{SI}} = \frac{\text{A}}{\text{m}}$, $[\mathbf{B}]_{\text{SI}} = \frac{\text{N}}{\text{Am}}$. ρ is the electric (volume) charge density, with units $\frac{\text{C}}{\text{m}^3}$, and $\mathbf{J}$ is the electric current density, with units $[\mathbf{J}]_{\text{SI}} = \frac{\text{A}}{\text{m}^2}$.

Let us make one final remark before moving forward to electrodynamics. The fact that the curl of $\mathbf{E}$ is zero means that it can be expressed as a gradient of some scalar potential, or in other words, as a so-called *conservative vector field*:

$$\mathbf{E} = -\nabla V$$

since we know that (continuously differentiable) vector fields are conservative if and only if they are curl-free. Similarly, using the fact that the divergence of any curl of a vector field is zero $\nabla \cdot (\nabla \times \mathbf{A}) = 0$, we can express $\mathbf{B}$ in terms of a vector potential $\mathbf{A}$:

$$\mathbf{B} = \nabla \times \mathbf{A}$$

Let us now expand (1). Introducing $\mu : \Omega \rightarrow \mathbb{R}$ as the magnetic permeability, with units $[\mu]_{\text{SI}} = \frac{H}{m} = \frac{N}{A^2}$, and assuming that $\mathbf{B}$ and $\mathbf{H}$ are related by $\mathbf{H} = \frac{\mathbf{B}}{\mu}$ (which will be motivated within Section 2.1), we have:

$$\nabla \times \mathbf{B} = \nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} = \mu_0 \mathbf{J}$$

Here $\nabla^2 = \Delta$ is the Laplacian operator, $\Delta = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$. Since we could now add any field whose curl is zero to $\mathbf{A}$ and not change the physical electric field, one can use these extra degrees of freedom to specify V and $\mathbf{A}$ further, by only allowing zero-divergence fields for $\mathbf{A}$. Similarly, one could add any constant to V . With this, the equations above become Poisson's equation:

$$\nabla^2 \mathbf{A} = -\mu_0 \mathbf{J}, \quad \nabla^2 V = -\frac{\rho}{\varepsilon_0}$$

where ε is the electrical permittivity, and comes up in $\mathbf{D} = \varepsilon \mathbf{E}$. With this we finalize our discussion of electrostatics.

2.1 Maxwell's equations

In this section, we shall first introduce the relevant equations, then explain the units involved, and finally try to present some physical intuition about their behavior. We start by introducing the equations that govern the propagation of electromagnetic waves:

$$\textbf{Amp\`ere's Law, "fixed":} \quad (\text{integral form}) \quad \frac{\partial}{\partial t} \iint_S \mathbf{D} \cdot d\mathbf{S} = \oint_{\partial S} \mathbf{H} \cdot d\mathbf{L} - \iint_S \mathbf{J} \cdot d\mathbf{S} \quad (2a)$$

$$(\text{differential form}) \quad \frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J} \quad (2b)$$

$$\textbf{Faraday's Law:} \quad (\text{integral form}) \quad \frac{\partial}{\partial t} \iint_S \mathbf{B} \cdot d\mathbf{S} = -\oint_{\partial S} \mathbf{E} \cdot d\mathbf{L} - \iint_S \mathbf{M} \cdot d\mathbf{S} \quad (3a)$$

$$(\text{differential form}) \quad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} - \mathbf{M} \quad (3b)$$

$$\textbf{Gauss' Law, electric field:} \quad (\text{integral form}) \quad \oiint_{\partial \Omega} \mathbf{D} \cdot d\mathbf{S} = \iiint_{\Omega} \rho dV \quad (4a)$$

$$(\text{differential form}) \quad \nabla \cdot \mathbf{D} = \rho \quad (4b)$$

$$\textbf{Absence of magnetic charges:} \quad (\text{integral form}) \quad \oiint_{\partial \Omega} \mathbf{B} \cdot d\mathbf{S} = 0 \quad (5a)$$

$$(\text{differential form}) \quad \nabla \cdot \mathbf{B} = 0 \quad (5b)$$

These equations are named after Scottish mathematical physicist James Clerk Maxwell, and have been often called a great unification of electricity, light and magnetism into one field of electromagnetism. Some standard resources on these equations could be found for example in John David Jackson's *Classical Electrodynamics* [19], or in David J. Griffiths' *Introduction to Electrodynamics* [15]. As we shall soon explain, Maxwell modified Ampère's original law, creating an altered version which we refer to as "fixed".

In the above equations, $\mathcal{S}$ is an arbitrary compact 2D surface with a piecewise smooth 1D boundary denoted as $\partial\mathcal{S}$. Moreover, Ω is an arbitrary compact 3D volume, with its piecewise smooth 2D boundary denoted as $\partial\Omega$.

Furthermore, $\sigma, \varepsilon : \Omega \rightarrow \mathbb{R}$ are the electrical conductivity, and electric permittivity, respectively, with units $[\sigma]_{\text{SI}} = \frac{S}{m}$, $[\varepsilon]_{\text{SI}} = \frac{F}{m}$. We denote by $\mathbf{M}$ the magnetic current density, with units $[\mathbf{M}]_{\text{SI}} = \frac{V}{m^2}$.

Note that Faraday's Law does not normally appear with this magnetic current density, and the absence of physical magnetic charges would imply that this current cannot exist. We shall see in a moment the computational reason for introducing this fictitious current.

Now, in order to understand how all the equations are coupled, a relationship linking $\mathbf{D}$, $\mathbf{E}$ and $\mathbf{H}$, $\mathbf{B}$ pairwise is needed. This is done through the so-called *constitutive equations*.

$$\mathbf{D} = \varepsilon \mathbf{E} + \text{polarization}, \quad \mathbf{H} = \frac{1}{\mu} \mathbf{B} - \text{magnetization}$$

This is the most general form of these relations, however human tissues cannot develop or exhibit either polarization or magnetization, so we shall use the simplified equations:

$$\mathbf{D} = \varepsilon \mathbf{E}, \quad \mathbf{H} = \frac{1}{\mu} \mathbf{B} \tag{6}$$

Before we spend some time discussing the physical interpretation of Maxwell's equations, let us mention that usually their differential forms are presented, for readability. The integral forms are obtained by applying the Kelvin–Stokes Theorem and the Divergence Theorem, given in (7), to the differential forms of the equations.

$$\oint_{\partial\mathcal{S}} \mathbf{F} d\mathbf{L} = \iint_{\mathcal{S}} \nabla \times \mathbf{F} d\mathbf{S}, \quad \iiint_V (\nabla \cdot \mathbf{F}) dV = \oint\oint_{\partial V} (\mathbf{F} \cdot \mathbf{n}) dS \tag{7}$$

Here $\mathbf{n}$ is the outer unit normal vector to the surface ∂V . Now, let us discuss the physical interpretation of Maxwell's equations. Gauss' Law (4b) states that any divergence in the electric displacement, and consequently the electric field (due to the constitutive equations), is given by the electrical charge contained. Equation (5b) tells us that the converse statement for the magnetic field does not hold. That is, there is no known magnetic charge.

The integral forms of these equations, (4a) and (5a), serve to specify the volumes and surfaces involved in the statements. In this sense, they help us obtain a more concrete picture of the statements, and are much more helpful in practice, in order to gain intuition about all four equations. This will be especially helpful later on, throughout the entire transition from these analytic statements towards discrete equivalents.

Faraday's Law (3b) states that over a given surface, a changing magnetic flux induces an electric field around itself, specifically across the boundary of this surface (according to the right-hand rule). We do not attribute any physical interpretation to the magnetic current at this point.

We finally arrive at the most interesting equation, Ampère's Law, "fixed" (2b). Originally, Ampère's Law did not contain the so-called *displacement current* $\frac{\partial \mathbf{D}}{\partial t}$ term. This equation was initially observed in terms of steady state phenomena ($\frac{\partial}{\partial t}(\text{any field}) = 0$) for the case $\nabla \cdot \mathbf{J} = 0$, which can be retrieved by taking the curl of the equation without the displacement current.

Maxwell's addition was to introduce the displacement current $\mathbf{J}_d := \frac{\partial \mathbf{D}}{\partial t}$, motivated by the suspicion that the equations should be symmetric, as is the case for many phenomena. That is, he suspected that if a changing magnetic flux can produce an electric field, then a changing electric flux should produce a magnetic field.

First, let us look at the continuity equation for charge and current:

$$\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = 0$$

Now substitute (the time derivative of) Gauss' Law (4b) into the above:

$$\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = \nabla \cdot \left(\mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \right) = 0$$

So Maxwell thought to replace $\mathbf{J}$ with $\mathbf{J} + \mathbf{J}_d$, which turns Ampère's Law into a law that is consistent with time-changing fields. Finally, the remaining current $\mathbf{J}$ can be further split into two terms:

$$\mathbf{J} = \mathbf{J}_{\text{source}} + \mathbf{J}_{\text{conduction}}$$

The source current may be any arbitrarily imposed source, but the fact that an electric field flowing through a material with $\sigma \neq 0$ generates a current is a well-known fact:

$$\text{Ohm's Law: } \mathbf{J}_{\text{conduction}} = \sigma \mathbf{E}$$

We can also interpret this in another way: σ defines the ratio of electric energy that is lost, and turned into heat. This will be elaborated on later, but in a similar manner, we can define magnetic losses:

$$\mathbf{M} = \mathbf{M}_{\text{source}} + \sigma^* \mathbf{H}$$

Here we introduce the nonphysical *magnetic conductivity* σ^* , with units $[\sigma^*]_{\text{SI}} = \frac{\Omega}{m} = \frac{V}{Am}$. This term is a purely theoretical construct, which serves to make the equations symmetric. With this, we finalize the introduction of Maxwell's equations.

2.1.1 Field propagation in vacuum and conductors

Let us visualize the electric and magnetic fields for a simple case: plane wave propagation. One way to categorize types of tissues, from the electromagnetic point of view, is through their conductivity σ . Tissues with no conductivity, such as vacuum or air, are called *lossless*, because none of the electromagnetic energy is "lost" and converted to heat, as

can be seen in Ampère's Law. Tissues that satisfy $\sigma > 0$ are coined *lossy*. One important remark to make is that in a lossless medium, the electric and magnetic fields are in phase. The following is an example of a sinusoidal wave propagation along the x -axis, where $\mathbf{E}$ is polarized (oriented) in the z -direction, and $\mathbf{B}$ is polarized in the y -direction:

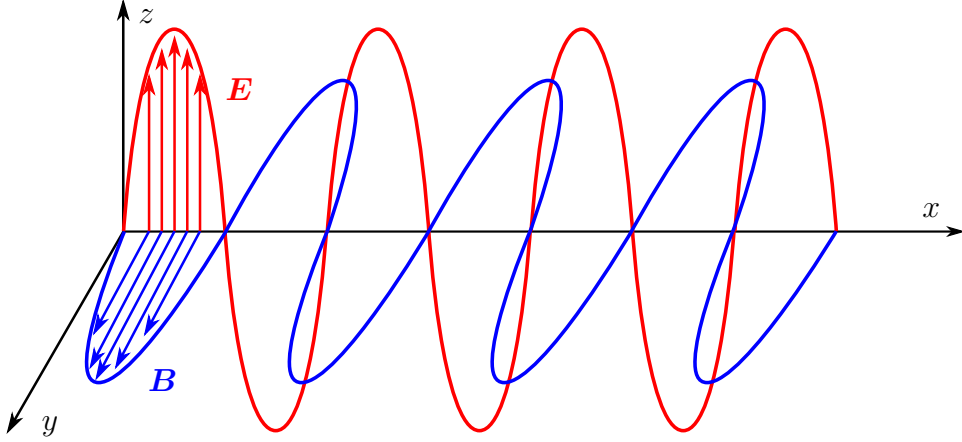


Figure 4: E and B fields in phase.

We shall derive this soon for more general mediums, but it is known that in vacuum, the relationship between the amplitudes of the fields is the following:

$$\frac{|\mathbf{B}(x)|}{|\mathbf{E}(x)|} = \frac{1}{c}$$

where c is the speed of light in vacuum. Since plane wave propagation through vacuum is lossless, this ratio is actually preserved pointwise everywhere.

In a lossy material however, this relationship changes. To observe this, let us apply curl to Faraday and Ampère's laws. Assuming no source currents or charges are present, we obtain the following equations:

$$\nabla \times \left(\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_{\text{conduction}} \right) = \nabla \times \nabla \times \mathbf{H}, \quad \nabla \times \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \nabla \times \mathbf{E}$$

Using the vector identity

$$\nabla \times (\nabla \times \mathbf{V}) = \nabla(\nabla \cdot \mathbf{V}) - \nabla^2 \mathbf{V} = \nabla(\nabla \cdot \mathbf{V}) - \Delta \mathbf{V}$$

together with the lack of charge ($\rho = 0$), which results in zero divergence of both $\mathbf{E}$ and $\mathbf{B}$ from (4b) and (5b), we can simplify further:

$$\nabla \times \left(\frac{\partial \mathbf{D}}{\partial t} + \sigma \mathbf{E} \right) = -\Delta \mathbf{H}, \quad \nabla \times \frac{\partial \mathbf{B}}{\partial t} = \Delta \mathbf{E}$$

Then, applying the constitutive relations (6) in a homogeneous medium yields:

$$\begin{aligned} \nabla \times \left(\varepsilon \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E} \right) &= -\Delta \left(\frac{\mathbf{B}}{\mu} \right), & \mu \nabla \times \frac{\partial \mathbf{H}}{\partial t} &= \Delta \mathbf{E} \\ \left(\sigma + \varepsilon \frac{\partial}{\partial t} \right) (\nabla \times \mathbf{E}) &= -\frac{1}{\mu} \Delta \mathbf{B}, & \frac{\partial}{\partial t} (\mu \nabla \times \mathbf{H}) &= \Delta \mathbf{E} \end{aligned}$$

Applying (2b) and (3b) once more yields:

$$\left(\sigma + \varepsilon \frac{\partial}{\partial t}\right) \left(\frac{\partial \mathbf{B}}{\partial t}\right) = \frac{1}{\mu} \Delta \mathbf{B}, \quad \frac{\partial}{\partial t} \left(\mu \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \mu \sigma \mathbf{E}\right) = \Delta \mathbf{E}$$

Which finally leads to these two wave equations:

$$\Delta \mathbf{E} = \mu \varepsilon \frac{\partial^2}{\partial t^2} \mathbf{E} + \mu \sigma \frac{\partial}{\partial t} \mathbf{E} \quad (8)$$

$$\Delta \mathbf{B} = \mu \varepsilon \frac{\partial^2}{\partial t^2} \mathbf{B} + \mu \sigma \frac{\partial}{\partial t} \mathbf{B} \quad (9)$$

Equations (8) and (9) admit so-called *plane waves* as solutions, which are constant frequency electromagnetic waves (of frequency ω), whose wave fronts (surfaces of constant phase) are infinite planes. These planes are perpendicular to the direction-defining *wave vector* $\mathbf{k} := k\mathbf{x}$, which in our case points along the x -axis. The scalar k is usually called the *wave number*. With this in mind, let us implicitly define our wave number as:

$$\tilde{k}^2 := \mu \varepsilon \omega^2 + i \mu \sigma \omega$$

then the plane waves listed below satisfy our wave equations (8) and (9).

$$\begin{aligned} \mathbf{E}(x, t) &= \mathbf{E}_0 \exp\left(i(\tilde{k}x - \omega t)\right) \\ \mathbf{B}(x, t) &= \mathbf{B}_0 \exp\left(i(\tilde{k}x - \omega t)\right) \end{aligned}$$

If we now solve for $\tilde{k}$ we obtain

$$\tilde{k} = \frac{\omega}{c\sqrt{2}} \sqrt{\sqrt{1 + \left(\frac{\sigma}{\varepsilon\omega}\right)^2} + 1} + i \frac{\omega}{c\sqrt{2}} \sqrt{\sqrt{1 + \left(\frac{\sigma}{\varepsilon\omega}\right)^2} - 1}$$

We notice that the amplitude of the waves decreases with distance due to the imaginary part of $\tilde{k}$. We denote by $\Im(\cdot) : \mathbb{C} \rightarrow \mathbb{R}$ the imaginary part, and $\Re(\cdot) : \mathbb{C} \rightarrow \mathbb{R}$ the real part of a complex number, respectively. We can rewrite the plane wave equations as:

$$\begin{aligned} E_y(x, t) &= E_{y0} \exp\left(-x\Im(\tilde{k})\right) \exp\left(i(\Re(\tilde{k})x - \omega t)\right) \\ B_z(x, t) &= B_{z0} \exp\left(-x\Im(\tilde{k})\right) \exp\left(i(\Re(\tilde{k})x - \omega t)\right) \end{aligned} \quad (10)$$

Let us note however, that the wave equations impose fewer restrictions than the full Maxwell equations. For example, we can still gain information about the relative amplitudes of the two fields, by plugging in our solutions (10) into Faraday's Law. Applying $\frac{\partial}{\partial t}(\cdot)$ to B , and $-\nabla \times (\cdot)$ to E , we obtain:

$$B_z(x, t) = E_y(x, t) \frac{\tilde{k}}{\omega}$$

We can observe that the fields remain perpendicular, but there is one qualitative difference from the lossless case: a difference in phase between the fields has been introduced. To see this, let us first rewrite $\tilde{k}$.

$$\tilde{k} = |\tilde{k}|e^{i\varphi}$$

$$\text{where } |\tilde{k}| = \omega \sqrt{\varepsilon\mu} \sqrt{1 + \left(\frac{\sigma}{\varepsilon\omega}\right)^2}, \quad \varphi = \tan^{-1} \left(\frac{\Im(\tilde{k})}{\Re(\tilde{k})} \right)$$

Therefore, the complex amplitudes of the fields are related as follows:

$$B_0 e^{i\varphi_B} = \frac{|\tilde{k}| e^{i\varphi}}{\omega} E_0 e^{i\varphi_E}$$

Thus, the phase relationship between the two fields is given by φ :

$$\varphi_B = \varphi_E + \varphi$$

and the real amplitudes of the fields by:

$$\frac{B_0}{E_0} = \sqrt{\varepsilon\mu} \sqrt{1 + \left(\frac{\sigma}{\varepsilon\omega}\right)^2}$$

Summing up, the real electric and magnetic fields are the following:

$$\begin{aligned} \mathbf{B}(x, t) &= \begin{pmatrix} 0 \\ 0 \\ B_0 \end{pmatrix} \exp\left(-\Im(\tilde{k})x\right) \cos(\Re(\tilde{k})x - \omega t + \varphi_E + \varphi) \\ \mathbf{E}(x, t) &= \begin{pmatrix} 0 \\ E_0 \\ 0 \end{pmatrix} \exp\left(-\Im(\tilde{k})x\right) \cos(\Re(\tilde{k})x - \omega t + \varphi_E) \end{aligned}$$

In the figure below we visualize this phase difference and point out the exponential decay of the amplitude:

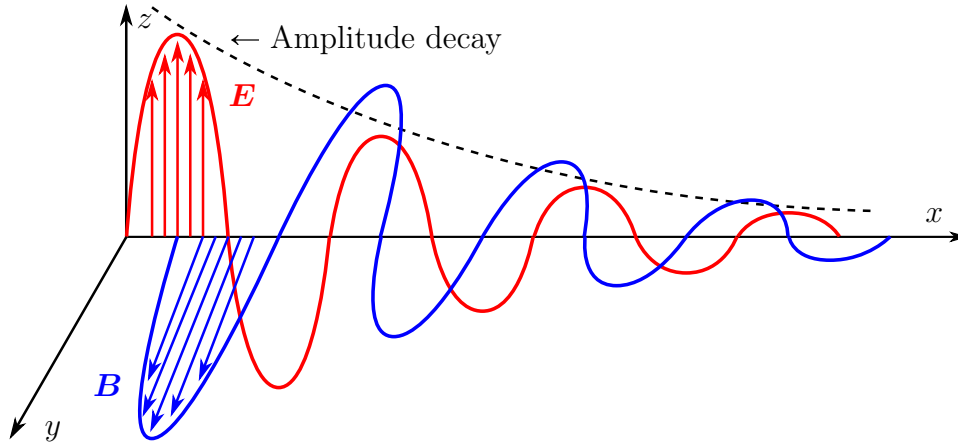


Figure 5: Phase shift in lossy (homogeneous) mediums.

Having gained some more intuition about the way electromagnetic fields propagate in both vacuum and lossy materials, and how their phase and amplitude are affected, we can proceed to the other relevant equations.

2.2 Bioheat equation and tissue damage

In order to simulate the impact of the electromagnetic field on a given biological tissue, one needs to specify how heat is produced, since temperature is the main quantifier in the evaluation of tissue damage. To this end, we define the bioheat equation:

$$\rho_{\text{kg}} C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + Q$$

where $\rho_{\text{kg}} \left[\frac{\text{kg}}{\text{m}^3} \right]$ is the mass density (to be distinguished from our usual charge density ρ), $C \left[\frac{\text{J}}{\text{K}} \right]$ is the heat capacity, $T[\text{K}]$ is the temperature, $\lambda \left[\frac{\text{W}}{\text{mK}} \right]$ is the thermal conductivity, and $Q \left[\frac{\text{J}}{\text{m}^3 \text{s}} \right]$ defines heat sources or heat sinks. Q is further separated into:

$$Q = Q_{\text{perfusion}} + Q_{\text{source}}$$

where $Q_{\text{perfusion}}$ is the heat sink due to blood perfusion in the tissue, and Q_{source} is the heat source (or sink), which in our case will be defined pointwise as:

$$Q_{\text{source}}(\mathbf{r}) := \sigma(\mathbf{r}) \|\mathbf{E}(\mathbf{r})\|^2$$

Tissue parameter values, both thermal and dielectric (related to the electromagnetic equations), will be discussed in Section 6. It is worth mentioning that while the area of experimental parameter evaluation is not recent, it is ongoing, and there are numerous biological tissues that are not completely characterized. As mentioned, heating is the main source of so-called *tissue damage*, or tissue coagulation. We will define tissue damage based on the Arrhenius formalism tissue damage integral [7]:

$$D(x, t) = A \int_0^t \exp \left(-\frac{E}{RT(x, \tau)} \right) d\tau$$

where $D[1]$ is the degree of tissue damage, $R \left[\frac{\text{J}}{\text{molK}} \right]$ is the universal gas constant, $A \left[\frac{1}{\text{s}} \right]$ is a “frequency factor”, $E \left[\frac{\text{J}}{\text{mol}} \right]$ is the activation energy for irreversible damage, and $T : \Omega \times [0, t]$ with units $[K]$ is the temperature.

This is one of the more involved tissue damage models. Other options are the *Cumulative equivalent minutes* model, developed by Sapaerto and Dewey [37], which defines thermal effects in terms of how many minutes of heating at 43deg Celsius would be needed to obtain the same result. Probably the simplest option is to define some threshold temperature above which the tissue is considered destroyed, which is what we shall do, as motivated below.

We shall later compare the temperature distribution produced by our complete electrodynamic model with that given by another (reference point) model, which employs a static approximation of Maxwell’s equations. That reference model will use (qualitatively) the same heat solver, but does not estimate the tissue damage caused by heat. Both heat solvers perform explicit time-stepping. Thus, for all intents and purposes, the final comparison shall be carried out between the resulting temperatures, or equivalently, by looking at a relevant temperature threshold.

2.3 The Field Equivalence Principle

We shall now introduce one of the most important building blocks of both theoretical and numerical electrodynamics, the *Field Equivalence Principle*. Intuitively, this method involves replacing certain sources of electromagnetic fields, with other types of sources. Consider the following situation:

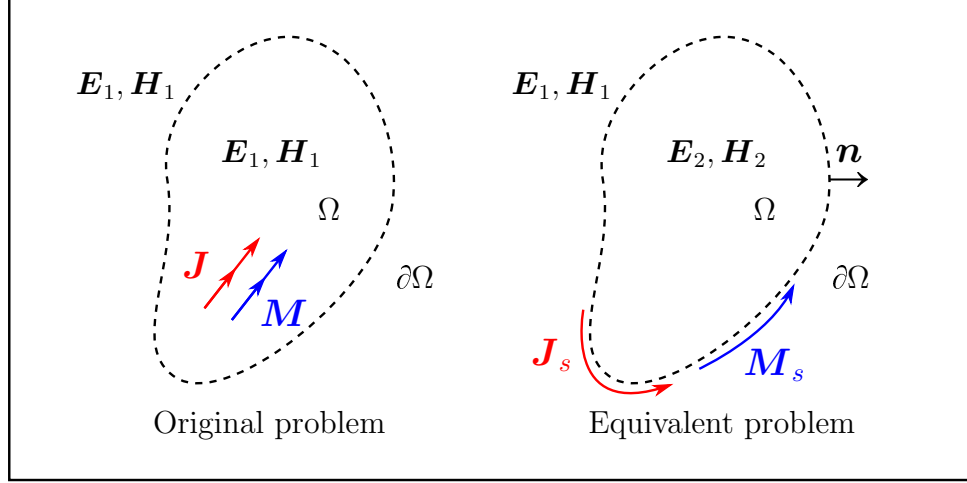


Figure 6: Illustration of the FEP.

Assume there are some sources of electromagnetic waves inside Ω , denoted by $\mathbf{J}$ and $\mathbf{M}$, which radiate fields outwards. The boundary $\partial\Omega$ of Ω is an arbitrary virtual construct, which does not necessarily have any physical counterpart. Then the Field Equivalence Principle (hereon FEP) can be phrased in broad terms as follows:

Given the problem on the left in Figure [6], find an “equivalent” problem in the following sense: the radiated fields outside of Ω must be the same as in the original problem.

Now, as stated, this description is vague, however that is not unexpected, since this is not a uniqueness statement. There are in fact infinitely many equivalent problems that one can formulate in such a manner. The way in which this equivalent problem is built, is by replacing the sources inside Ω with equivalent sources, given by so-called *surface current densities* $\mathbf{J}_s$ and $\mathbf{M}_s$, which have units defined by $[\mathbf{J}_s]_{\text{SI}} = m[\mathbf{J}]_{\text{SI}}$, $[\mathbf{M}_s]_{\text{SI}} = m[\mathbf{M}]_{\text{SI}}$. A proper physically meaningful definition will be given in Section 3.2.1. For now let us mention that they are defined as improper integrals of their volumetric counterparts, over infinitesimally small volumes or areas.

Let us first acknowledge some historical aspects before we formalize this discussion further. The principle we have introduced is mentioned under different names, and in different variations: Field Equivalence Principle, Huygens’ principle, Love’s equivalence principle, Schelkunoff’s equivalence principle, Volume equivalence principle, etc. The earliest form of this concept was investigated by Christiaan Huygens, who introduced it in his *Traité de la Lumière* [16] in 1690. Silvanus P. Thompson translated Huygens’ work into English in 1912 [17], which thereafter gave rise to the term *Huygens’ principle*, stated as follows:

“Each point on a primary wavefront can be considered to be a new source of a secondary spherical wave and that a secondary wavefront can be constructed as the envelope of these secondary spherical waves.” [20]

This can be interpreted visually in the example below. Huygens did not explain initially why the wavefronts of the points travel only forward, and there is no backward wavefront created, and simply assumed this to be the case. The new wavefront, displayed in green, is comprised of the envelope of all spherical waves present on the old planar wavefront.

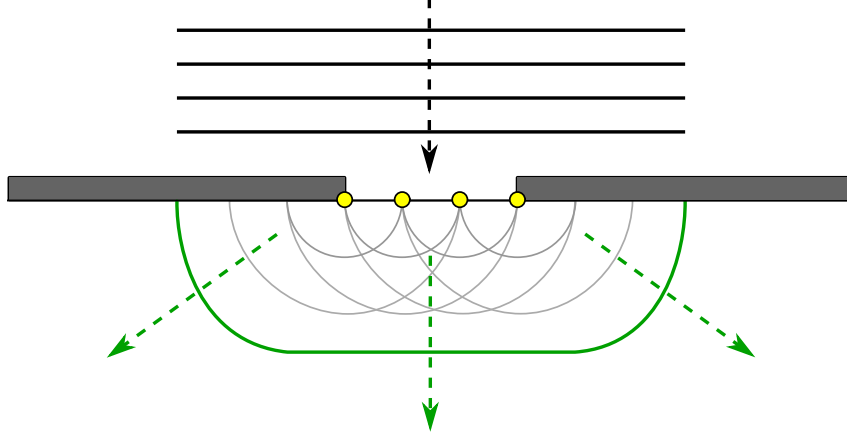


Figure 7: Huygens' principle illustrated.

The first rigorous mathematical analysis of this principle started with Helmholtz in 1859, which was done for steady-state monochromatic (single-frequency) waves, and then also by Kirchhoff in 1882 for time-dependent scenarios. In the context of Maxwell's equations, the first to investigate an equivalent formulation in terms of the vector quantities $\mathbf{E}$ and $\mathbf{H}$ was Augustus Edward Hough Love in 1901 [25]. Love introduced the concept of equivalent surface current, which would act as the intermediate source of spherical waves, whose envelope would compose the further wavefront. In his formulation the fields inside Ω are identically zero.

Schelkunoff extended this result, by allowing arbitrary fields to be present inside Ω (and thus on both sides of $\partial\Omega$). This result is known as Schelkunoff's equivalence principle. If we now look back at Figure [6], we see that the equivalent problem on the right-hand side is a formulation of Schelkunoff's equivalence principle.

Let us continue by formalizing the statement. In the equivalent problem, the sources $\mathbf{J}$ and $\mathbf{M}$ are removed, and replaced pointwise locally by equivalent surface current densities, given by:

$$\mathbf{J}_s = \mathbf{n} \times (\mathbf{H}_1 - \mathbf{H}_2)|_{\partial\Omega} \quad (11)$$

$$\mathbf{M}_s = -\mathbf{n} \times (\mathbf{E}_1 - \mathbf{E}_2)|_{\partial\Omega} \quad (12)$$

The main ingredient needed in proving the FEP, is the inherent boundary condition that arises at interfaces, which is precisely given by (11) and (12). In order to derive this, let us consider the following:

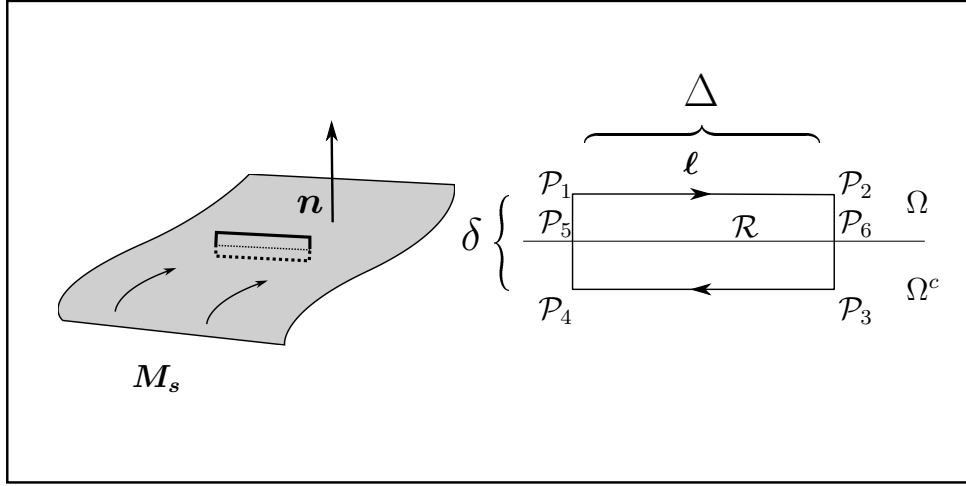


Figure 8: Integration contour.

Let us assume that there is a surface separating Ω and its complement (with respect to the 2D space it is embedded into) Ω^c , and a rectangle perpendicular to this surface, given by the points $\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_3, \mathcal{P}_4$, which form the closed loop $\ell := \overrightarrow{\mathcal{P}_1 \mathcal{P}_2 \mathcal{P}_3 \mathcal{P}_4}$, enclosing the rectangular surface $\mathcal{R}$. Assume that the width Δ of the rectangle is small enough that all quantities are constant in the direction parallel to the surface.

Let $E_{1\parallel}$ be the parallel (to the surface) component of the electrical field inside Ω , and $E_{2\parallel}$ the analogue for Ω^c . If we apply Faraday's Law in integral form, we obtain the following:

$$\oint_{\ell} \mathbf{E} \cdot d\mathbf{L} = - \iint_{\mathcal{R}} \mathbf{M} \cdot d\mathbf{S} - \frac{d}{dt} \iint_{\mathcal{R}} \mathbf{B} \cdot d\mathbf{S}$$

If we now assume that the height δ of the rectangle $\mathcal{R}$ is infinitesimal, then the surface of $\mathcal{R} \rightarrow 0$, and if $\mathbf{B}$ is bounded on this surface, then the rightmost term vanishes.

$$\Rightarrow \int_{\mathcal{P}_1}^{\mathcal{P}_2} \mathbf{E} \cdot d\mathbf{L} + \int_{\mathcal{P}_2}^{\mathcal{P}_3} \mathbf{E} \cdot d\mathbf{L} + \int_{\mathcal{P}_3}^{\mathcal{P}_4} \mathbf{E} \cdot d\mathbf{L} + \int_{\mathcal{P}_4}^{\mathcal{P}_1} \mathbf{E} \cdot d\mathbf{L} = - \iint_{\mathcal{R}} \mathbf{M} \cdot d\mathbf{S} \quad (13)$$

If we now implicitly define a surface current density $\mathbf{M}_s$ through

$$\iint_{\mathcal{R}} \mathbf{M} \cdot d\mathbf{S} = \int_{\mathcal{P}_5}^{\mathcal{P}_6} \mathbf{M}_s \cdot d\mathbf{L} = \Delta \cdot \mathbf{M}_s$$

and assume that $\mathbf{E}$ is also bounded on $\mathcal{R}$, the two terms on the left-hand side of (13), which integrate perpendicularly to the interface, cancel out due to the infinitesimal δ .

$$\Rightarrow \int_{\mathcal{P}_5}^{\mathcal{P}_6} (\mathbf{E}_{1\parallel} - \mathbf{E}_{2\parallel}) \cdot d\mathbf{L} = \Delta(\mathbf{E}_{1\parallel} - \mathbf{E}_{2\parallel}) = -\Delta \mathbf{M}_s \quad \Leftrightarrow \quad (\mathbf{E}_{1\parallel} - \mathbf{E}_{2\parallel}) = -\mathbf{M}_s$$

In other words, if $\mathbf{n}$ is the unit normal pointing from Ω^c into Ω :

$$\mathbf{n} \times (\mathbf{E}_1 - \mathbf{E}_2) = -\mathbf{M}_s$$

which is exactly (12). In a completely analogous manner, one obtains (11). Here we can note that these currents are a purely mathematical construct, and do not have a physical equivalent. They are simply tools to correct the discrepancy in fields across the surface, as far as Maxwell's equations are concerned.

With this in mind, we see that this new construct satisfies Faraday and Ampère's laws, both across the interface, and, assuming this was the case for the original problem, outside Ω as well. If the newly specified fields $\mathbf{E}, \mathbf{H}$ inside Ω are also consistent with Maxwell's equations (which is true for uniformly zero fields in particular), then both problems are consistent with Maxwell's equations.

The applicability of the FEP method is now clear, together with its difficulties. Assume that the electromagnetic field is known (or can be reliably measured or approximated) on a surface of the computational domain. Then all physical structures and sources of energy (contained by this surface) can be replaced by a homogeneous volume with zero (or otherwise specified) electromagnetic fields. The use case of this for our simulations will range from numerical proof of concepts, to possibly simulating (or rather replacing) a physical antenna within tissue.

2.4 Energy

In this section we shall shortly present the concept of energy in the electromagnetic context. We know from classical electrodynamics that the expression for electromagnetic energy density (in vacuum) is the following:

$$U_{\text{EM}} = \frac{1}{2} \int_{\Omega} \left(\varepsilon_0 E^2 + \frac{1}{\mu_0} B^2 \right) dV$$

where E, B are the (real) amplitudes of the electric and magnetic fields. Let us derive this. We know from magnetostatics ([15], p. 204) that given a charge q , moving at speed v inside an electromagnetic field, the net force acting on it is:

$$\mathbf{F} = q [\mathbf{E} + (\mathbf{v} \times \mathbf{B})]$$

This equation is known as the **Lorentz Force Law**, and is a fundamental axiom of electromagnetism. Now, let us assume we have some charge and current density that produces the electromagnetic field given by $\mathbf{E}, \mathbf{B}$. If within the next infinitesimal time window dt the charges move with speed $\mathbf{v}$, how much work is done by the electromagnetic fields on these charges?

For an infinitesimal volume dV we know that the electric charge $q = \rho dV$, and that the current density is given by the moving charge density $\mathbf{J} = \rho \mathbf{v}$. If we integrate over a volume Ω which contains all the charges and currents, this means that the rate of work shall be:

$$\frac{dW}{dt} = \int_{\Omega} \mathbf{E} \cdot \mathbf{J} dV$$

noting that $\mathbf{E} \cdot \mathbf{J}$ is the work done per unit volume, per unit time, i.e. *power* per unit volume, so power density. Let us rewrite this quantity to factor out $\mathbf{J}$, using Maxwell's equations. From Ampère's Law we have:

$$\mathbf{E} \cdot \mathbf{J} = \frac{1}{\mu_0} \mathbf{E} \cdot (\nabla \times \mathbf{B}) - \varepsilon_0 \mathbf{E} \cdot \frac{\partial}{\partial t} \mathbf{E} \quad (14)$$

Using the following vector identity:

$$\nabla \cdot (\mathbf{V} \times \mathbf{W}) = \mathbf{W} \cdot (\nabla \times \mathbf{V}) - \mathbf{V} \cdot (\nabla \times \mathbf{W})$$

and applying Faraday's Law, we obtain:

$$\mathbf{E} \cdot (\nabla \times \mathbf{B}) = -\mathbf{B} \cdot \frac{\partial}{\partial t} \mathbf{E} - \nabla \cdot (\mathbf{E} \times \mathbf{B})$$

Furthermore, we arrive at the following forms:

$$\mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial t} = \frac{1}{2} \frac{\partial}{\partial t} (B^2), \quad \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} = \frac{1}{2} \frac{\partial}{\partial t} (E^2)$$

With this we can rewrite (14) as:

$$\mathbf{E} \cdot \mathbf{J} = -\frac{1}{2} \frac{\partial}{\partial t} \left(\varepsilon_0 E^2 + \frac{1}{\mu_0} B^2 \right) - \frac{1}{\mu_0} \nabla \cdot (\mathbf{E} \times \mathbf{B})$$

If we use the Divergence Theorem on the second term from the RHS, and plug it into the expression of the rate of work, we arrive at:

$$\frac{\partial W}{\partial t} = -\frac{\partial}{\partial t} \int_{\Omega} \frac{1}{2} \left(\varepsilon_0 E^2 + \frac{1}{\mu_0} B^2 \right) dV - \frac{1}{\mu_0} \oint_{\partial\Omega} (\mathbf{E} \times \mathbf{B}) dS$$

This is known as **Poynting's Theorem**. The LHS is the power delivered to the volume Ω , the first term of the RHS is the rate of loss of electromagnetic energy within the volume $\partial_t U_{\text{EM}}$, and the second term is the rate of energy transport out of the volume (through $\partial\Omega$).

The **Poynting vector**, which points in the direction of energy transport, is:

$$\mathbf{S} := \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B}$$

which quantifies energy per unit area per unit time. Finally, if we denote by U_{MEC} the mechanical energy density as given by

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial t} \int_{\Omega} U_{\text{MEC}} dV$$

then we can rewrite Poynting's Theorem in differential form:

$$\frac{\partial}{\partial t} (U_{\text{MEC}} + U_{\text{EM}}) = -\nabla \cdot \mathbf{S}$$

It is worth mentioning that performing a discrete check of the conservation of U_{MEC} is one of the heuristics to evaluate numerical schemes solving Maxwell's equations. Furthermore, in hyperthermia patient treatment interventions (both computationally and continuously in the operating room) the input power is defined on a generator. This generator then transports the energy, usually through a coaxial cable, to the applicator.

The transport of energy is not perfect, and less than 100% of the energy leaving the generator reaches the tip of the applicator. When simulating a pipeline involving this generator component, this fact has to be taken into account in order to not overestimate the delivered thermal dose.

Before we move over to the next section, let us summarize the main equations we shall be interested in. These are (i) be the bioheat equation, which was not discretized by the author, but by Tim Kröger, Inga Altrogge and Tobias Preußner [21], with a Finite Element discretization in space, and various discretization methods in time:

$$\rho_{\text{kg}} C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + Q$$

and (ii) Maxwell's equations, which will be our main focus:

$$\begin{aligned} \frac{\partial \mathbf{D}}{\partial t} &= \nabla \times \mathbf{H} - \mathbf{J}, & \frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \mathbf{E} - \mathbf{M} \\ \nabla \cdot \mathbf{D} &= \rho, & \nabla \cdot \mathbf{B} &= 0 \end{aligned}$$

Chapter 3

Discretization

In this chapter we shall present the discretization method that we used for Maxwell's equations, and various properties and aspects of this process. As mentioned before, once this is done, the heat solver shall interpret the output of the discrete solutions to Maxwell's equations in terms of an isotropic hexahedral Finite Element mesh. We shall also mention that in this work there is no grid adaptivity implemented, with respect to either the spatial or temporal discretizations. While possible, adaptivity would be quite technically involved (requiring work in so-called *sub-voxel accuracy* and interface matching similar to that of the FEP). Furthermore, the code written for this research was developed with the end goal of GPU parallelization in mind.

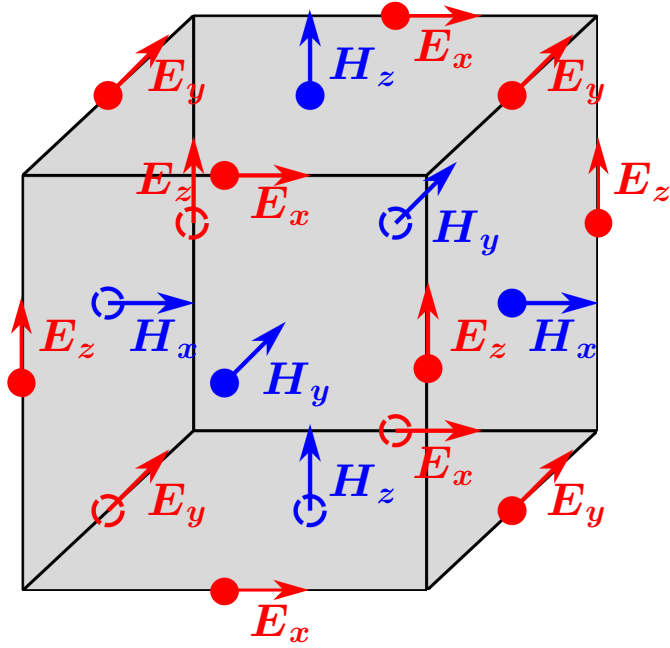
3.1 Finite-difference time-domain

Arguably the most used discretization method for time-dependent Maxwell's equations has been Yee's scheme, introduced by Kane S. Yee, in his seminal 1966 paper *Numerical Solution of Initial Boundary Value Problems Involving Maxwell's Equations in Isotropic Media* [46]. This method is now most often referred to as the *finite-difference time-domain* method, or FDTD. It involves a finite difference stencil for both the spatial and temporal discretizations. In relation to what was available at the time, but also more importantly to what has been used since, Yee's scheme has proven to be one of the most widely used. Some of the major reasons are:

1. Solving for both the electric and magnetic fields simultaneously, as opposed to using potential methods to reduce Maxwell's equations to a wave equation, where one solves for only one of the fields.
2. Simplicity of the discretization.
3. Discrete conservation of the divergence of the fields.

As can be seen below in Figure [9], the main idea of the Yee algorithm is to space out the electric and magnetic fields as follows: given a hexahedral gridding of the physical space, the $\mathbf{E}$ components are placed on the midpoints of the edges of grid cells, and the $\mathbf{H}$ components are placed in the midpoints of the grid cell faces.

These correspond with the component directions, for example the E_x component is placed on the midpoint of an edge aligned with the x -axis, the H_x component is placed at the midpoint of a face perpendicular to the x -axis, and so on.

Figure 9: Yee grid cell, with staggered E and H grids.

Another very important feature to notice, which leads to discrete conservation of the divergence of the fields, is that not only does this grid provide an intuitive placement of pointwise evaluation positions, but also of integration contours. Faraday's Law and Ampère's Law can be readily applied to a given component together with the four surrounding dual components.

Furthermore, given a material interface provided by the hexahedral mesh, the continuity of field components is preserved across the interface as long as it is parallel to one of the axes (which is readily true when the interface is rasterized by the grid).

In terms of temporal discretization, Yee's algorithm employs the so-called *leapfrog* scheme. Illustrated in Figure [10], this algorithm involves evaluating all E field points at integer multiples of the temporal step Δ_t , and the H field at half-integer points $n\Delta_t + \frac{1}{2}$, $n \in \mathbb{N}$. Each time the electric field is updated, it uses the intermediate magnetic field values, and vice-versa.

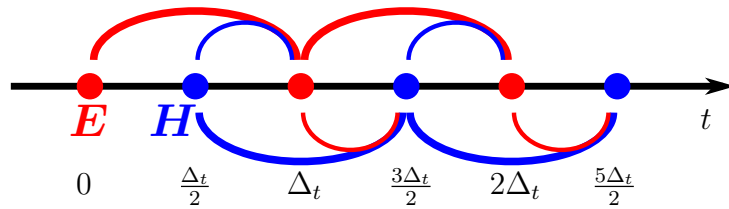


Figure 10: Leapfrog time stepping scheme.

The main importance of this is that it removes the issue of simultaneous evaluation of the equations given by Faraday and Ampère's laws, namely the apparent inability to evaluate both at the same time.

Before specifying the actual algorithm steps, let us define the notation. We note here that unless necessary, we shall try to keep the assumptions to a minimum, and only make them locally where needed. Assume Ω_h is a cuboid grid of size $N_x \times N_y \times N_z$ with spacing

$\Delta_x, \Delta_y, \Delta_z$, and let Δ_t be the temporal step to be used in the leapfrog scheme.

For any analytic or discrete field, or any parameter quantity f (which is a function of both space and time), the evaluation of this quantity at the grid point $(i\Delta_x, j\Delta_y, k\Delta_z)$ (with $i \in \{0, \dots, N_x\}$, $j \in \{0, \dots, N_y\}$, $k \in \{0, \dots, N_z\}$), and at the discrete time point $n\Delta_t$ is denoted by $f|_{i,j,k}^n$, i.e.

$$f|_{i,j,k}^n := f(i\Delta_x, j\Delta_y, k\Delta_z, n\Delta_t)$$

Now, we mentioned a finite-difference discretization in space, which is performed as follows for the derivative in the x -direction, and analogously for the other four directions (y, z, t):

$$\frac{\partial}{\partial x} f|_{i,j,k}^n = \frac{f|_{i+\frac{1}{2},j,k}^n - f|_{i-\frac{1}{2},j,k}^n}{\Delta_x} + O(\Delta_x^2) \quad (15)$$

which follows immediately from a Taylor series expansion of $f((i + \frac{1}{2})\Delta_x, j\Delta_y, k\Delta_z)$ and $f((i - \frac{1}{2})\Delta_x, j\Delta_y, k\Delta_z)$ around $(i\Delta_x, j\Delta_y, k\Delta_z)$. The main importance of this choice of step size is that a derivative of a field at one point can be computed with the readily available discrete field values, which are separated by half a step in both time and space. In the same manner, we can retrieve the corresponding discretization in time:

$$\frac{\partial}{\partial t} f|_{i,j,k}^n = \frac{f|_{i,j,k}^{n+\frac{1}{2}} - f|_{i,j,k}^{n-\frac{1}{2}}}{\Delta_t} + O(\Delta_t^2) \quad (16)$$

As a result of the choice of truncation, one would expect that the numerical scheme is second order accurate in both space and time. We could of course construct schemes with larger difference stencils, and thus higher convergence order, but most applications prefer the second order scheme because the smaller stencil allows more geometric flexibility. With a higher order scheme and a larger stencil, and when dealing with heterogeneities, it may happen that stencil evaluations pertaining to a derivative in one type of material take place “several materials away”, depending on the geometry. This normally leads to numerical instability, and would require a nontrivial amount of effort to circumvent.

3.1.1 Yee’s algorithm

The algorithm put forward by Yee consists of the following steps:

1. Discretize all derivatives according to Equation (15) and (16)
2. Transform the resulting equations into *update equations* by splitting up the contributions of the time derivative to both sides of the equations
3. Given known E field values up to the time point $k\Delta_t$, evaluate the magnetic field update equation to obtain $H^{k+\frac{1}{2}}$
4. Evaluate the electric field update equation to obtain E^{k+1}
5. Repeat steps 3 and 4 until the desired total simulation time is reached

Now, let us see how the first two steps are carried out in practice. Looking at the x -coordinate of (2b), let us assume that during the time elapsed in our electromagnetic simulation, the permittivity ε stays constant in time. As we shall observe later, even if

this may not be exactly true, we still need to make this assumption when breaking down time (actually temperature) dependence into constant steps. We now have:

$$\frac{\partial}{\partial t} E_x = \frac{1}{\varepsilon} \left(\frac{\partial}{\partial y} H_z - \frac{\partial}{\partial z} H_y - (\sigma E_x + J_{\text{source},x}) \right)$$

Let us first write and illustrate this discretization in 1D. This means we are working with the E_z and H_y fields for example, where E_z are evaluated at integer points in space and time, and H_y are evaluated at half-integer points. If both conductivities σ, σ^* are zero and we have no source current, the update equation becomes:

$$\varepsilon \frac{E_z|_i^n - E_z|_i^{n+1}}{\Delta t} = \frac{H_y|_{i+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} \Leftrightarrow$$

$$E_z|_i^{n+1} = E_z|_i^n + \frac{\Delta t}{\varepsilon \Delta x} \left(H_y|_{i+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2}}^{n+\frac{1}{2}} \right)$$

The update idea is illustrated in Figure [11] in 1D, for ease of visualization.

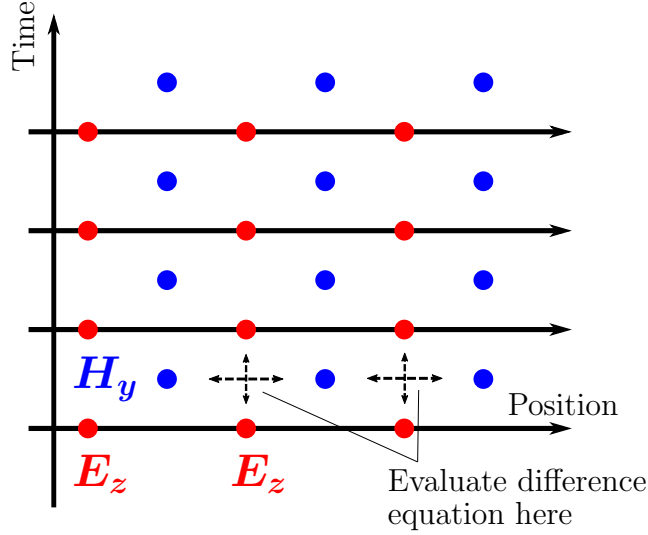


Figure 11: Visualization of the time stepping scheme.

Now, without making any assumptions about σ, σ^* , and if we consider nonzero electric and magnetic currents $\mathbf{J}$ and $\mathbf{M}$, the 3D update equations for E_z , H_x and H_y are:

$$E_z|_{i,j,k+\frac{1}{2}}^{n+1} = \frac{1 - \frac{\sigma \Delta t}{2\varepsilon}}{1 + \frac{\sigma \Delta t}{2\varepsilon}} E_z|_{i,j,k+\frac{1}{2}}^n +$$

$$+ \frac{\frac{\Delta t}{\varepsilon}}{1 + \frac{\sigma \Delta t}{2\varepsilon}} \left(\frac{H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} - \frac{H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y} - J_{\text{source},z}|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} \right) \quad (17)$$

$$H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1 - \frac{\sigma^* \Delta t}{2\mu}}{1 + \frac{\sigma^* \Delta t}{2\mu}} H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n-\frac{1}{2}} +$$

$$+ \frac{\frac{\Delta t}{\mu}}{1 + \frac{\sigma^* \Delta t}{2\mu}} \left(\frac{E_y|_{i,j+\frac{1}{2},k+1}^n - E_y|_{i,j+\frac{1}{2},k}^n}{\Delta z} - \frac{E_z|_{i,j+1,k+\frac{1}{2}}^n - E_z|_{i,j,k+\frac{1}{2}}^n}{\Delta y} - M_{\text{source},x}|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n \right) \quad (18)$$

$$\begin{aligned}
H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1 - \frac{\sigma^* \Delta_t}{2\mu}}{1 + \frac{\sigma^* \Delta_t}{2\mu}} H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n-\frac{1}{2}} + \\
&+ \frac{\frac{\Delta_t}{\mu}}{1 + \frac{\sigma^* \Delta_t}{2\mu}} \left(\frac{E_z|_{i+1,j,k+\frac{1}{2}}^n - E_z|_{i,j,k+\frac{1}{2}}^n}{\Delta_x} - \frac{E_x|_{i+\frac{1}{2},j,k+1}^n - E_x|_{i+\frac{1}{2},j,k}^n}{\Delta_z} - M_{\text{source},y}|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n \right)
\end{aligned} \tag{19}$$

Before we address the other three update equations, let us take a moment to make a few remarks. First, the three equations (17),(18),(19) form what is called the *transverse magnetic* z case, or TM^z case, since the magnetic field is transverse to the z -direction.

This is one of the two ways to define a 2D restriction of Maxwell's equations. The analogous formulation is the *transverse electric*, or TE^z case, where E_x, E_y, H_z fields are considered. The TE^z and TM^z formulations (or modes, as they are sometimes referred to) complement each other, and form the full 3D equations.

Furthermore, let us clarify that the following parameter-dependent coefficients

$$\frac{1 - \frac{\sigma \Delta_t}{2\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}}, \quad \frac{1 - \frac{\sigma^* \Delta_t}{2\mu}}{1 + \frac{\sigma^* \Delta_t}{2\mu}}, \quad \frac{\frac{\Delta_t}{\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}}, \quad \frac{\frac{\Delta_t}{\mu}}{1 + \frac{\sigma^* \Delta_t}{2\mu}}$$

are all evaluated at the position of the field whose update equation they are part of, i.e.

$$\begin{aligned}
E_z|_{i,j,k+\frac{1}{2}}^{n+1} &= \frac{1 - \frac{\sigma_{i,j,k+\frac{1}{2}} \Delta_t}{2\varepsilon_{i,j,k+\frac{1}{2}}}}{1 + \frac{\sigma_{i,j,k+\frac{1}{2}} \Delta_t}{2\varepsilon_{i,j,k+\frac{1}{2}}}} E_z|_{i,j,k+\frac{1}{2}}^n + \frac{\frac{\Delta_t}{\varepsilon_{i,j,k+\frac{1}{2}}}}{1 + \frac{\sigma_{i,j,k+\frac{1}{2}} \Delta_t}{2\varepsilon_{i,j,k+\frac{1}{2}}}} \left(\dots \right) \\
H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1 - \frac{\sigma_{i,j+\frac{1}{2},k+\frac{1}{2}}^* \Delta_t}{2\mu_{i,j+\frac{1}{2},k+\frac{1}{2}}}}{1 + \frac{\sigma_{i,j+\frac{1}{2},k+\frac{1}{2}}^* \Delta_t}{2\mu_{i,j+\frac{1}{2},k+\frac{1}{2}}}} H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\frac{\Delta_t}{\mu_{i,j+\frac{1}{2},k+\frac{1}{2}}}}{1 + \frac{\sigma_{i,j+\frac{1}{2},k+\frac{1}{2}}^* \Delta_t}{2\mu_{i,j+\frac{1}{2},k+\frac{1}{2}}}} \left(\dots \right) \\
H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1 - \frac{\sigma_{i+\frac{1}{2},j,k+\frac{1}{2}}^* \Delta_t}{2\mu_{i+\frac{1}{2},j,k+\frac{1}{2}}}}{1 + \frac{\sigma_{i+\frac{1}{2},j,k+\frac{1}{2}}^* \Delta_t}{2\mu_{i+\frac{1}{2},j,k+\frac{1}{2}}}} H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\frac{\Delta_t}{\mu_{i+\frac{1}{2},j,k+\frac{1}{2}}}}{1 + \frac{\sigma_{i+\frac{1}{2},j,k+\frac{1}{2}}^* \Delta_t}{2\mu_{i+\frac{1}{2},j,k+\frac{1}{2}}}} \left(\dots \right)
\end{aligned}$$

Throughout all of our further use of FDTD, we shall assume that all parameters are constant in time (only w.r.t the electromagnetic equations). Hence, we suppress the time index in the coefficients above. It is also noteworthy that the terms of the form σE_w , $w \in \{x, y, z\}$ would normally be evaluated at half integer time steps, and those of the form $\sigma^* H_w$ at integer steps, contrary to their field value counterparts. What is most often done is to perform a so-called *semi-implicit* approximation, namely:

$$E_w|_{i+\mathbb{1}_w(x),j+\mathbb{1}_w(y),k+\mathbb{1}_w(z)}^{n+\frac{1}{2}} = \frac{E_w|_{i+\mathbb{1}_w(x),j+\mathbb{1}_w(y),k+\mathbb{1}_w(z)}^n + E_w|_{i+\mathbb{1}_w(x),j+\mathbb{1}_w(y),k+\mathbb{1}_w(z)}^n}{2}$$

where $\mathbb{1}_w(x) = 1$ if $x = w$, and 0 otherwise. If we define $\mathbf{0}_w(\cdot) := 1 - \mathbb{1}_w(\cdot)$, we obtain the corresponding expression for dealing with the $\sigma^* H_w$ term:

$$H_w|_{i+\mathbf{0}_w(x),j+\mathbf{0}_w(y),k+\mathbf{0}_w(z)}^n = \frac{H_w|_{i+\mathbf{0}_w(x),j+\mathbf{0}_w(y),k+\mathbf{0}_w(z)}^{n+\frac{1}{2}} + H_w|_{i+\mathbf{0}_w(x),j+\mathbf{0}_w(y),k+\mathbf{0}_w(z)}^{n-\frac{1}{2}}}{2}$$

With this in mind, we can write out the TE^z mode equations:

$$\begin{aligned} H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} &= \frac{1 - \frac{\sigma^* \Delta_t}{2\mu}}{1 + \frac{\sigma^* \Delta_t}{2\mu}} H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n-\frac{1}{2}} + \\ &+ \frac{\frac{\Delta_t}{\mu}}{1 + \frac{\sigma^* \Delta_t}{2\mu}} \left(\frac{E_x|_{i,j+\frac{1}{2},k+1}^n - E_x|_{i,j+\frac{1}{2},k}^n}{\Delta_y} - \frac{E_y|_{i,j+1,k+\frac{1}{2}}^n - E_y|_{i,j,k+\frac{1}{2}}^n}{\Delta_x} - M_{\text{source},z}|_{i+\frac{1}{2},j+\frac{1}{2},k}^n \right) \end{aligned} \quad (20)$$

$$\begin{aligned} E_x|_{i+\frac{1}{2},j,k}^{n+1} &= \frac{1 - \frac{\sigma \Delta_t}{2\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}} E_x|_{i+\frac{1}{2},j,k}^n + \\ &+ \frac{\frac{\Delta_t}{\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}} \left(\frac{H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - H_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta_y} - \frac{H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i+\frac{1}{2},j,k-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta_z} - J_{\text{source},x}|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} \right) \end{aligned} \quad (21)$$

$$\begin{aligned} E_y|_{i,j+\frac{1}{2},k}^{n+1} &= \frac{1 - \frac{\sigma \Delta_t}{2\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}} E_y|_{i,j+\frac{1}{2},k}^n + \\ &+ \frac{\frac{\Delta_t}{\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}} \left(\frac{H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta_x} - \frac{H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - H_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta_y} - J_{\text{source},y}|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} \right) \end{aligned} \quad (22)$$

Once more, we evaluate all coefficients involving $\sigma, \sigma^*, \varepsilon, \mu$ at the position of the field being updated. With these equations, one can easily and independently compute the update value of either field at a grid vertex, requiring the latest values of both fields. This can be easily parallelized, which is another major reason for the widespread use of FDTD for solving Maxwell's equations.

Finally, we shall mention without proof the necessary condition for stability of the FDTD numerical scheme. The Courant-Friedrichs-Lewy (CFL) condition was introduced in 1928 by Richard Courant, Kurt Friedrichs and Hans Lewy [8]:

$$\Delta_t \leq \frac{1}{c_{\max} \sqrt{\frac{1}{\Delta_x^2} + \frac{1}{\Delta_y^2} + \frac{1}{\Delta_z^2}}}$$

where $c_{\max}$ is the maximum speed of light in the computational domain. For a regular grid, this becomes:

$$S_c := \frac{c_{\max} \Delta_t}{\Delta_x} \leq \frac{1}{\sqrt{3}} =: S_{c,\max}$$

Here S_c is referred to as the *Courant number* (or ratio), and $S_{c,\max}$ is the upper bound imposed by the CFL condition. With this we conclude the description of the basic FDTD building blocks for solving Maxwell's equations: the finite-difference update equations.

The reader is referred to either Taflov and Hagness' textbook on Computational Electrodynamics [43], or Schneider's textbook on the Finite-Difference Time-Domain method [38] for further reading on Yee's algorithm.

3.1.2 Divergence conservation

We have previously alluded to a property of Yee's discretization process without proof, namely the discrete conservation of divergence. We shall now prove that the numerical scheme we have introduced thus far preserves the initial divergence, which is given by the charge density ρ for the electric flux, or zero for the magnetic flux.

Looking at the integral forms, let us integrate (5a) over a Yee cell (Figure [9]) in free space (vacuum, $\varepsilon = \varepsilon_0, \mu = \mu_0$). Let us also specify what assumptions we make about quantities defined on our grid, when investigating them analytically. Any quantity $f|_{i,j,k,n}$ shall be considered piecewise constant on the cube below, and averaged between such cubes.

$$\begin{aligned}
& \left[i - \frac{\Delta_x}{2}, i + \frac{\Delta_x}{2} \right] \times \left[j - \frac{\Delta_x}{2}, j + \frac{\Delta_y}{2} \right] \times \left[k - \frac{\Delta_z}{2}, k + \frac{\Delta_z}{2} \right] \times \left[n - \frac{\Delta_t}{2}, n + \frac{\Delta_t}{2} \right] \\
& \Rightarrow \frac{\partial}{\partial t} \oint\!\!\!\oint_{\text{Yee cell}} \mathbf{B} \cdot d\mathbf{S} = \mu_0 \frac{\partial}{\partial t} \left[\Delta_y \Delta_z \left(H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}} - H_x|_{i+1,j+\frac{1}{2},k+\frac{1}{2}} \right) + \right. \\
& \quad + \Delta_x \Delta_z \left(H_y|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}} \right) + \\
& \quad \left. + \Delta_x \Delta_y \left(H_z|_{i+\frac{1}{2},j+\frac{1}{2},k+1} - H_z|_{i+\frac{1}{2},j+\frac{1}{2},k} \right) \right] \quad (23)
\end{aligned}$$

We shall now replace all time derivatives of H_w terms with the finite differences that are given by Yee's algorithm, and define $t_1 := H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}} - H_x|_{i+1,j+\frac{1}{2},k+\frac{1}{2}}$, $t_2 := H_y|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}$, $t_3 := H_z|_{i+\frac{1}{2},j+\frac{1}{2},k+1} - H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}$.

$$\begin{aligned}
t_1 = & \left(\frac{E_z|_{i+1,j+1,k+\frac{1}{2}} - E_z|_{i+1,j,k+\frac{1}{2}}}{\Delta_y} - \frac{E_y|_{i+1,j+\frac{1}{2},k+1} - E_y|_{i+1,j+\frac{1}{2},k}}{\Delta_z} \right) - \\
& - \left(\frac{E_z|_{i,j+1,k+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}}{\Delta_y} - \frac{E_y|_{i,j+\frac{1}{2},k+1} - E_y|_{i,j+\frac{1}{2},k}}{\Delta_z} \right) \quad (24)
\end{aligned}$$

$$\begin{aligned}
t_2 = & \left(\frac{E_x|_{i+\frac{1}{2},j+1,k+1} - E_x|_{i+\frac{1}{2},j+1,k}}{\Delta_z} - \frac{E_z|_{i+1,j+1,k+\frac{1}{2}} - E_z|_{i,j+1,k+\frac{1}{2}}}{\Delta_x} \right) - \\
& - \left(\frac{E_x|_{i+\frac{1}{2},j,k+1} - E_x|_{i+\frac{1}{2},j,k}}{\Delta_z} - \frac{E_z|_{i+1,j,k+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}}{\Delta_x} \right) \quad (25)
\end{aligned}$$

$$\begin{aligned}
t_3 = & \left(\frac{E_y|_{i+1,j+\frac{1}{2},k+1} - E_y|_{i,j+\frac{1}{2},k+1}}{\Delta_x} - \frac{E_x|_{i+\frac{1}{2},j+1,k+1} - E_x|_{i+\frac{1}{2},j,k+1}}{\Delta_y} \right) - \\
& - \left(\frac{E_y|_{i+1,j+\frac{1}{2},k} - E_y|_{i,j+\frac{1}{2},k}}{\Delta_x} - \frac{E_x|_{i+\frac{1}{2},j+1,k} - E_x|_{i+\frac{1}{2},j,k}}{\Delta_y} \right) \quad (26)
\end{aligned}$$

Summing these three terms yields:

$$\frac{\partial}{\partial t} \oint\!\!\!\oint_{\text{Yee cell}} \mathbf{B} \cdot d\mathbf{S} = 0 \Leftrightarrow \oint\!\!\!\oint_{\text{Yee cell}} \mathbf{B}(t) \cdot d\mathbf{S} = \oint\!\!\!\oint_{\text{Yee cell}} \mathbf{B}(0) \cdot d\mathbf{S} = 0$$

Thus, the magnetic flux preserves its value. The corresponding result for Gauss' Law is straightforward, and the divergence given by the initial electrical charge ρ is preserved.

3.1.3 Integral interpretation of difference equations

One useful property of Yee's scheme is the possibility to interpret and visualize the geometric interaction of the grids in terms of the integral equations. This primarily establishes an intuition linking the two forms of the equations, differential and integral. In Figure [12] we illustrate a combination of field components, placed accordingly in staggered grids.

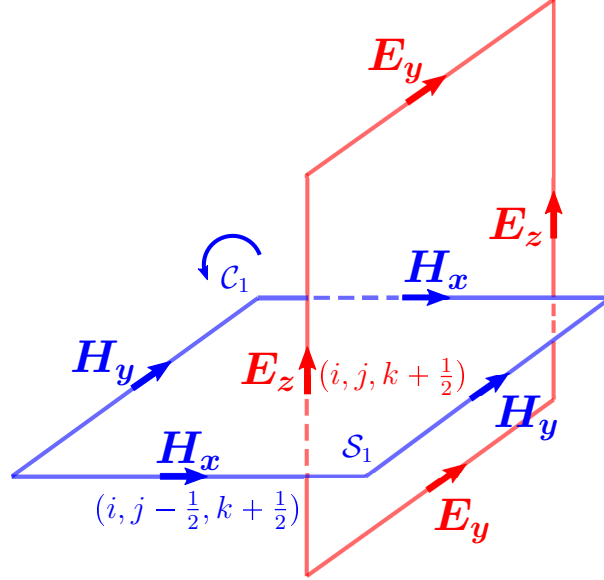


Figure 12: TM^z integral contour within the Yee grid.

We can observe a “ring” of magnetic field components around E_z , and another one formed by electric field components around H_x . Denote the magnetic field contour by $\mathcal{C}_1$.

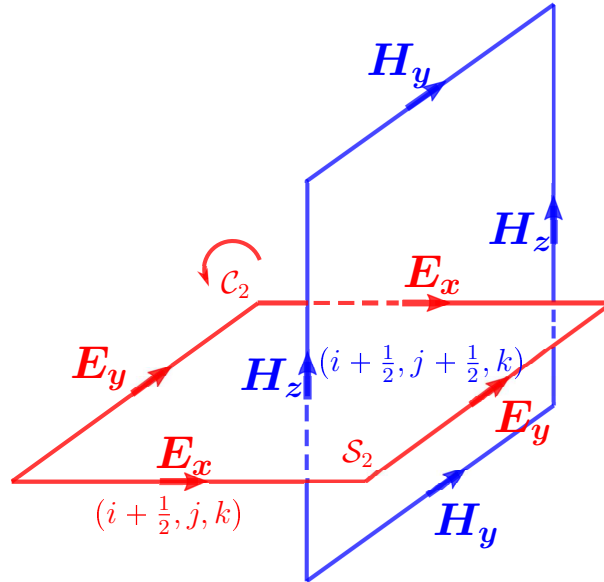


Figure 13: TE^z integral contour inside the Yee grid.

Analogously, we denote by $\mathcal{C}_2$ the electric field integration contour in Figure [13]. One could name $\mathcal{C}_1$ the TM^z integral contour, and $\mathcal{C}_2$ the TE^z integral contour. The (closed) surfaces enclosed by them are denoted as $\mathcal{S}_1$ and $\mathcal{S}_2$ respectively. Let us now highlight the equivalence of the differential and integral forms of the equations on these discrete grids.

Firstly, we need to apply Ampère's Law along the contour $\mathcal{C}_1$. Now, in the Yee grid, we assume that field values are constant within the cube of dimensions $\Delta_x \times \Delta_y \times \Delta_z$ whose midpoint is the position of the field component. With this in mind, we compute

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\mathcal{S}_1} \mathbf{D} \cdot d\mathbf{S} &= \oint_{\mathcal{C}_1} \mathbf{H} \cdot d\mathbf{L} \\ \Leftrightarrow \frac{\partial}{\partial t} \int_{\mathcal{S}_1} \varepsilon_0 E_z|_{i,j,k+\frac{1}{2}} dS &= \Delta_y H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}} + \Delta_x H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}} \\ &\quad - \Delta_y H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}} - \Delta_x H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}} \end{aligned} \quad (27)$$

$$\begin{aligned} \Leftrightarrow \Delta_x \Delta_y \varepsilon_0 \frac{E_z|_{i,j,k+\frac{1}{2}}^{n+1} - E_z|_{i,j,k+\frac{1}{2}}^n}{\Delta_t} &= \Delta_y H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} + \Delta_x H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} \\ &\quad - \Delta_y H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \Delta_x H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} \end{aligned} \quad (28)$$

$$\begin{aligned} \Leftrightarrow E_z|_{i,j,k+\frac{1}{2}}^{n+1} &= E_z|_{i,j,k+\frac{1}{2}}^n + \frac{\Delta_t}{\varepsilon_0 \Delta_x} \left(H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} \right) \\ &\quad + \frac{\Delta_t}{\varepsilon_0 \Delta_y} \left(H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} \right) \end{aligned} \quad (29)$$

which we recognize as the vacuum version of the Yee update equation. The converse result for Faraday's Law and contour $\mathcal{C}_2$ is completely straightforward. With this, we finalize the parallel between the integral formulations and the finite difference grid implementation of the differential formulations.

As we shall see in the next section, this parallel is also particularly helpful for dealing with geometric structures which are finer than the available grid. This entire analysis particularly applies to thin wires, which are often components of electromagnetic antennas. The continuous analysis can be carried out while embedded into the discrete grid, and the result distributed correspondingly to discrete field values.

3.2 Sources and current densities

Let us now discuss ways of introducing energy into our computational domain. This is required in order to have a computational way to replicate the energy introduced into the tissue by a MWA applicator. A first method is to essentially define a Dirichlet boundary condition on one (or several) nodes, which is called a **hard source**. This needs to be provided as a time dependent function. For example, at time step n , the following would be defined at lattice node (i, j, k) :

$$E_z|_{i,j,k}^n = E_0 \sin(2\pi f_0 n \Delta_t) \quad (30)$$

In 3D, this source would produce a spherical wave, such as that of an infinitesimal length dipole, but we shall return to this in more depth in the following subsection.

The sine wave in (30) can be replaced by any time-dependent function, however usually sine or cosine functions are used, or variations of a Gaussian pulse, such as:

$$E_z|_{i,j,k}^n = E_0 \exp\left(-\left(\frac{n - n_0}{n_{\text{decay}}}\right)^2\right) \quad (31)$$

where the n_0 parameter is selected such that $n_0 \geq n_{\text{decay}}$, and a smooth transition from zero is achieved.

A third option is to combine (30) and (31), in order to obtain a Gauss-modulated sine wave, i.e. a wave whose amplitude is given by a Gaussian pulse:

$$E_z|_{i,j,k}^n = E_0 \exp\left(-\left(\frac{n - n_0}{n_{\text{decay}}}\right)^2\right) \sin(2\pi f_0 (n - n_0) \Delta_t)$$

One problem that arises with this type of energy insertion is the following: when a wave encounters a node where such a **hard source** is defined, this node will produce a nonphysical reflection of that wave, due to the tangential component of the electrical field being specified, without any consideration of incident fields. One can show that this happens irrespective of the type of pulse (sinusoidal or Gaussian), and irrespective of whether the value being set as a Dirichlet condition is zero or not.

This can be especially problematic when one wishes to study some harmonic (periodic) behavior, where such nonphysical reflections can permanently pollute the numerical solution. One way to fix this issue would be to simply stop introducing energy through such a source after a given time, essentially “turning it off”. However, this would not work if the desired inserted energy is periodic. What happens in practice is that a harmonic source can only be left active for as long as no waves reach the point of origin.

As opposed to Dirichlet conditions, another method of specifying a source of energy at a grid point is the so-called *soft source*. This involves defining a Dirichlet condition not on any of the six $\mathbf{E}$ or $\mathbf{H}$ components, but on the electric or magnetic currents $\mathbf{J}$ and $\mathbf{M}$.

$$\text{Harmonic example: } J_z|_{i,j,k}^n = J_0 \sin(2\pi f_0 n \Delta_t)$$

One important advantage of the soft source over the hard source is that it allows incident waves to pass through undistorted and unreflected. To observe this, one needs only to

look at the update equations involving the currents, where their influence can be seen to be purely additive, and splittable from the usual update formulas.

3.2.1 Current and current densities

Let us now have a closer look at current sources. A quick check of the equations shows us that $\mathbf{J}$ and $\mathbf{M}$ are indeed *volume current densities*, with units:

$$[\mathbf{J}]_{\text{SI}} = \frac{A}{m^2}, \quad [\mathbf{M}]_{\text{SI}} = \frac{V}{m^2}$$

One way to visualize this is the following: imagine a cylinder with infinitesimal cross sectional area $da_{\perp}$ which runs parallel to the flow of current, as in Figure [14].

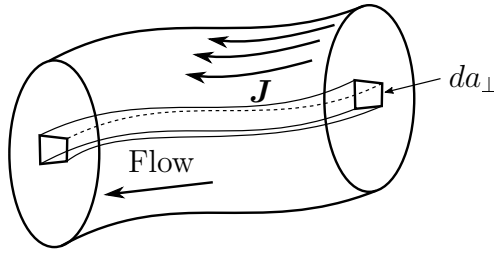


Figure 14: Volume current flowing through a “tube”

It then follows that the total current I_{tube} through this tube (with units $[I_{\text{tube}}]_{\text{SI}} = A$) is:

$$I_{\text{tube}} = \int_{\text{tube}} \mathbf{J} \cdot d\mathbf{V}$$

One other way to introduce current is through a *surface current density*, $\mathbf{J}_s$ (sometimes also denoted by $\mathbf{K}$), with units $\frac{A}{m}$. Here one considers a surface of infinitesimal width $dl_{\perp}$, which is parallel to the flow of current, as illustrated in Figure [15].

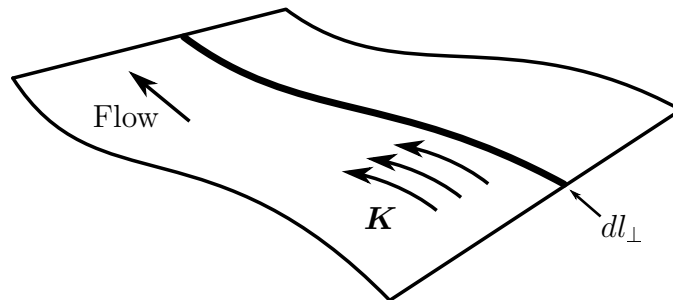


Figure 15: Surface current flowing through a surface

In this case we can define the total current through the surface I_{surface} (with units $[I_{\text{surface}}]_{\text{SI}} = A$):

$$I_{\text{surface}} = \int_{\text{surface}} \mathbf{J}_s \cdot d\mathbf{S}$$

Finally, one can define in an analogous manner a *line current density*, with units $[\mathbf{J}_l]_{\text{SI}} = A$, where $I_{\text{line}} = \int_{\text{line}} \mathbf{J}_l \cdot d\mathbf{L}$. With this in mind, let us understand what happens when a soft source is defined in a Yee lattice. If one wants to define a current at a given node (i, j, k) , one assigns time-varying functions to (volume) current density components, such as $\mathbf{J}_z|_{i,j,k}^n = f(n\Delta_t)$ or $\mathbf{M}_z|_{i,j,k}^n = g(n\Delta_t)$.

Let us approach this from the point of view of current, and not current density. If one wants to impose a given current I_z at the node mentioned previously, then the lattice (grid) current density would have to be defined as:

$$J_z|_{i,j,k} = \frac{I_z|_{i,j,k}}{\Delta_x \Delta_y}$$

where Δ_x, Δ_y are the lattice x - and y -direction steps. This fact shall prove to be useful later on, when we shall provide a discrete formulation of the Field Equivalence Principle.

3.2.2 The Hertzian dipole and currents

We now introduce a theoretical construct derived from the classical dipole antenna. The Hertzian dipole consists of an idealized infinitesimal-width cylinder, thus approximated by a wire or line segment, carrying a constant current I along its entire length. This is realized by considering two charges, $+q$ and $-q$, placed at a distance δl apart, as illustrated in Figure [16].

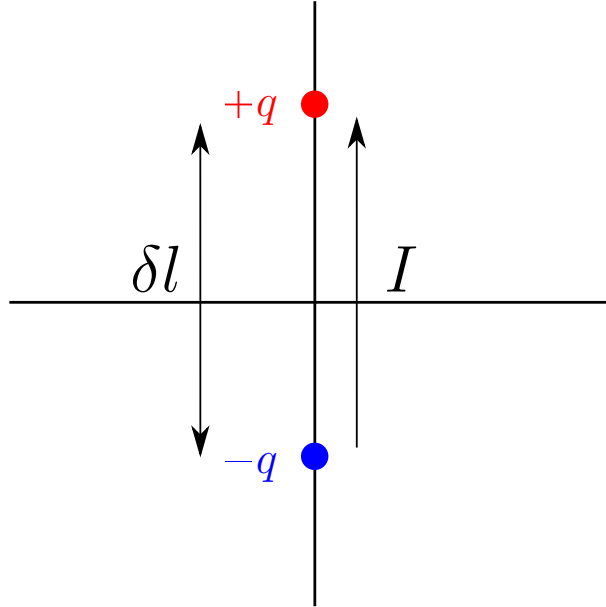


Figure 16: Ideal (point) dipole.

This pair of charges constitutes an *electric dipole*. For such a dipole, we introduce the notion of *dipole moment* $\mathbf{p}$:

$$\mathbf{p} := \text{charge} \cdot \text{displacement vector} \quad (= 2q\delta l \text{ in our case})$$

One should note the vector quantities, since orientation obviously plays a role. It is important to remark that in our case, when the distance $\delta l \rightarrow 0$, which constitutes this

idealized, or point dipole, the charges $q \rightarrow \infty$. This has to happen in such a way that $\exists \lim_{\delta l \rightarrow \infty} p$, and the norms of the charges are scaled in such a way that maintains the dipole moment constant, irrespective of the distance between the charges. This is essentially an improper integral, where the domain of integration has infinitesimal size.

This (finite) dipole moment is the crucial quantity that one should refer to when discussing infinitesimal dipoles. One way to relate this to the current densities we have been working with is the following: suppose we have a (compact) volume $\mathcal{V}$ containing the two charges defining the dipole moment $\mathbf{p}$, then the following holds:

$$\int_{\mathcal{V}} \mathbf{J} dV = \frac{d\mathbf{p}}{dt}$$

Now, the main reason we introduced this infinitesimal dipole, is due to the fact that the field radiated by such a “point charge” in vacuum, or free space, is known analytically. Most textbooks formulate this field in terms of a harmonic situation, where all fields vary according to $\exp(i\omega t)$. However, in the most general case, for a given dipole moment

$$\mathbf{p}(r, t) := \mathbf{p} \left(t - \frac{r}{c} \right)$$

the $\mathbf{E}$ and $\mathbf{H}$ fields radiated by a point dipole are [6]:

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \left(-\frac{\ddot{\mathbf{p}}}{c^2 r} - \frac{\dot{\mathbf{p}}}{cr^2} + \frac{3(\dot{\mathbf{p}} \cdot \mathbf{r}) \cdot \mathbf{r}}{cr^4} + \frac{(\ddot{\mathbf{p}} \cdot \mathbf{r}) \cdot \mathbf{r}}{c^2 r^3} + \frac{3(\mathbf{p} \cdot \mathbf{r}) \cdot \mathbf{r}}{r^5} - \frac{\mathbf{p}}{r^3} \right) \quad (32)$$

$$\mathbf{H}(\mathbf{r}) = \frac{1}{4\pi} \left(\frac{\ddot{\mathbf{p}} \times \mathbf{r}}{cr^2} + \frac{\dot{\mathbf{p}} \times \mathbf{r}}{r^3} \right) \quad (33)$$

where $\mathbf{r}$ is the position where the fields are evaluated, c is the speed of light in vacuum, and $\ddot{\mathbf{p}}, \dot{\mathbf{p}}$ are the second and first-order derivatives of the dipole moment with respect to time. We suppressed the time dependence of the fields and dipole moment for ease of notation. Regions of the domain, and thus regions of the fields, are sometimes referred to depending on their distance from the antenna. These are labeled as near field, intermediate field, and far field. Depending on this distance from the antenna, applications quite often ignore several of the terms from the formula above, if they are not the most influential.

Given this information, one would ask the natural question: can we use these analytical fields to check how accurate the FDTD simulation is? In order to answer this, we need to first analyze the following two questions:

1. Given an analytical point dipole of moment $\mathbf{p}$, what hard point source E_z do we need to impose in order to obtain the equivalent numerical electromagnetic field?
2. Assume we find such an equivalent hard source, what would we need to impose on a pointwise value of the volume current density in order to replicate it? In other words, how do we build an equivalent soft source?

Let us first note that in essence, if we wish to replicate the field produced by a point dipole, and assume the length of such a dipole is δl , then for a constant line current

$$\text{density } I_l, \text{ we have a total current } I = \int_{-\delta l/2}^{+\delta l/2} I_l dL = \delta l I_l.$$

Let us start with question (2), and work our way back to answering (1) as well. What we have to do now is basically a sub-cell resolution analysis of point sources in the Yee grid. When one evaluates a current density J_z at a grid point, the question is, what do we assume about the values between neighboring current nodes?

The natural supposition is that we have piecewise constant values, given by the discrete grid nodes. If that is the case, then in order to achieve an accurate conservation of quantities, we need a pointwise node evaluation of a field to be assumed constant throughout the entire Yee cell. For example, if we have a given (source) current impressed at a point of the grid:

$$I_z|_{i,j,k}^{n\Delta_t} = I_{\text{source}}(n\Delta_t)$$

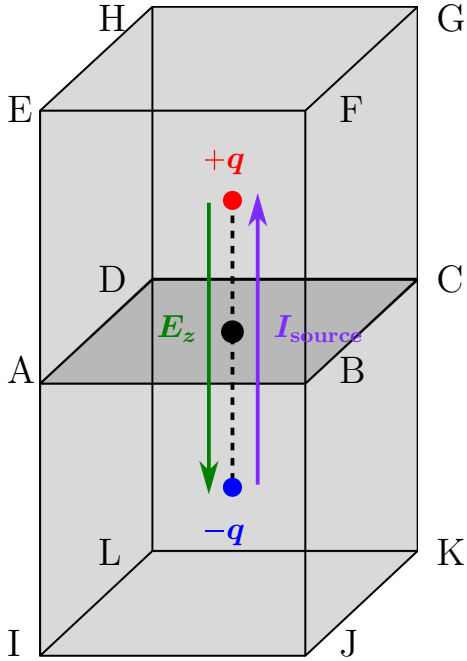
then the J_z term in the update equations will become:

$$J_z|_{i,j,k} = \frac{I_z|_{i,j,k}^{n\Delta_t}}{\Delta_x \Delta_y} \quad \left(\text{with units } \frac{A}{m^2} \right)$$

We can now see that for a given Yee cell of volume $\Delta_x \Delta_y \Delta_z$, if we integrate both quantities, we obtain $I_{\text{source}} \Delta_z$. This gives us a dipole defined by the dipole moment:

$$\mathbf{p}_{\text{discrete}} := \int \left(\int_{\text{Yee cell}} \mathbf{J} \cdot d\mathbf{V} \right) dt = \int I_{\text{source}}(t) \Delta_z dt = \Delta_z \int I_{\text{source}}(t) dt$$

By computing the so-called *discrete lattice capacitance*, and assuming an even grid spacing $\Delta_x = \Delta_y = \Delta_z = \Delta_h$, one can derive a relationship between an imposed Dirichlet hard source $E_{\text{source}}(t)$ and a soft current source given by $I_{\text{source}}(t)$, at a lattice point (i, j, k) . This fact has been investigated by Bérenger [11], and goes as follows:



Let $+q$ and $-q$ be two charges centered in the cubes from Figure [17]. Let there be an E_z node in the center between the two lattice cells, and an I_{source} defined at the same position.

If we now apply Ampère's Law (in integral form) to the total volume of the two cells, we see that E_z has to be of the form:

$$E_z(t) = -\frac{c}{\varepsilon_0 \Delta_x \Delta_y} \int_{-\infty}^t I_s(\tau) d\tau$$

where c is some unknown constant that we need to determine. To simplify the computations, we assume a uniform spatial discretization ($\Delta_x = \Delta_y = \Delta_z = \Delta_h$).

Figure 17: I_{source} and E_z placement.

Let us now take a step back. We want to relate the electrical field on the faces of the lattice cells to the enclosed charges. Let us start with the definition of capacitance:

$$C = \frac{q}{V}$$

where q is the enclosed charge, and V the voltage between the charges. We now state the continuity equation below for convenience:

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t}$$

where ρ is the charge density (with units $[\rho]_{SI} = \frac{C}{m^3}$). If we consider a filamentary (1D curve) current source, and apply the continuity equation, then electric charge will be deposited at the endpoints of this filament.

Let Ω be a volume that encloses an endpoint of this filament, and thus contains the deposited charge. Let $\partial\Omega$ be its bounding surface, and q_{enclosed} the deposited charge at this endpoint, enclosed in Ω . Then we have:

$$-\int_{-\infty}^t \left(\oiint_{\partial\Omega} \mathbf{J}(\mathbf{r}, \tau) \cdot d\mathbf{S} \right) d\tau = \int_{-\infty}^t I(\tau) d\tau = q_{\text{enclosed}}(t)$$

Here $I(t)$ is the total current that enters the volume Ω . Now, if we apply Gauss' Law in integral form to a Yee lattice cell, denoted by Λ , containing a charge q_{enclosed} , we obtain:

$$\begin{aligned} q_{\text{enclosed}} &= \iiint_{\Lambda} \rho dV = \varepsilon_0 \oiint_{\partial\Lambda} \mathbf{E} \cdot d\mathbf{S} = \varepsilon_0 \sum_{i=1}^6 \oiint_{\text{face}_i(\Lambda)} \mathbf{E} \cdot d\mathbf{S} = \varepsilon_0 \sum_{i=1}^6 \Delta_h^2 \frac{1}{\Delta_h^2} \oiint_{\text{face}_i(\Lambda)} \mathbf{E} \cdot d\mathbf{S} = \\ &= 6\varepsilon_0 \Delta_h^2 \oiint_{\text{face}_i(\Lambda)} \mathbf{E} \cdot d\mathbf{S} = 6\varepsilon_0 \Delta_h^2 \left\| \oiint_{\text{face}_i(\Lambda)} \mathbf{E} \cdot d\mathbf{S} \right\| = 6\varepsilon_0 \Delta_h^2 E_{\text{face}} \end{aligned}$$

which we can summarize into:

$$q_{\text{enclosed}} = 6\varepsilon_0 \Delta_h^2 E_{\text{face}} \quad (34)$$

Here we have defined E_{face} as the (vector l^2 -) norm of the average integral of the electric field over one cell face:

$$E_{\text{face}} := \frac{1}{\Delta_h^2} \left\| \oiint_{\text{face}_i(\Lambda)} \mathbf{E} \cdot d\mathbf{S} \right\|$$

which is the same for all six faces, due to symmetry of the situation (charge at the center of the lattice cell). Let us see what the voltage would be in the semi-discrete case. If we have two charges of equal magnitude and opposite sign in adjacent Yee cells, the difference in potential between them is (p. 189 [43]):

$$V = 2\Delta_h E_{\text{face}} \quad (35)$$

If we now combine (35) and (34), and plug them into the definition of capacitance, we obtain our discrete grid capacitance:

$$C_{\text{discrete}} = 3\varepsilon_0\Delta_h$$

Now, if we observe Figure [17], and assume the two charges are placed on either side of an electric field component $E_z(i, j, k)$, we have:

$$E_z(i, j, k, t) = -2E_{\text{face}} = -\frac{q(t)}{3\varepsilon_0\Delta_h^2}$$

However, we know that charge is given by the integral of the current in this dipole:

$$E_z(i, j, k, t) = -\frac{1}{3\varepsilon_0\Delta_h^2} \int_{-\infty}^t I_s(\tau) d\tau$$

so we have found our constant $c = \frac{1}{3}$ from earlier. Note that this final result matches the intuition of how E_z and I_s contribute to the update equations: the electrical field is fixed at every step, and I_s is added to the electric field value at each time step, so one expects E_z to be some sort of integral of I_s .

At this moment we have a workflow to evaluate equivalent hard and soft sources: given a (z -directed) hard source at a point (i, j, k) , defined by:

$$E_z(i, j, k, t) = f(t)$$

we can find the equivalent current and current density sources as follows:

$$I_s(t) = -3\varepsilon_0\Delta_h^2 \frac{d}{dt} E_z(t) \quad \Leftrightarrow \quad J_z(t) = -3\varepsilon_0 \frac{d}{dt} E_z(t)$$

This concludes our analysis of equivalent hard and soft sources, and provides the basis to compare the behavior of these three quantities of interest: electromagnetic field produced by a *hard source*, by a *soft source*, and the analytical result in vacuum. This shall be used later on for numerical accuracy validation.

3.3 Total-field/Scattered-field technique

The so-called *total-field/scattered-field* technique, hereon abbreviated TFSF, was created as a result of a recurring application necessity: the ability to introduce a plane wave into an FDTD simulation. This technique can be interpreted as a discrete version of the Field Equivalence Principle, as we shall highlight later on. Furthermore, this technique allows significant flexibility when defining sources of energy, which is clearly helpful for our goal application.

This introduction of TFSF was motivated by the desire to study the interaction of various plane waves with complex structures. The trivial approach to obtain such an interaction is to place objects, or scatterers, far away from the electromagnetic sources, such that the wavefronts are quasi-planar by the time they reach them. However, this procedure has the obvious drawback of requiring an overly large computational domain.

Furthermore, to cite Taflove [43], several desirable properties were difficult to obtain:

1. The ability to specify an arbitrary direction, polarization, and duration.
2. A perfectly planar wavefront, that is perpendicular to the direction of propagation.
3. A constant amplitude across any plane perpendicular to the direction of propagation.

Yee [46] had some rudimentary implementation of such a plane wave source in his seminal paper, involving setting Dirichlet conditions on all nodes in the lattice. However, this method still required significantly large computational domains, and suffered from distortions when interacting with the boundary of the domain. As a result, it has seen very limited use since.

The breakthrough in defining plane wave sources, which is regularly used to this day, was brought by the TFSF method, initially formulated in 1980 by Merewether, Fisher and Smith [27], and then in 1982 by Umashankar and Taflove [44]. The TFSF method conclusively achieved the goal of introducing long duration and harmonic plane wave sources.

TFSF Idea

The main ingredient required in formulating the TFSF method is the linearity of Maxwell's equations. The crucial idea is to split up both $\mathbf{E}$ and $\mathbf{H}$ into two parts, the *incident* and *scattered* fields:

$$\mathbf{E}_{\text{total}} = \mathbf{E}_{\text{incident}} + \mathbf{E}_{\text{scattered}}$$

$$\mathbf{H}_{\text{total}} = \mathbf{H}_{\text{incident}} + \mathbf{H}_{\text{scattered}}$$

The incident fields are those given by the desired incident plane wave, and are assumed to be known apriori, everywhere in the computational grid. The scattered field is the unknown field which results from the interaction of the incident field with the physical structures of interest inside the lattice.

It is important to remark that these two split components can be updated independently with the usual FDTD equations. Let us now interpret this splitting visually. In Figure [18] we introduce the illustration of this scattering idea.

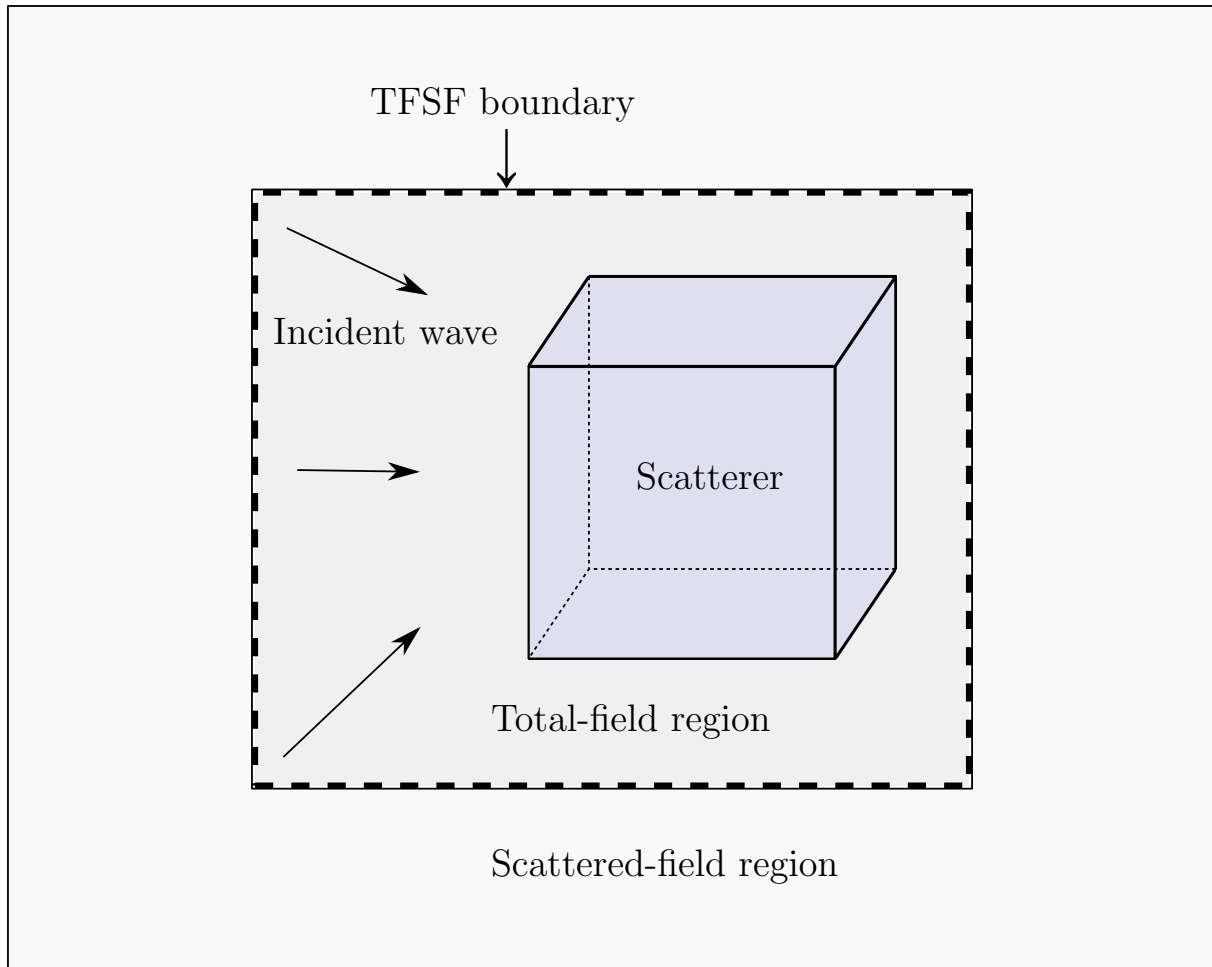


Figure 18: Total-field scattered-field sample use case.

Our region of interest is split into two parts (volumes): the total-field (TF) region, and the scattered-field (SF) region. The boundary surface between the two regions is non-physical, and should ideally be positioned such that there are no electromagnetic field nodes exactly on the surface. If the TFSF boundary intersects grid nodes, one is faced with an ambiguity when deciding which region they belong to.

The plane wave is produced on this TFSF boundary, it then proceeds to interact with the scatterer, and then finally disappears from the domain. However, the scattered wave resulting from this interaction remains in the grid.

One can now already identify the analogy to the FEP technique presented earlier. This TFSF boundary is the correspondent of the boundary delimiting Ω in that case. Specifying the incident plane wave (through TFSF) inside the total-field region is equivalent to specifying the fields $\mathbf{E}, \mathbf{H}$ inside Ω . Discretely, we perform the FDTD updates on the total field inside the total-field region, and separately on the scattered field inside the scattered-field region. Let us now analyze a 1D example of this technique, in order to understand how it is carried out in practice.

1D TFSF

In Figure [19] we introduce a one-dimensional FDTD grid.

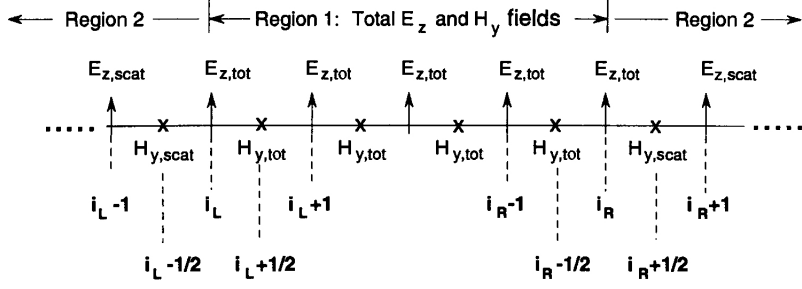


Figure 19: 1D FDTD grid, taken from [43], p. 195.

If we are working in vacuum, we use the following update equation:

$$E_z|_i^{n+1} = E_z|_i^n + \frac{\Delta t}{\varepsilon_0 \Delta x} \left(H_y|_{i+1/2}^{n+1/2} - H_y|_{i-1/2}^{n+1/2} \right)$$

This equation is valid if all three field values are contained in the same region (TF or SF). If we now apply this update at grid point i_L on the left side, we obtain

$$E_{z,\text{total}}|_{i_L}^{n+1} = E_{z,\text{total}}|_{i_L}^n + \frac{\Delta t}{\varepsilon_0 \Delta x} \left(H_{y,\text{total}}|_{i_L+1/2}^{n+1/2} - H_{y,\text{scattered}}|_{i_L-1/2}^{n+1/2} \right)$$

which is inconsistent and false. In order to correct this inconsistency, we need to subtract an additional $H_{y,\text{incident}}$ term from the right-hand side, as follows:

$$-H_{y,\text{total}} = -H_{y,\text{scattered}} - H_{y,\text{incident}} \Rightarrow$$

$$E_{z,\text{total}}|_{i_L}^{n+1} = E_{z,\text{total}}|_{i_L}^n + \frac{\Delta t}{\varepsilon_0 \Delta x} \left(H_{y,\text{total}}|_{i_L+1/2}^{n+1/2} - H_{y,\text{scattered}}|_{i_L-1/2}^{n+1/2} \right) - \frac{\Delta t}{\varepsilon_0 \Delta x} H_{y,\text{incident}}|_{i_L-1/2}^{n+1/2}$$

Now, let us turn to the update equation for the magnetic field, at node $i_L - 1$, where we will need to perform a similar correction. The usual FDTD update would be:

$$H_{y,\text{scattered}}|_{i_L-1}^{n+1/2} = H_{y,\text{scattered}}|_{i_L-1}^{n-1/2} + \frac{\Delta t}{\mu_0 \Delta x} \left(E_{z,\text{total}}|_{i_L}^n - E_{z,\text{scattered}}|_{i_L-1}^n \right)$$

And the corrected version of the equation is

$$H_{y,\text{scattered}}|_{i_L-1}^{n+1/2} = H_{y,\text{scattered}}|_{i_L-1}^{n-1/2} + \frac{\Delta t}{\mu_0 \Delta x} \left(E_{z,\text{total}}|_{i_L}^n - E_{z,\text{scattered}}|_{i_L-1}^n \right) - \frac{\Delta t}{\mu_0 \Delta x} E_{z,\text{incident}}|_{i_L}^n$$

This two step correction procedure would have to be performed at the other end of the TFSF interface (i_R) as well, with a change in sign due to the different direction. Let $[\cdot]_{\text{usual}}$ denote the unmodified FDTD update expression of the given argument. We can then write the corrected equations as follows:

$$E_z|_{i_R}^{n+1} = [E_z|_{i_R}^{n+1}]_{\text{usual}} + \frac{\Delta t}{\varepsilon_0 \Delta x} H_{y,\text{incident}}|_{i_R+1/2}^{n+1/2} \quad (36)$$

$$H_y|_{i_R+1/2}^{n+1/2} = [H_y|_{i_R+1/2}^{n+1/2}]_{\text{usual}} + \frac{\Delta t}{\mu_0 \Delta x} E_{z,\text{incident}}|_{i_R}^n \quad (37)$$

The results of a 1D simulation employing the corrections (36) and (37) can be seen in Figure [20]. In the second half, a so-called *perfect electric conductor* (PEC) is realized in the center node of the total-field region, by setting a Dirichlet condition of $E_z = 0$ at that position. This Dirichlet condition behaves as a mirror for the incident wave.

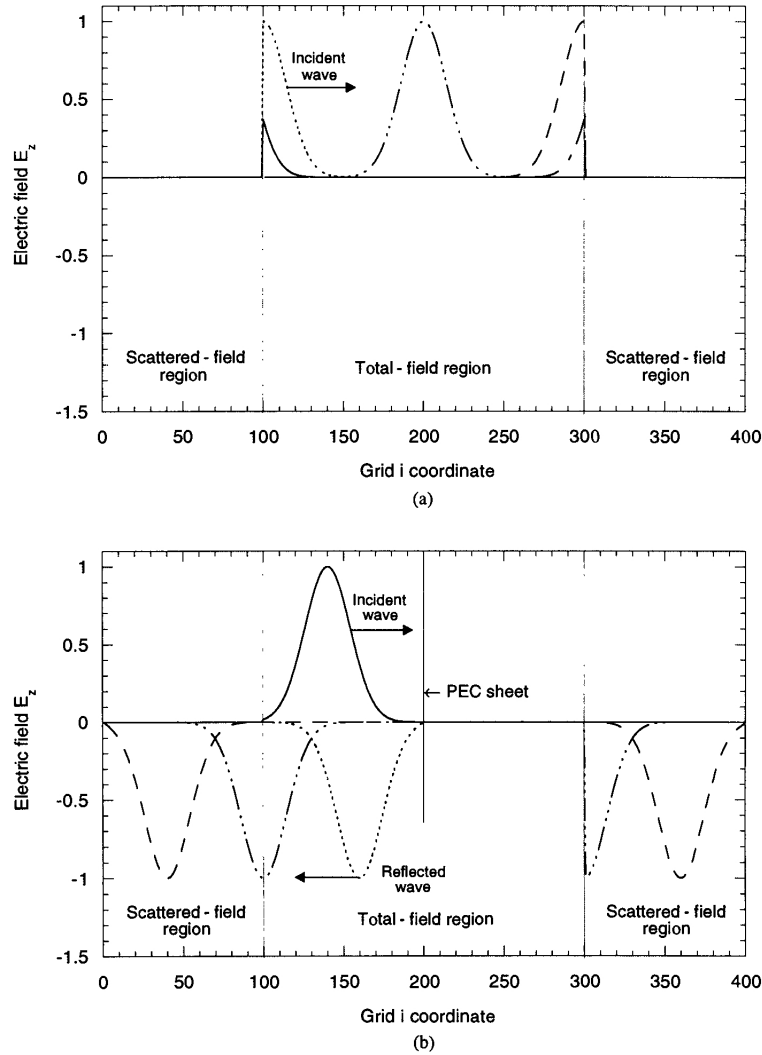


Figure 20: One-dimensional Yee grid TFSF implementation. Taken from [43], p. 202.

(a): vacuum parameters in the entire grid.

(b): PEC “mirror” placed in the center of the total-field region.

Seeing as this equation correction can be performed as a “post-processing” step, we can implement the regular FDTD update uniformly in the entire domain, and then correct it for the necessary nodes. Let us now see how this TFSF update process is applied in 2D. The transition to 3D will then be very natural.

In Figure [21], Ω_1 represents the total-field zone, and Ω_2 the scattered-field zone. We employ a TM^z mode here, i.e. only E_z , H_x and H_y nodes are present. The dotted line denotes the virtual TFSF boundary between the two zones. The right-oriented arrows are H_x nodes, the upward ones H_y nodes, and the points are E_z nodes.

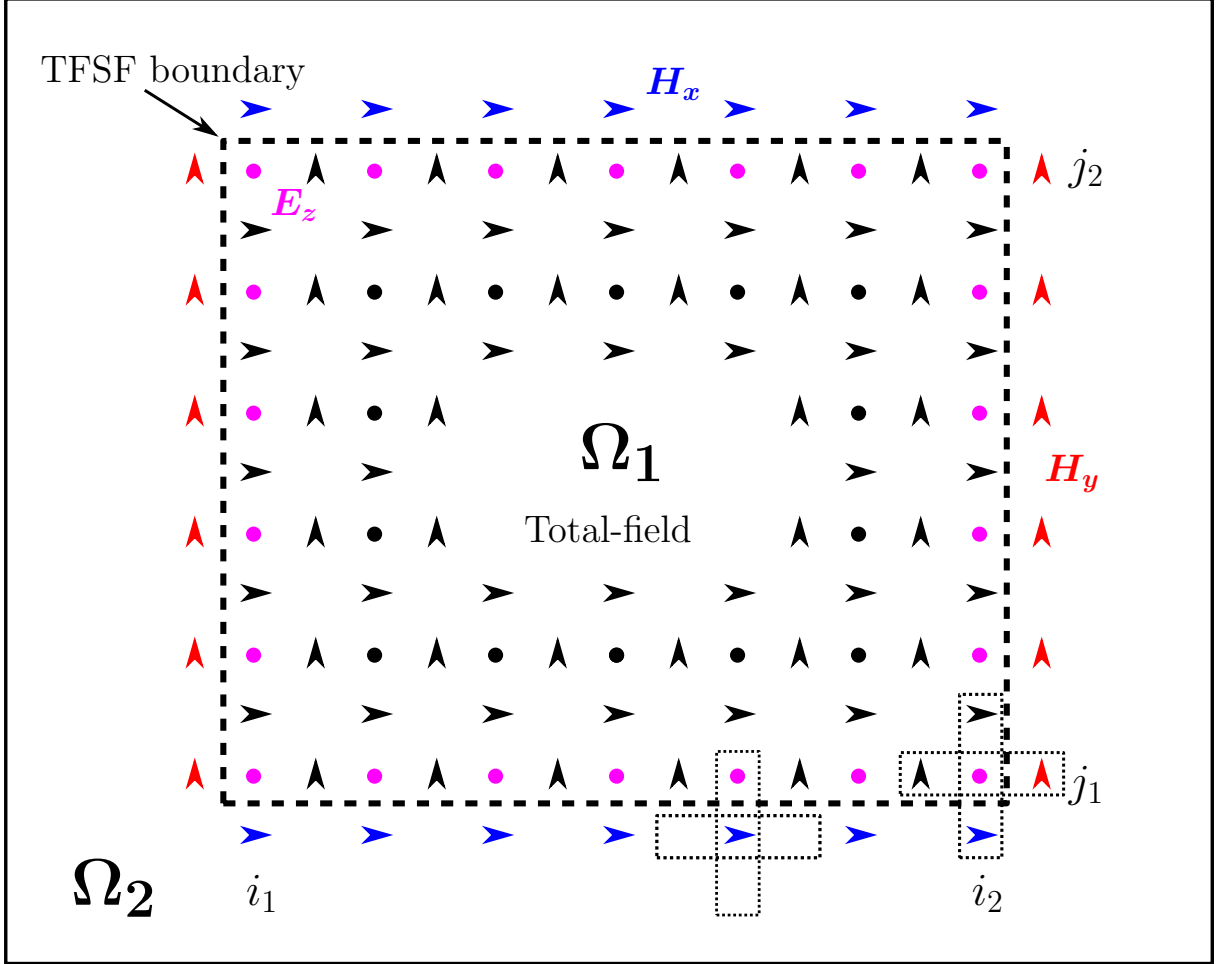


Figure 21: Two-dimensional TFSF geometry.

The blue H_x , red H_y and purple E_z nodes are those that require a consistency correction, such that their FDTD update is correct. While determining which nodes require this correction becomes more and more tedious, especially as is the case for 3D, there is a simple heuristic we can highlight that simplifies this process.

Let us observe the lower right side of the TFSF boundary in Figure [21]. In order to determine whether we need to make such a consistency correction, we iterate over all nodes of all fields. We then check the FDTD stencil (denoted here by the dotted rectangles) used to update that node. If it contains any (spatial) nodes that are not part of the same region (TF or SF) as the updated node, then they are flagged for correction.

For example, the stencil of the lower right E_z node contains the rightward H_y node, and the lower H_x node in another region. Let us see what the update equations look like. We shall assume that the leftmost E_z nodes are located at x -coordinate i_1 , and the rightmost at i_2 . Similarly, the bottom ones are located at y -coordinate j_1 , and the top ones at j_2 . It then follows that the red H_y nodes on the left are positioned at the $i_1 - 1/2$ x -coordinate, and the bottom blue H_x nodes at y -coordinate $j_1 - 1/2$.

On the left side of the TFSF interface ($i_1, j \in \{j_1, \dots, j_2\}$) we have the following correction:

$$E_z|_{i_1,j}^{n+1} = [E_z|_{i_1,j}^{n+1}]_{\text{usual}} - \frac{\Delta t}{\varepsilon_0 \Delta_x} H_{y,\text{incident}}|_{i_1-1/2,j}^{n+1/2}$$

Due to the change in direction, on the right side ($i_2, j \in \{j_1, \dots, j_2\}$) the correction is:

$$E_z|_{i_2,j}^{n+1} = [E_z|_{i_2,j}^{n+1}]_{\text{usual}} + \frac{\Delta t}{\varepsilon_0 \Delta_x} H_{y,\text{incident}}|_{i_2+1/2,j}^{n+1/2}$$

Similarly, for the bottom side ($j_1, i \in \{i_1, \dots, i_2\}$) we obtain:

$$E_z|_{i,j_1}^{n+1} = [E_z|_{i,j_1}^{n+1}]_{\text{usual}} + \frac{\Delta t}{\varepsilon_0 \Delta_y} H_{x,\text{incident}}|_{i,j_1-1/2}^{n+1/2}$$

And finally the top side ($j_2, i \in \{i_1, \dots, i_2\}$) corrections are the following:

$$E_z|_{i,j_2}^{n+1} = [E_z|_{i,j_2}^{n+1}]_{\text{usual}} - \frac{\Delta t}{\varepsilon_0 \Delta_y} H_{x,\text{incident}}|_{i,j_2+1/2}^{n+1/2}$$

This concludes the consistency corrections for E_z . For H_x we have the following:

$$(j_1 - 1/2, i \in \{i_1, \dots, i_2\}) : H_x|_{i,j_1-1/2}^{n+1} = [H_x|_{i,j_1-1/2}^{n+1}]_{\text{usual}} + \frac{\Delta t}{\varepsilon_0 \Delta_y} E_{z,\text{incident}}|_{i,(j_1-1/2)+1/2}^{n+1/2}$$

$$(j_2 + 1/2, i \in \{i_1, \dots, i_2\}) : H_x|_{i,j_2+1/2}^{n+1} = [H_x|_{i,j_2+1/2}^{n+1}]_{\text{usual}} - \frac{\Delta t}{\varepsilon_0 \Delta_y} E_{z,\text{incident}}|_{i,(j_2+1/2)-1/2}^{n+1/2}$$

Similarly, we correct H_y according to:

$$(i_1 - 1/2, j \in \{j_1, \dots, j_2\}) : H_y|_{i_1-1/2,j}^{n+1} = [H_y|_{i_1-1/2,j}^{n+1}]_{\text{usual}} - \frac{\Delta t}{\varepsilon_0 \Delta_x} E_{z,\text{incident}}|_{(i_1-1/2)+1/2,j}^{n+1/2}$$

$$(i_2 + 1/2, j \in \{j_1, \dots, j_2\}) : H_y|_{i_2+1/2,j}^{n+1} = [H_y|_{i_2+1/2,j}^{n+1}]_{\text{usual}} + \frac{\Delta t}{\varepsilon_0 \Delta_x} E_{z,\text{incident}}|_{(i_2+1/2)-1/2,j}^{n+1/2}$$

While it can be tedious to follow the signs dictating the corrections, we can observe a pattern that relates this further to the FEP. Let $\mathbf{n} = (n_x, n_y)$ be the outer normal defined on the TFSF boundary, pointing from Ω_1 into Ω_2 (from TF into SF). We then have on x -aligned boundaries, where $\mathbf{n} = (0, n_y)$, the following updates for E_z total field nodes:

$$E_z|_{i,j}^{n+1} = [E_z|_{i,j}^{n+1}]_{\text{usual}} - n_y \frac{\Delta t}{\varepsilon_0 \Delta_y} H_{x,\text{incident}}|_{i,j+n_y/2}^{n+1/2}$$

For y -aligned boundaries ($\mathbf{n} = (n_x, 0)$), we have for TF E_z nodes:

$$E_z|_{i,j}^{n+1} = [E_z|_{i,j}^{n+1}]_{\text{usual}} + n_x \frac{\Delta t}{\varepsilon_0 \Delta_x} H_{y,\text{incident}}|_{i+n_x/2,j}^{n+1/2}$$

If we now abuse the notation of the $\mathbf{H}$ field slightly, we see that the following holds:

$$E_z|_{i,j}^{n+1} = [E_z|_{i,j}^{n+1}]_{\text{usual}} + \frac{\Delta t}{\varepsilon_0 \Delta_x} \mathbf{n} \times \mathbf{H}_{\text{incident}}|_{i,j}^{n+1/2}$$

Defining $J_z := \mathbf{n} \times \frac{\mathbf{H}_{\text{incident}}}{\Delta_h} \Big|_z$, and assuming a uniform spatial discretization, we obtain:

$$E_z|_{i,j}^{n+1} = [E_z|_{i,j}^{n+1}]_{\text{usual}} + \frac{\Delta_t}{\varepsilon_0} J_z|_{i,j}^{n+1/2}$$

Hence, we have rephrased the TFSF correction as an equation involving a volume current density, defined just as in the FEP, where the surface current density is given by $J_{z,\text{surface}} := \mathbf{n} \times \mathbf{H}_{\text{incident}} \Big|_z$.

Let us now investigate the scattered-field H field nodes:

$$x\text{-aligned boundaries : } H_x|_{i,j+n_y/2}^{n+1} = [H_x|_{i,j+n_y/2}^{n+1}]_{\text{usual}} - n_y \frac{\Delta_t}{\varepsilon_0 \Delta_y} E_{z,\text{incident}}|_{i,j}^{n+1/2}$$

$$y\text{-aligned boundaries : } H_y|_{i+n_x/2,j}^{n+1} = [H_y|_{i+n_x/2,j}^{n+1}]_{\text{usual}} + n_x \frac{\Delta_t}{\varepsilon_0 \Delta_x} E_{z,\text{incident}}|_{i,j}^{n+1/2}$$

Equivalating this to a form involving a cross product and a surface current would be less revealing, due to the missing field components we have in 2D. However, this analogy becomes even more evident for the 3D consistency correction formulas. To that end, and as a straightforward step from 2D, let us state the 3D TFSF correction formulas:

$$E_x|_{i,j,k}^{n+1} = [E_x|_{i,j,k}^{n+1}]_{\text{usual}} + n_y \frac{\Delta_t}{\varepsilon_0 \Delta_h} H_{z,\text{incident}}|_{i,j+n_y/2,k}^{n+1/2}$$

$$E_x|_{i,j,k}^{n+1} = [E_x|_{i,j,k}^{n+1}]_{\text{usual}} - n_z \frac{\Delta_t}{\varepsilon_0 \Delta_h} H_{y,\text{incident}}|_{i,j,k+n_z/2}^{n+1/2}$$

If we now add these two equations, and denote by $(\cdot)_x$ the x -component of a vector:

$$E_x|_{i,j,k}^{n+1} = [E_x|_{i,j,k}^{n+1}]_{\text{usual}} + \frac{\Delta_t}{\varepsilon_0 \Delta_h} \left(\mathbf{n} \times \mathbf{H}_{\text{incident}}|_{i,j,k}^{n+1/2} \right)_x$$

In the same fashion we obtain the following:

$$E_y|_{i,j,k}^{n+1} = [E_y|_{i,j,k}^{n+1}]_{\text{usual}} + \frac{\Delta_t}{\varepsilon_0 \Delta_h} \left(\mathbf{n} \times \mathbf{H}_{\text{incident}}|_{i,j,k}^{n+1/2} \right)_y$$

$$E_z|_{i,j,k}^{n+1} = [E_z|_{i,j,k}^{n+1}]_{\text{usual}} + \frac{\Delta_t}{\varepsilon_0 \Delta_h} \left(\mathbf{n} \times \mathbf{H}_{\text{incident}}|_{i,j,k}^{n+1/2} \right)_z$$

$$\Rightarrow \mathbf{E}|_{i,j,k}^{n+1} = [\mathbf{E}|_{i,j,k}^{n+1}]_{\text{usual}} + \frac{\Delta_t}{\varepsilon_0 \Delta_h} \mathbf{n} \times \mathbf{H}_{\text{incident}}|_{i,j,k}^{n+1/2} \quad (38)$$

Following the same steps, one can retrieve the corresponding magnetic field correction:

$$\mathbf{H}|_{i,j,k}^{n+1} = [\mathbf{H}|_{i,j,k}^{n+1}]_{\text{usual}} - \frac{\Delta_t}{\mu_0 \Delta_h} \mathbf{n} \times \mathbf{E}_{\text{incident}}|_{i,j,k}^{n+1/2} \quad (39)$$

In conclusion, we have found exactly the same equation (in discrete form) for the TFSF consistency corrections, as for the surface current corrections in the FEP. The sign discrepancy comes from the flipped convention of the normal vector between the TFSF figure and the FEP one.

Thus, the main difficulty that arises in translating FEP into a discrete form, namely the TFSF technique, lies in defining the boundaries for all six fields properly. A very important note to make is that while for our TFSF example the virtual separating surface had a “nice” rectangular shape, in practice there is no such constraint imposed. The virtual TFSF boundary can be arbitrarily complex, which can lead to issues with sub-voxel accuracy, but also interesting applications (such as replacing antennas).

Finally, we should note that for the Yee grid, it is particularly helpful to define the virtual TFSF boundary at coordinate values that are *not* of the form $\frac{k}{2}, k \in \mathbb{Z}$. This eliminates any ambiguity about which of the two TFSF regions the grid nodes belong to.

3.4 TFSF application: plane wave

Thus far we have described the TFSF technique, and shown how to derive it from the FEP. Let us now highlight some details about how to introduce a plane wave into an FDTD grid. We shall note that essentially, there is nothing restricting us to plane waves in this entire process. Any electromagnetic fields (whose values we know at any point in space and time) can be specified as a source of energy with the TFSF method.

For the following discussion, we shall refer to Figure [21] for guidance. We will now continue our thought process in 2D. Let us consider a rectangular TFSF interface as displayed in Figure [22]. We shall proceed to specify an incident plane wave, whose direction of propagation is given by a (normalized) wave vector $\mathbf{k} = (k_x, k_y)$. The angle between $\mathbf{k}$ and the x -axis is α .

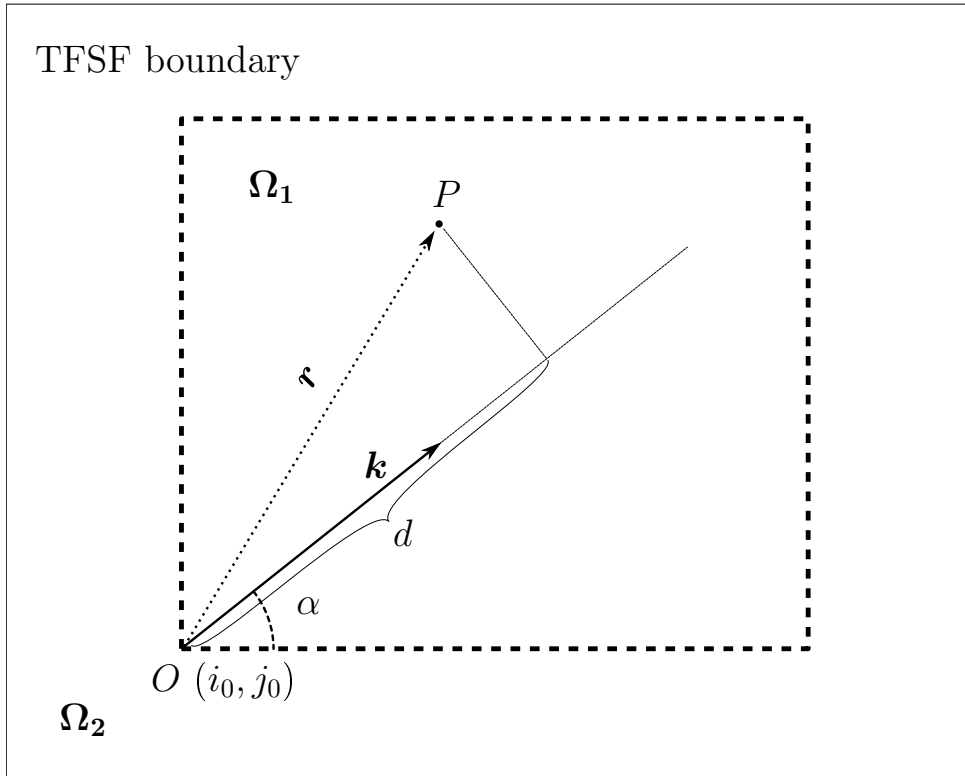


Figure 22: Incident plane wave on TFSF boundary.

Without loss of generality, let us assume that point O at (i_0, j_0) would be the first point of contact of the plane wave with the total field region. Let there be a point in the grid, P , given by the position vector $\mathbf{r}$. The wave reaches this point after n_{offset} time steps:

$$n_{\text{offset}} = \frac{d\Delta_h}{\tilde{v}_p(\alpha)}$$

where d is the distance along the direction of the wave propagation, from O to P , defined by $d := \mathbf{k} \cdot \mathbf{r}$. Furthermore, $\tilde{v}_p(\alpha)$ is the numerical propagation speed of the wave for an angle of α . The way in which $\tilde{v}_p(\alpha)$ differs from the speed of light in vacuum shall be detailed in Section 3.6. The wavevector and position vector can be expressed as follows:

$$\mathbf{k} = \mathbf{n}_x \cos(\alpha) + \mathbf{n}_y \sin(\alpha)$$

$$\mathbf{r} = (i_P - i_0)\mathbf{n}_x + (j_P - j_0)\mathbf{n}_y$$

where $\mathbf{n}_x, \mathbf{n}_y$ are coordinate vectors. The incident E and H fields can be computed analytically everywhere on and around the TFSF boundary. Normally this can be quite numerically intense, however there is an adaption we can employ which is only valid for this plane wave case. We can simulate a 1D wave propagation on an auxiliary grid, and interpolate the results. We shall then need to polarize (distribute) these 1D fields to our 3D fields. This process will then only require us to numerically evaluate the analytical formulas at the 1D grid origin.

Furthermore, as will be detailed in Section 3.6, the numerical wave velocity is smaller than the physical one. This discrepancy also varies in magnitude according to the direction of travel of the wave. Hence, when we perform the FDTD update in 1D, we are required to take this into account through a factor that scales up the speed of propagation:

$$E_{\text{incident}}|_i^{n+1} = E_{\text{incident}}|_i^n + \frac{\Delta t}{\left(\frac{\tilde{v}_p(\alpha=0^\circ)}{\tilde{v}_p(\alpha)}\right) \varepsilon_o \Delta_h} \left(H_{\text{incident}}|_{i-1/2}^{n+1/2} - H_{\text{incident}}|_{i+1/2}^{n+1/2} \right)$$

$$H_{\text{incident}}|_{i+1/2}^{n+1/2} = H_{\text{incident}}|_{i+1/2}^{n-1/2} + \frac{\Delta t}{\left(\frac{\tilde{v}_p(\alpha=0^\circ)}{\tilde{v}_p(\alpha)}\right) \mu_o \Delta_h} \left(E_{\text{incident}}|_i^n - E_{\text{incident}}|_{i+1}^n \right)$$

This update is performed at a position i in the 1D grid. We remark that the first node of the 1D grid, $E_{\text{incident}}|_{i_0}$, has to coincide with the “first” electrical field node in the bottom left of the 2D total-field region.

Let us now see how we can interpolate the 1D values, in order to match them to the 2D grid. If $\lfloor \cdot \rfloor$ is the floor function ($\lfloor x \rfloor := \max\{m \in \mathbb{Z} | m \leq x\}$), let us define the following:

$$d_{\mathbb{R},E} := d - \lfloor d \rfloor$$

$$d_{\mathbb{R},H} := d + \frac{1}{2} - \left\lfloor d + \frac{1}{2} \right\rfloor$$

$$E_{\text{incident}}|_d^n = (1 - d_{\mathbb{R},E})E_{\text{incident}}|_{i_0 + \lfloor d_{\mathbb{R},E} \rfloor}^n + d_{\mathbb{R},E}E_{\text{incident}}|_{i_0 + \lfloor d_{\mathbb{R},E} \rfloor + 1}^n \quad (40)$$

$$H_{\text{incident}}|_d^{n+1/2} = (1 - d_{\mathbb{R},H})H_{\text{incident}}|_{i_0 - 1/2 + \lfloor d_{\mathbb{R},H} \rfloor}^{n+1/2} + d_{\mathbb{R},H}H_{\text{incident}}|_{i_0 - 1/2 + \lfloor d_{\mathbb{R},H} \rfloor + 1}^{n+1/2} \quad (41)$$

Now that we have interpolated the 1D field values, we can compute the 2D vector fields:

$$E_{z,\text{incident}}|_d^n = E_{\text{incident}}|_d^n$$

$$H_{x,\text{incident}}|_d^{n+1/2} = H_{\text{incident}}|_d^{n+1/2} \sin(\alpha)$$

$$H_{y,\text{incident}}|_d^{n+1/2} = -H_{\text{incident}}|_d^{n+1/2} \cos(\alpha)$$

where E_{incident} and H_{incident} are taken from (40) and (41). This concludes the theoretical preparations for the plane-wave TFSF application. Let us now turn to some visual results.

In Figure [23], a perfect electric conductor (PEC) rectangle is defined in the center (by enforcing all electrical field components to be zero). The incident wave is introduced at the bottom left, leaves the domain after reaching the top right, and the reflection off of the PEC cube remains in the domain.

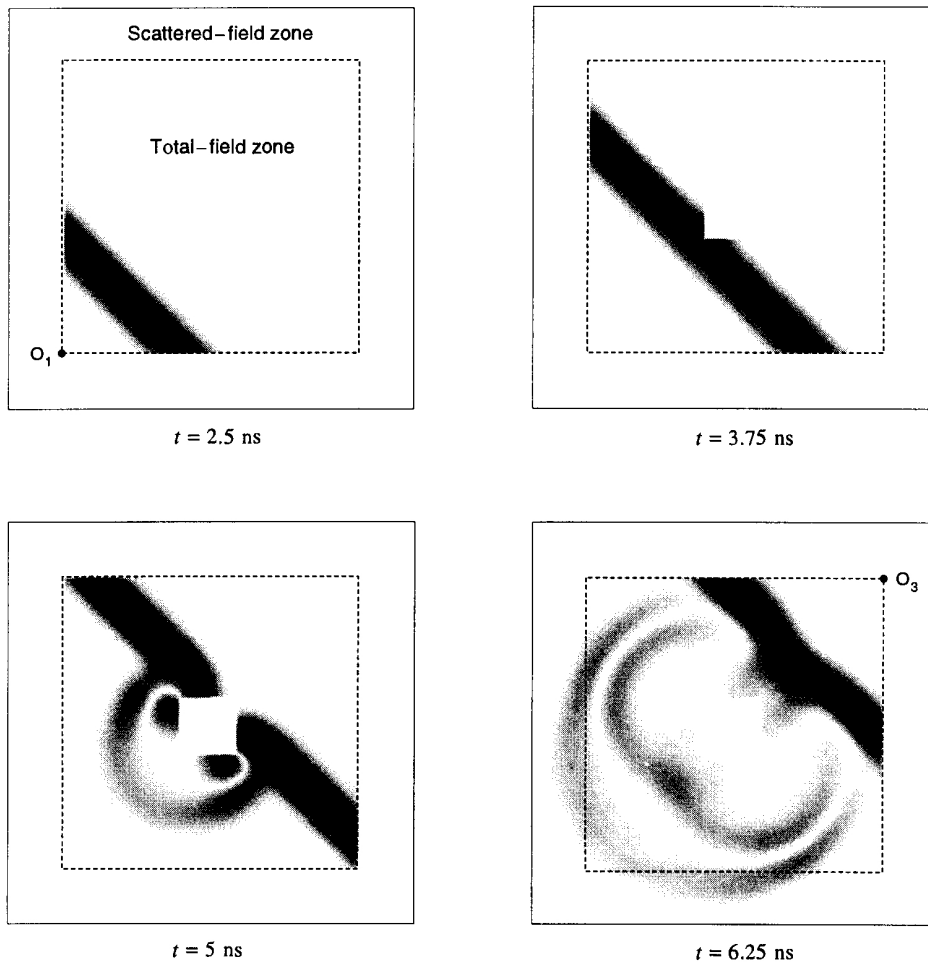


Figure 23: 2D TFSF plane wave interaction with PEC cube. Taken from [43], p. 214.

We observe that the TFSF boundary is essentially transparent for the scattered wave, allowing it to travel through unimpeded. With this we conclude the 2D example, and take the final step to the 3D implementation.

3D Plane wave

In three dimensions, we have eight possible points of “initial contact” of the incident plane wave with the TFSF interface. Let us once more assume without loss of generality that the contact point is the bottom left corner, given by coordinates (i_0, j_0, k_0) . The wave vector defining our 3D plane wave is illustrated in Figure [24].

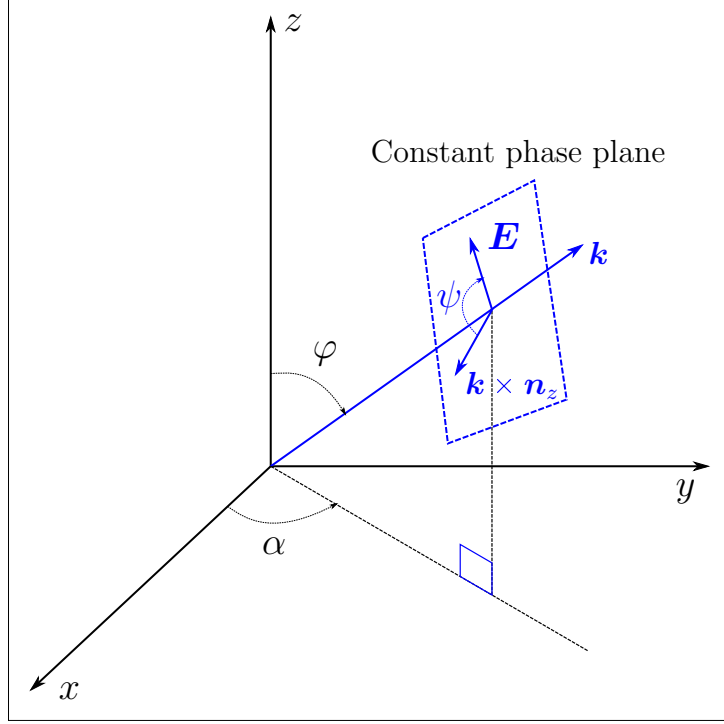


Figure 24: 3D plane wave polarization.

We now have two angles defining the wavevector $\mathbf{k}$, α and φ , as follows:

$$\mathbf{k} = \mathbf{n}_x \sin(\varphi) \cos(\alpha) + \mathbf{n}_y \sin(\varphi) \sin(\alpha) + \mathbf{n}_z \cos(\varphi)$$

Defining $d := \mathbf{k} \cdot \mathbf{r}$, we can use the same interpolation method as we have for the 2D case, in order to obtain the values of the 1D wave at the correct 3D positions. Once this is done, we can polarize the 1D wave as follows:

$$\begin{aligned} H_{x,\text{incident}}|_d^{n+1/2} &= H_{\text{incident}}|_d^{n+1/2} (\sin(\psi) \sin(\alpha) + \cos(\psi) \cos(\varphi) \cos(\alpha)) \\ H_{y,\text{incident}}|_d^{n+1/2} &= H_{\text{incident}}|_d^{n+1/2} (-\sin(\psi) \cos(\alpha) + \cos(\psi) \cos(\varphi) \cos(\alpha)) \\ H_{z,\text{incident}}|_d^{n+1/2} &= H_{\text{incident}}|_d^{n+1/2} (-\cos(\psi) \sin(\alpha)) \end{aligned} \quad (42)$$

$$\begin{aligned} E_{x,\text{incident}}|_d^n &= E_{\text{incident}}|_d^n (\cos(\psi) \sin(\alpha) - \sin(\psi) \cos(\varphi) \cos(\alpha)) \\ E_{y,\text{incident}}|_d^n &= E_{\text{incident}}|_d^n (-\cos(\psi) \cos(\alpha) - \sin(\psi) \cos(\varphi) \sin(\alpha)) \\ E_{z,\text{incident}}|_d^n &= E_{\text{incident}}|_d^n (\sin(\psi) \sin(\alpha)) \end{aligned} \quad (43)$$

This concludes our section on how to apply the TFSF technique in order to introduce a plane wave. The values defined in (43) and (42) are used as the analytical solution needed to define the surface currents in (38) and (39).

3.5 Perfectly Matched Layer

One important limiting factor of electromagnetic simulations is the size of the domain. Frequently, one would wish to observe EM phenomena in regions much larger than one is able to simulate. Due to the unavailability of unbounded computational domains, one has to rely on computational workarounds in order to overcome this problem.

One possible solution is to introduce some type of dampening (absorbing) material at the outer edges of the computational domain. The first breakthrough in this direction was achieved by Jean-Pierre Bérenger's 1994 paper [3], titled "A perfectly matched layer for the absorption of electromagnetic waves", which is the origin of the title of this section.

Previously, methods were developed that could deal with a plane wave incident on a computational domain face. However, these methods could not properly deal with a non-planar wave impinging at an arbitrary angle. This is where the Perfectly Matched Layer (hereon PML) provides an advancement. The idea that Bérenger introduced was to artificially include an anisotropy of the fields. This would be done by splitting each field component into two further orthogonal components, and then defining consistent PDEs on all twelve components.

Afterwards, with the help of this anisotropy, one introduces loss in the direction normal to the material interface, while not altering tangential propagation. Let us consider a simple 2D TM^z example. Let us consider σ_x, σ_x^* and σ_y, σ_y^* to be conductivities associated with propagation in the x and y directions respectively. We shall now consider the plane wave incidence illustrated in Figure [25].

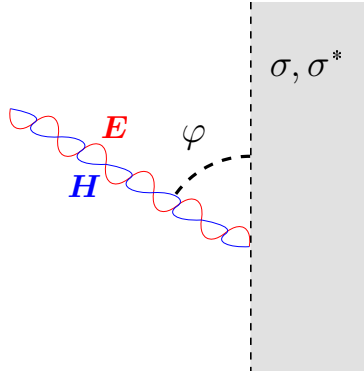


Figure 25: 2D TM^z plane wave.

For a given wave vector $\mathbf{k}_1 = \begin{pmatrix} \omega \sqrt{\mu_1 \varepsilon_1} \cos(\varphi) \\ \omega \sqrt{\mu_1 \varepsilon_1} \sin(\varphi) \end{pmatrix}$, the TM^z plane wave is defined as follows:

$$\check{\mathbf{E}}_{\text{incident}} = \mathbf{n}_z \exp(ik_{1x}x + ik_{1y}y)$$

where we use phasor notation for $\check{\mathbf{E}}$ (the expression also has to be multiplied with $\exp(i\omega t)$ to account for time dependence). Within the PML, the propagation is given by:

$$i\omega\mu_2 H_y + \sigma_x^* H_y = \frac{\partial E_z}{\partial x}, \quad i\omega\mu_2 H_x + \sigma_y^* H_x = -\frac{\partial E_z}{\partial y}$$

$$i\omega\varepsilon_2 E_z + \sigma_x E_z = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}$$

As we can see, there is no immediately obvious way to impose anisotropy on the third equation. It is at this point that we apply Bérenger's idea, to split the field into two components (which by themselves are not physically meaningful):

$$E_z = E_{zx} + E_{zy}$$

These two split components satisfy the following:

$$i\omega\varepsilon_2 E_{zx} + \sigma_x E_{zx} = \frac{\partial H_y}{\partial x} \quad (44)$$

$$i\omega\varepsilon_2 E_{zy} + \sigma_y E_{zy} = -\frac{\partial H_x}{\partial y} \quad (45)$$

At this point, in order to simplify notation, we shall introduce the following functions:

$$s_w = \ell_w + \frac{\sigma_w}{i\omega\varepsilon_2}, \quad s_w^* = \ell_w + \frac{\sigma_w^*}{i\omega\mu_2}$$

Where $\ell_w = 1$ for our purposes, and we use the subscript w to denote any of the x, y, z directions. We can then rewrite (44) and (45) as follows:

$$\begin{aligned} i\omega\varepsilon_2 s_x E_{zx} &= \frac{\partial H_y}{\partial x} \\ i\omega\varepsilon_2 s_y E_{zy} &= -\frac{\partial H_x}{\partial y} \\ i\omega\mu_2 s_x^* H_y &= \frac{\partial(E_{zx} + E_{zy})}{\partial x} \\ i\omega\mu_2 s_y^* H_x &= -\frac{\partial(E_{zx} + E_{zy})}{\partial y} \end{aligned}$$

Taking one more partial derivative and substituting, we obtain:

$$\begin{aligned} -\omega^2 \mu_2 \varepsilon_2 (E_{zx} + E_{zy}) &= \left(\frac{1}{s_x^*} \frac{\partial}{\partial x} \frac{1}{s_x} \frac{\partial}{\partial x} + \frac{1}{s_y^*} \frac{\partial}{\partial y} \frac{1}{s_y} \frac{\partial}{\partial y} \right) (E_{zx} + E_{zy}) \\ \Leftrightarrow \left(\frac{1}{s_x^*} \frac{\partial}{\partial x} \frac{1}{s_x} \frac{\partial}{\partial x} + \frac{1}{s_y^*} \frac{\partial}{\partial y} \frac{1}{s_y} \frac{\partial}{\partial y} \right) E_z &= 0 \end{aligned}$$

Let us now define the wave *transmission* coefficient Γ and the wave *reflection* coefficient τ , satisfying $\tau = 1 + \Gamma$. Then for the PML medium, the spatial dependence is as follows:

$$\check{E}_{z,\text{transmitted}} = \tau \exp(i\sqrt{s_x^* s_x} k_{2x} x + i\sqrt{s_y^* s_y} k_{2y} y)$$

Furthermore, the following has to be satisfied:

$$k_{2x}^2 + k_{2y}^2 = \omega^2 \mu_2 \varepsilon_2$$

The spatial dependence of the magnetic field transmitted into the PML is:

$$\check{H}_{y,\text{transmitted}} = \frac{1}{i\omega\mu_2 s_x^*} \frac{\partial E_{z,\text{transmitted}}}{\partial x} = -\frac{k_{2x}}{\omega\mu_2} \sqrt{\frac{s_x}{s_x^*}} E_{z,\text{transmitted}}$$

The tangential fields must match at the interface, which for the H_y field yields:

$$1 - \Gamma = \frac{\mu_1 k_{2x}}{\mu_2 k_{1x}} \sqrt{\frac{s_x}{s_x^*}} \tau$$

If we now use $1 + \Gamma = \tau$, we can solve for the coefficients:

$$\begin{aligned}\tau &= \frac{2\frac{k_{1x}}{\mu_1}}{\frac{k_{1x}}{\mu_1} + \frac{k_{2x}}{\mu_2} \sqrt{\frac{s_x}{s_x^*}}} \\ \Gamma &= \frac{\frac{k_{1x}}{\mu_1} - \frac{k_{2x}}{\mu_2} \sqrt{\frac{s_x}{s_x^*}}}{\frac{k_{1x}}{\mu_1} + \frac{k_{2x}}{\mu_2} \sqrt{\frac{s_x}{s_x^*}}}\end{aligned}$$

We expect to have no reflection ($\Gamma = 0$). If we first set $\mu_2 = \mu_1$ and $\varepsilon_1 = \varepsilon_2$, we obtain:

$$k_{2x} = \sqrt{\omega^2 \mu_2 \varepsilon_2 - k_{2y}^2} = \sqrt{\omega^2 \mu_1 \varepsilon_1 - k_{2y}^2} \quad (46)$$

In order to match the phase along the interface, the following has to hold:

$$\sqrt{s_y s_y^*} k_{2y} = k_{1y}$$

If we now claim there is no loss tangential to the interface ($\sigma_y = \sigma_y^* = 0$), which yields $s_y = s_y^* = 1$, we have that $k_{2y} = k_{1y}$. We can plug this into (46), and obtain $k_{2x} = k_{1x}$, and then furthermore:

$$\Gamma = \frac{1 - \sqrt{\frac{s_x}{s_x^*}}}{1 + \sqrt{\frac{s_x}{s_x^*}}}$$

Thus, in order to obtain a perfect match, i.e. no reflection, we require $s_x = s_x^*$, which means $\frac{\sigma_x}{\varepsilon_2} = \frac{\sigma_x^*}{\mu_2}$. We can now conclude with the set of all conditions necessary for a perfect x -direction PML matching condition, from vacuum:

$$\begin{aligned}\varepsilon_1 &= \varepsilon_2 \\ \mu_1 &= \mu_2 \\ \frac{\sigma_x}{\varepsilon_2} &= \frac{\sigma_x^*}{\mu_2} \\ \sigma_y &= \sigma_y^* = 0\end{aligned} \quad (47)$$

When (47) are satisfied, the amplitude of the plane wave traveling through the PML region is given by:

$$\begin{aligned}\exp(is_x k_{1x} x + ik_{1y} y) &= \exp\left(i\left(1 + \frac{\sigma_x}{i\omega\varepsilon_1}\right) k_{1x} x + ik_{1y} y\right) \\ &= \exp\left(-\frac{k_{1x}\sigma_x}{\omega\varepsilon_1}\right) \exp(ik_{1x} x + ik_{1y} y)\end{aligned}$$

The consequence is that for a nonzero σ_w , the wave will attenuate exponentially along the x -direction. One very important note to make is that this entire construct is nonphysical. In other words, the PML loss-inducing σ_w has no connection with the physical conductivity involved in the dielectric loss term $\mathbf{J} = \sigma \mathbf{E}$. Let us now investigate an alternative way to formulate the PML concept.

3.5.1 Uniaxial PML

Let us consider again the case of a harmonic plane wave, traveling in a 3D region. We consider a propagation from an isotropic medium in the region $x < 0$, into an anisotropic medium in $x > 0$. The $x > 0$ medium shall be referred to as “uniaxial”, since it is assumed to only have varying (anisotropic) material properties along the x -axis. More generally, material parameters associated with propagation in the w -direction ($w \in \{x, y, z\}$) only vary along the w -axis. This is defined by the permittivity and permeability tensors

$$\boldsymbol{\varepsilon}_2 = \begin{bmatrix} \varepsilon_{2x} & 0 & 0 \\ 0 & \varepsilon_{2yz} & 0 \\ 0 & 0 & \varepsilon_{2yz} \end{bmatrix} \quad \boldsymbol{\mu}_2 = \begin{bmatrix} \mu_{2x} & 0 & 0 \\ 0 & \mu_{2yz} & 0 \\ 0 & 0 & \mu_{2yz} \end{bmatrix}$$

Using phasor notation, let us assume the plane wave is propagating in region 1 ($x < 0$) according to $\widetilde{\mathbf{H}} = \mathbf{H}_0 \exp(-i\mathbf{k}_1 \cdot (x, y))$. The wave in region 2 ($x > 0$) will then also be a plane wave:

$$\begin{aligned} \mathbf{k}_2 \times \widetilde{\mathbf{E}} &= \omega \boldsymbol{\mu}_2 \widetilde{\mathbf{H}}, \quad \mathbf{k}_2 \times \widetilde{\mathbf{H}} = -\omega \boldsymbol{\varepsilon}_2 \widetilde{\mathbf{E}} \\ \Rightarrow \mathbf{k}_2 \times (\boldsymbol{\varepsilon}_2 \mathbf{k}_2) \times \widetilde{\mathbf{H}} + \omega^2 \boldsymbol{\mu}_2 \widetilde{\mathbf{H}} &= 0 \end{aligned}$$

which in expanded matrix form is

$$\begin{bmatrix} \kappa_2^2 c - k_{2y}^2 \varepsilon_{2yz}^{-1} & k_{2x} k_{2y} \varepsilon_{2yz}^{-1} & 0 \\ k_{2x} k_{2y} \varepsilon_{2yz}^{-1} & \kappa_2^2 \mu_{2yz}^{-1} & 0 \\ 0 & 0 & \kappa_2^2 \mu_{2yz} - k_{2x}^2 \varepsilon_{2yz}^{-1} - k_{2y}^2 \varepsilon_{2x} \end{bmatrix} \begin{bmatrix} \widetilde{H}_x \\ \widetilde{H}_y \\ \widetilde{H}_z \end{bmatrix} = 0$$

Here we defined $\kappa_2 := \omega \sqrt{\mu_{2x} \varepsilon_{2x}}$, $\kappa_1 := \omega \sqrt{\mu_{21} \varepsilon_1}$. We can interpret the first two equations as TE_z mode equations, and the third as TM_z mode. If we now denote $e_{i\mathbf{k}1} := \exp(ik_{1x}x + ik_{1y}y)$, we can express the fields in zone 1 as:

$$\begin{aligned} \widetilde{\mathbf{H}}_1 &= \mathbf{n}_z H_0 (1 + \Gamma \exp(-2ik_{1x}x)) e_{i\mathbf{k}1} \\ \widetilde{\mathbf{E}}_1 &= \left(-\mathbf{n}_x \frac{k_{1y}}{\omega \varepsilon_{1x}} (1 + \Gamma \exp(-2ik_{1x}x)) + \mathbf{n}_y \frac{k_{1x}}{\omega \varepsilon_{1x}} (1 - \Gamma \exp(-2ik_{1x}x)) \right) H_0 e_{i\mathbf{k}1} \end{aligned}$$

The wave propagated into zone 2 is then:

$$\begin{aligned} \widetilde{\mathbf{H}}_2 &= \mathbf{n}_z H_0 \tau \exp(ik_{2x}x + ik_{2y}y) \\ \widetilde{\mathbf{E}}_2 &= \tau \left(-\mathbf{n}_x \frac{k_{1y}}{\omega \varepsilon_{1x}} + \mathbf{n}_y \frac{k_{1x}}{\omega \varepsilon_{1x}} \right) H_0 \exp(ik_{2x}x + ik_{2y}y) \end{aligned}$$

Enforcing continuity of the fields at the interface, we obtain:

$$\Gamma = \frac{k_{1x} - k_{2x} \varepsilon_{2yz}^{-1}}{k_{1x} + k_{2x} \varepsilon_{2yz}^{-1}}, \quad \tau = \frac{2k_{1x}}{k_{1x} + k_{2x} \varepsilon_{2yz}^{-1}}, \quad k_{2y} = k_{1y} \quad (48)$$

If we look back at the TE_z equations, and use the third part of (48), we have:

$$k_{2x} = \sqrt{\kappa_2^2 \varepsilon_{2yz} \mu_{2yz} - k_{1y}^2 \varepsilon_{2x}^{-1} \varepsilon_{2yz}}$$

Thus, if we enforce $\varepsilon_1 = \varepsilon_2$, $\mu_1 = \mu_2$, $\mu_{2yz} = \varepsilon_{2yz}$, $\varepsilon_{2x}^{-1} = \varepsilon_{2yz}$, then $\kappa_1 = \kappa_2$, and furthermore

$$k_{2x} = \sqrt{(\kappa_1^2 - k_{1y}^2) \varepsilon_{2yz}^2} = \varepsilon_{2yz} \sqrt{\kappa_1^2 - k_{1y}^2} = \varepsilon_{2yz} k_{1x} \quad (49)$$

We observe that substituting (49) into (48) leads to $\Gamma = 0$ for all x -components of the wavevector, thus we achieve a reflectionless transmission, regardless of the angle of incidence. In a completely analogous manner, we can repeat the same computation for the TM_z equation, and obtain $\varepsilon_{2yz} = \mu_{2yz}, \mu_{2x}^{-1} = \mu_{2yz}$ as the requirements for total transmission ($\tau = 1$). In other words, the following relationship has to hold:

$$\boldsymbol{\varepsilon}_2 = \varepsilon_1 \mathbf{s}, \quad \boldsymbol{\mu}_2 = \mu_1 \mathbf{s}; \quad \mathbf{s} = \begin{bmatrix} s_x^{-1} & 0 & 0 \\ 0 & s_x & 0 \\ 0 & 0 & s_x \end{bmatrix}$$

We can specify propagation with these material parameters everywhere in the computational domain, as follows:

$$\nabla \times \check{\mathbf{H}} = -i\omega\varepsilon\mathbf{s}\check{\mathbf{E}}, \quad \nabla \times \check{\mathbf{E}} = i\omega\mu\mathbf{s}\check{\mathbf{H}}$$

if we redefine $\mathbf{s}$ as

$$\mathbf{s} = \begin{bmatrix} s_x^{-1} & 0 & 0 \\ 0 & s_x & 0 \\ 0 & 0 & s_x \end{bmatrix} \begin{bmatrix} s_y & 0 & 0 \\ 0 & s_y^{-1} & 0 \\ 0 & 0 & s_y \end{bmatrix} \begin{bmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & s_z^{-1} \end{bmatrix} = \begin{bmatrix} s_x^{-1}s_y s_z & 0 & 0 \\ 0 & s_x s_y^{-1} s_z & 0 \\ 0 & 0 & s_x s_y s_z^{-1} \end{bmatrix}$$

Let us now see how well this PML layer should theoretically dampen waves. Let us assume a PML thickness of d voxels on each side of the computational domain. We shall now use a plane wave solution, and plug it into the modified propagation equations within the UPML. One can show ([43], p. 306) that the total reflection for the round-trip to the the outer wall of the domain is the following, for an incidence angle of φ :

$$R(\varphi) = \exp\left(-2\eta\left(\int_0^d \sigma_w(x)dx\right)\cos(\varphi)\right) = \exp\left(-\frac{2\eta_0}{\sqrt{\varepsilon_r}}\left(\int_0^d \sigma_w(x)dx\right)\cos(\varphi)\right) \quad (50)$$

where η is the wave impedance inside the PML region, η_0 is wave impedance of vacuum, and ε_r is the relative permittivity. We see that the closer φ approaches 90° , the stronger the reflected wave. However, with a linear increase in d or η we have an exponential decrease in the reflection amplitude. Hence, in principle we will want to maximize σ_w , especially to mitigate the influence of the angle.

As is the case for the PML, the UPML is not applicable to lossy mediums in its current formulation. However, it would be able to handle inhomogeneous materials that have varying permittivity ε . If we look at the modified equations involving the $\mathbf{s}$ tensors, with some work one can show that Gauss' Law (or rather, a slightly modified version that has to hold in this case) does not hold if $\mathbf{s}$ is discontinuous in the transversal directions, inside the UPML. Of course, our σ_w is arbitrarily defined, and one could for example modify it locally as to maintain all s_w continuous in the tangential direction. An easier solution would be to instead define s_w in terms of the vacuum permittivity:

$$s_w = \ell_w + \frac{\sigma_w}{i\omega\varepsilon_0}$$

This definition is allowed, since our choice of s_w was arbitrary. However, this does change the propagation behavior through the material, leading to a modified reflection:

$$R(\varphi) = \exp\left(-2\eta_0\sqrt{\varepsilon_r}\left(\int_0^d \sigma_w(x)dx\right)\cos(\varphi)\right)$$

Hence, if we wish to have a permittivity-independent absorption behavior within the UPML, we need to scale (normalize) the σ_w 's. For this modified s_w definition, we shall divide the conductivities by the relative permittivity.

$$\sigma'_w(\mathbf{r}) := \frac{\sigma_w(\mathbf{r})}{\sqrt{\varepsilon_r(\mathbf{r})}} \Rightarrow s_w := \ell_w + \frac{\sigma'_w}{i\omega\varepsilon_0}$$

In this form, the $\mathbf{s}$ tensors would be able to yield the desired absorption behavior, independent of the local permittivity within the UPML.

Discrete UPML notes

In principle, one can deal with any change in material parameters across a PML interface, and still maintain a reflectionless absorption. However, in a discrete grid the large step discontinuity in σ_w leads to so-called *spurious wave reflection* at this interface. One way to subvert this is to gradually increase this parameter within the PML volume.

There are arbitrarily many ways of grading the parameters in the PML. Two of the most popular are polynomial and geometric. The most widespread is polynomial (of order m), which involves defining the $\mathbf{s}$ tensor as follows:

$$\sigma_x(x) = \left(\frac{x}{d}\right)^m \sigma_{x,\max}, \quad \ell_x(x) = 1 + (\ell_{x,\max} - 1) \left(\frac{x}{d}\right)^m$$

given for a PML thickness d . This ramps up $\sigma_x = 0$ at the interface to $\sigma_{x,\max}$ at the outer boundary, and $\ell_x = 1$ at the boundary to $\ell_x(d) = \ell_{x,\max}$. For this grading, the reflection factor is given by the following, according to (50):

$$R(\varphi) = \exp\left(-2\eta\sigma_{x,\max}d\cos(\varphi)\frac{1}{m+1}\right)$$

In most applications, $m \in [3, 4]$ is cited to be favorable [43]. For example, assume one knows d, m , and the desired reflection factor at normal incidence $R(0)$. Then one can compute $\sigma_{x,\max}$ as:

$$\sigma_{x,\max} = -\frac{(m+1)\ln(R(0))}{2\eta d}$$

Geometric grading involves defining the conductivity as:

$$\sigma_x(x) = (g^{\frac{1}{\Delta_h}})^x \sigma_{x,0}, \quad \ell_x(x) = (g^{\frac{1}{\Delta_h}})^x$$

where g is a scaling constant, Δ_h the spatial discretization spacing, and $\sigma_{x,0}$ is the conductivity at the interface with the computational domain. The resulting reflection is

$$R(\varphi) = \exp\left(-2\eta\sigma_{x,0}\Delta_h(g^{\frac{d}{\Delta_h}} - 1)\frac{\cos(\varphi)}{\ln(g)}\right)$$

If, as for the polynomial grading, we assume g, d and $R(0)$ to be known beforehand, we can compute the required $\sigma_{x,0}$ to achieve that reflection coefficient (usually $g \in [3, 4]$):

$$\sigma_{x,0} = -\frac{\ln(g)\ln(R(0))}{2\eta\Delta_h(g^{\frac{d}{\Delta_h}} - 1)}$$

Given this information, if one desires a factor of attenuation of $\exp(-16)$ for outgoing waves, i.e. $R(0) = \exp(-16)$, with a 10-cell thick polynomially-graded PML at the outer boundary, one needs to define the “optimal” $\sigma_{x,\max}$ as [43]:

$$\sigma_{x,\text{optimal}} = -\frac{(m+1)(-16)}{2\eta 10\Delta_h} = \frac{0.8(m+1)}{\eta\Delta_h}$$

FDTD UPML implementation

To simplify notation and computations, we shall assume that we are dealing with periodic fields (with the remark that this does not restrict the applicability of the result to such fields). Then we can formulate Ampère’s Law as:

$$\begin{bmatrix} \frac{\partial \check{H}_z}{\partial y} - \frac{\partial \check{H}_y}{\partial z} \\ \frac{\partial \check{H}_x}{\partial z} - \frac{\partial \check{H}_z}{\partial x} \\ \frac{\partial \check{H}_y}{\partial x} - \frac{\partial \check{H}_x}{\partial y} \end{bmatrix} = i\omega\epsilon \begin{bmatrix} s_x^{-1}s_y s_z & 0 & 0 \\ 0 & s_x s_y^{-1}s_z & 0 \\ 0 & 0 & s_x s_y s_z^{-1} \end{bmatrix} \begin{bmatrix} \check{E}_x \\ \check{E}_y \\ \check{E}_z \end{bmatrix}$$

We can also rewrite the constitutive relationships as follows:

$$\begin{aligned} \check{D}_x &= \frac{\epsilon s_z}{s_x} \check{E}_x, & \check{D}_y &= \frac{\epsilon s_x}{s_y} \check{E}_y, & \check{D}_z &= \frac{\epsilon s_y}{s_z} \check{E}_z \\ \Rightarrow \begin{bmatrix} \frac{\partial \check{H}_z}{\partial y} - \frac{\partial \check{H}_y}{\partial z} \\ \frac{\partial \check{H}_x}{\partial z} - \frac{\partial \check{H}_z}{\partial x} \\ \frac{\partial \check{H}_y}{\partial x} - \frac{\partial \check{H}_x}{\partial y} \end{bmatrix} &= i\omega \begin{bmatrix} s_y & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & s_x \end{bmatrix} \begin{bmatrix} \check{D}_x \\ \check{D}_y \\ \check{D}_z \end{bmatrix} \end{aligned}$$

We shall require one more step in order to arrive at a time-domain expression: an $i\omega f(\omega) \rightarrow \frac{\partial}{\partial t} f(t)$ inverse Fourier transform:

$$\begin{bmatrix} \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \\ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \\ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \end{bmatrix} = \frac{\partial}{\partial t} \begin{bmatrix} \ell_y & 0 & 0 \\ 0 & \ell_z & 0 \\ 0 & 0 & \ell_x \end{bmatrix} \begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} + \frac{1}{\epsilon} \begin{bmatrix} \sigma_y & 0 & 0 \\ 0 & \sigma_z & 0 \\ 0 & 0 & \sigma_x \end{bmatrix} \begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} \quad (51)$$

We can now discretize (51) according to the Yee scheme. The loss terms ℓ_w and σ_w are averaged in time. For D_x , this leads to the following explicit update:

$$\begin{aligned} D_x|_{i+1/2,j,k}^{n+1} &= \frac{2\epsilon_0\ell_y - \sigma_y\Delta_t}{2\epsilon_0\ell_y + \sigma_y\Delta_t} D_x|_{i+1/2,j,k}^{n+1} + \frac{2\epsilon_0\Delta_t}{2\epsilon_0\ell_y + \sigma_y\Delta_t} \cdot \\ &\cdot \left(\frac{H_z|_{i+1/2,j+1/2,k}^{n+1/2} - H_z|_{i+1/2,j-1/2,k}^{n+1/2}}{\Delta_y} - \frac{H_y|_{i+1/2,j,k+1/2}^{n+1/2} - H_y|_{i+1/2,j,k-1/2}^{n+1/2}}{\Delta_z} \right) \end{aligned} \quad (52)$$

If we now expand the constitutive relation for $\check{D}_x$, we obtain:

$$\begin{aligned} \check{D}_x \left(\ell_x + \frac{\sigma_x}{i\omega\epsilon_0} \right) &= \epsilon \check{E}_x \left(\ell_x + \frac{\sigma_x}{i\omega\epsilon_0} \right) \Big| \cdot i\omega, \text{ inverse Fourier transform} \\ \Leftrightarrow \frac{\partial}{\partial t} (\ell_x D_x) + \frac{\sigma_x}{\epsilon_0} D_x &= \epsilon \left(\frac{\partial}{\partial t} (\ell_z E_x) + \frac{\sigma_z}{\epsilon_0} E_x \right) \end{aligned}$$

We can now formulate the following update equation:

$$E_x|_{i+1/2,j,k}^{n+1} = \frac{2\varepsilon_0\ell_z - \sigma_z\Delta_t}{2\varepsilon_0\ell_z + \sigma_z\Delta_t} E_x|_{i+1/2,j,k}^{n+1} + \frac{1}{\varepsilon(2\varepsilon_0\ell_z + \sigma_z\Delta_t)} \cdot \left((2\varepsilon_0\ell_x + \sigma_x\Delta_t)D_x|_{i+1/2,j,k}^{n+1} - (2\varepsilon_0\ell_x - \sigma_x\Delta_t)D_x|_{i+1/2,j,k}^n \right) \quad (53)$$

Overall, we observe that the usual single equation that was needed for the update of E_x has now turned into two sequential steps. The first is (52), and the second is (53). Similarly, one obtains the two-step update equations for the magnetic field.

$$B_x|_{i,j+1/2,k+1/2}^{n+1/2} = \frac{2\varepsilon_0\ell_y - \sigma_y\Delta_t}{2\varepsilon_0\ell_y + \sigma_y\Delta_t} B_x|_{i,j+1/2,k+1/2}^{n-1/2} - \frac{2\varepsilon_0\Delta_t}{2\varepsilon_0\ell_y + \sigma_y\Delta_t} \cdot \left(\frac{E_z|_{i,j+1,k+1/2}^n - E_z|_{i,j-1,k+1/2}^n}{\Delta_y} - \frac{E_y|_{i,j+1/2,k+1}^n - E_y|_{i,j+1/2,k-1}^n}{\Delta_z} \right)$$

$$H_x|_{i,j+1/2,k+1/2}^{n+1/2} = \frac{2\varepsilon_0\ell_y - \sigma_y\Delta_t}{2\varepsilon_0\ell_y + \sigma_y\Delta_t} H_x|_{i,j+1/2,k+1/2}^{n-1/2} + \frac{1}{\mu(2\varepsilon_0\ell_z + \sigma_z\Delta_t)} \cdot \left((2\varepsilon_0\ell_x + \sigma_x\Delta_t)B_x|_{i,j+1/2,k+1/2}^{n+1/2} - (2\varepsilon_0\ell_x - \sigma_x\Delta_t)B_x|_{i,j+1/2,k+1/2}^{n-1/2} \right)$$

The corresponding equations for E_y, E_z, B_y, B_z are completely analogous. Let us shortly discuss the advantages and disadvantages that the UPML delivers. The main disadvantage is the doubling of the memory requirements, since we introduce two more fields that need to be stored and updated, $\mathbf{B}$ and $\mathbf{D}$. Furthermore, one also needs to take special care that heterogeneities (only w.r.t. permittivity) of the medium are properly accounted for. If this involves changes in conductivity, an extension of the model (as in [43], p. 332) will also be required.

The most important advantage of the UPML is the ability to absorb electromagnetic waves reaching the grid outer boundary. A clear advantage over the regular PML is the ability to have a uniform definition of the update equations throughout the computational domain. All that has to be ensured is that the values of the s_w 's change from 0 inside the physical computational domain, to whatever ramping is used inside the UPML subsets. With this we finalize the introduction of the UPML.

3.6 Numerical loss and numerical phase velocity

There are numerous sources treating the discussion on numerical phase velocity for lossless materials, see for example Taflov and Hagness' textbook [43]. Simply put, the discrete velocity of EM waves differs from the physical one. The same is true for dielectric loss. In the chapter at hand we shall quantify this discrepancy for the case of lossy materials, with a focus on numerical loss. Hereon in this section we shall use [42] for guidance, and fill in some of the gaps. Let us start our analysis with the 1D case. When we use time-averaging to evaluate the electrical field at non-integer time points in Maxwell's equations (which is desirable in order to preserve second order convergence in time), we obtain Yee's update equations, repeated here for convenience:

$$E_y^n(x_j) = \frac{1 - \frac{\sigma \Delta_t}{2\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}} E_y^{n-1}(x_j) - \frac{\frac{\Delta_t}{\varepsilon}}{1 + \frac{\sigma \Delta_t}{2\varepsilon}} \frac{H_z^{n-\frac{1}{2}}(x_{j+\frac{1}{2}}) - H_z^{n-\frac{1}{2}}(x_{j-\frac{1}{2}})}{\Delta_x}$$

$$H_z^{n+\frac{1}{2}}(x_{j+\frac{1}{2}}) = H_z^{n-\frac{1}{2}}(x_{j+\frac{1}{2}}) - \frac{\Delta_t}{\mu} \frac{E_y^n(x_{j+1}) - E_y^n(x_j)}{\Delta_x}$$

If we now consider a plane wave propagating through a lossy medium ($\sigma \neq 0$), then the electric and magnetic fields will have the following form:

$$E_y(x, t) = E_{y0} \exp \left(i(\tilde{k}x - \omega t) \right) \quad (54)$$

$$H_z(x, t) = H_{z0} \exp \left(i(\tilde{k}x - \omega t) \right) \quad (55)$$

where we denote with tilde discrete quantities that may differ from their physical counterparts. One knows from the analytical case that in lossy media the wave attenuates at a rate given by the imaginary part of the wavenumber [15]:

$$E_y(x, t) = E_{y0} \exp(i(\Re(k)x - \omega t)) \exp(-\Im(k)x)$$

$$H_z(x, t) = H_{z0} \exp(i(\Re(k)x - \omega t)) \exp(-\Im(k)x)$$

$$\text{where } k = \Re(k) + i\Im(k) =: \beta_\star + i\alpha_\star$$

We can define the discrete equivalent of k , denoted by $\tilde{k}$, which is given by the discrete analogue of Equations (54) and (55):

$$E_y(j\Delta_x, n\Delta_t) = E_{y0} \exp(i(\omega n\Delta_t - \beta j\Delta_x)) \exp(-\alpha j\Delta_x) \quad (56)$$

$$H_z((j + 1/2)\Delta_x, n\Delta_t) = H_{z0} \exp(i(\omega n\Delta_t - \beta(j + 1/2)\Delta_x)) \exp(-\alpha(j + 1/2)\Delta_x) \quad (57)$$

$$\text{where } \tilde{k} = \beta + i\alpha$$

One can work out $\alpha_\star, \beta_\star$ (p. 394 [15]) by applying curl ($\nabla \times$) to Faraday and Ampère's laws, and plugging in the plane wave solutions (54) and (55):

$$\alpha_\star = \omega \frac{1}{c\sqrt{2}} \sqrt{\sqrt{1 + \left(\frac{\sigma}{\varepsilon\omega}\right)^2} - 1} \quad (58)$$

$$\beta_\star = \omega \frac{1}{c\sqrt{2}} \sqrt{\sqrt{1 + \left(\frac{\sigma}{\varepsilon\omega}\right)^2} + 1} \left(\overset{\sigma \neq 0}{=} \frac{\omega\sigma\mu}{2\alpha_\star} \right) \quad (59)$$

It is also readily apparent that one retrieves the usual lossless formulas by plugging in $\sigma = 0$ into the above.

The next step is to plug in (56) and (57) into Yee's 1D update equations. If we do so, and afterwards divide by $\exp(i(\omega n \Delta_t - \beta j \Delta_x))$, we obtain:

$$E_{y0} \left(1 - e^{-i\omega\Delta_t} \frac{1 - \frac{\sigma\Delta_t}{2\varepsilon}}{1 + \frac{\sigma\Delta_t}{2\varepsilon}} \right) + H_{z0} \frac{\frac{\Delta_t}{\varepsilon}}{\Delta_x \left(1 + \frac{\sigma\Delta_t}{2\varepsilon} \right)} e^{-\frac{i\omega\Delta_t}{2}} \left(e^{-\frac{\tilde{k}\Delta_x}{2}} - e^{\frac{\tilde{k}\Delta_x}{2}} \right) = 0$$

$$E_{y0} \frac{\Delta_t}{\mu\Delta_x} \left(e^{-\tilde{k}\Delta_x} - 1 \right) + H_{z0} e^{-\frac{\tilde{k}\Delta_x}{2}} \left(e^{\frac{i\omega\Delta_t}{2}} - e^{-\frac{i\omega\Delta_t}{2}} \right) = 0$$

Which can be written as

$$\begin{bmatrix} e^{\frac{i\omega\Delta_t}{2}} - e^{-\frac{i\omega\Delta_t}{2}} \frac{1 - \frac{\sigma\Delta_t}{2\varepsilon}}{1 + \frac{\sigma\Delta_t}{2\varepsilon}} & \frac{\frac{\Delta_t}{\varepsilon}}{\Delta_x \left(1 + \frac{\sigma\Delta_t}{2\varepsilon} \right)} \left(e^{-\frac{\tilde{k}\Delta_x}{2}} - e^{\frac{\tilde{k}\Delta_x}{2}} \right) \\ \frac{\Delta_t}{\mu\Delta_x} \left(e^{-\frac{\tilde{k}\Delta_x}{2}} - e^{\frac{\tilde{k}\Delta_x}{2}} \right) & e^{\frac{i\omega\Delta_t}{2}} - e^{-\frac{i\omega\Delta_t}{2}} \end{bmatrix} \begin{bmatrix} E_{y0} \\ H_{z0} \end{bmatrix} = 0$$

$$\Leftrightarrow \begin{bmatrix} e^{\frac{i\omega\Delta_t}{2}} - e^{-\frac{i\omega\Delta_t}{2}} \frac{1 - \frac{\sigma\Delta_t}{2\varepsilon}}{1 + \frac{\sigma\Delta_t}{2\varepsilon}} & e^{i\varphi} \left(2 \frac{\frac{\Delta_t}{\varepsilon}}{\Delta_x \left(1 + \frac{\sigma\Delta_t}{2\varepsilon} \right)} \sinh \left(\frac{\tilde{k}\Delta_x}{2} \right) \right) \\ 2 \frac{\Delta_t}{\mu\Delta_x} \sinh \left(\frac{\tilde{k}\Delta_x}{2} \right) & e^{i\varphi} \left(e^{\frac{i\omega\Delta_t}{2}} - e^{-\frac{i\omega\Delta_t}{2}} \right) \end{bmatrix} \begin{bmatrix} E_{y0} \\ H_{z0} \end{bmatrix} = 0 \quad (60)$$

Where $e^{i\varphi}$ is the phase difference between the magnetic and electric field, due to the complex wavenumber k . To solve (60) we set the determinant of the matrix to zero, and notice that the phase difference cancels out, thus does not play a role any further:

$$\left(e^{\frac{i\omega\Delta_t}{2}} - e^{-\frac{i\omega\Delta_t}{2}} \frac{1 - \frac{\sigma\Delta_t}{2\varepsilon}}{1 + \frac{\sigma\Delta_t}{2\varepsilon}} \right) i \sin \left(\frac{\omega\Delta_t}{2} \right) = \frac{4\Delta_t^2}{\mu\Delta_x^2(\sigma\Delta_t + 2\varepsilon)} \sinh^2 \left(\frac{\tilde{k}\Delta_x}{2} \right)$$

We temporarily define $c := \frac{1 - \frac{\sigma\Delta_t}{2\varepsilon}}{1 + \frac{\sigma\Delta_t}{2\varepsilon}}$ for ease of notation, perform the following steps:

$$\Leftrightarrow \left((1 + c - c) e^{\frac{i\omega\Delta_t}{2}} - c e^{-\frac{i\omega\Delta_t}{2}} \right) i \sin \left(\frac{\omega\Delta_t}{2} \right) = \frac{4\Delta_t^2}{\mu\Delta_x^2(\sigma\Delta_t + 2\varepsilon)} \sinh^2 \left(\frac{\tilde{k}\Delta_x}{2} \right)$$

$$\Leftrightarrow \left((1 - c) e^{\frac{i\omega\Delta_t}{2}} + 2ic \sin \left(\frac{\omega\Delta_t}{2} \right) \right) i \sin \left(\frac{\omega\Delta_t}{2} \right) = \frac{4\Delta_t^2}{\mu\Delta_x^2(\sigma\Delta_t + 2\varepsilon)} \sinh^2 \left(\frac{\tilde{k}\Delta_x}{2} \right)$$

With a bit more work, we reach the following more readable form:

$$\Leftrightarrow -\sin^2 \left(\frac{\omega\Delta_t}{2} \right) \left(1 + c - \frac{i(1 - c)}{\tan \left(\frac{\omega\Delta_t}{2} \right)} \right) = \frac{4\Delta_t^2}{\mu\Delta_x^2(\sigma\Delta_t + 2\varepsilon)} \sinh^2 \left(\frac{\tilde{k}\Delta_x}{2} \right) \quad (61)$$

Applying $\Re(\cdot)$ and $\Im(\cdot)$ to (61), we obtain:

$$(1 + c) \sin^2 \left(\frac{\omega\Delta_t}{2} \right) = \frac{2\Delta_t^2}{\mu\Delta_x^2(\sigma\Delta_t + 2\varepsilon)} (1 - \cosh(\alpha\Delta_x) \cos(\beta\Delta_x))$$

$$(1 - c) \sin(\omega\Delta_t) = \frac{4\Delta_t^2}{\mu\Delta_x^2(\sigma\Delta_t + 2\varepsilon)} \sinh(\alpha\Delta_x) \sin(\beta\Delta_x)$$

If one follows the same steps with a plane wave in 3D, the resulting equations will be:

$$(1 + c) \sin^2 \left(\frac{\omega \Delta_t}{2} \right) = \frac{2\Delta_t^2}{\mu(\sigma \Delta_t + 2\varepsilon)} \sum_{w \in \{x,y,z\}} \frac{1 - \cosh(\alpha_w \Delta_w) \cos(\beta_w \Delta_w)}{\Delta_w^2}$$

$$(1 - c) \sin(\omega \Delta_t) = \frac{4\Delta_t^2}{\mu(\sigma \Delta_t + 2\varepsilon)} \sum_{w \in \{x,y,z\}} \frac{\sinh(\alpha_w \Delta_w) \sin(\beta_w \Delta_w)}{\Delta_w^2}$$

If we move now a bit further with the 1D equations, re-expanding c yields:

$$2\varepsilon\mu \sin^2 \left(\frac{\omega \Delta_t}{2} \right) = \frac{\Delta_t^2}{\Delta_x^2} (1 - \cosh(\alpha \Delta_x) \cos(\beta \Delta_x)) \quad (62)$$

$$\sigma \sin(\omega \Delta_t) = \frac{2\Delta_t}{\mu \Delta_x^2} \sinh(\alpha \Delta_x) \sin(\beta \Delta_x) \quad (63)$$

Now would be a good point to note that, as seen in (58), if $\sigma = 0$, then equation (63) is identically zero. Furthermore, (62) retrieves the lossless variant of the numerical dispersion equation. Let us also rewrite the equations slightly.

$$\begin{aligned} \frac{\omega^2 \sin^2 \left(\frac{\omega \Delta_t}{2} \right)}{c^2 \left(\frac{\omega \Delta_t}{2} \right)^2} &= \frac{2(1 - \cosh(\alpha \Delta_x) \cos(\beta \Delta_x))}{\Delta_x^2} \\ \downarrow \Delta_t \rightarrow 0 & \quad \downarrow \Delta_x \rightarrow 0 \\ \frac{\omega^2}{c^2} & \quad \beta_\star^2 - \alpha_\star^2 \\ \Leftrightarrow \frac{\omega^2}{c^2} &= \beta_\star^2 - \alpha_\star^2 \end{aligned}$$

Where $\alpha_\star$ and $\beta_\star$ are the *physical* loss and dispersion, given by $\Re(k), \Im(k)$ in (58), (59).

$$\begin{aligned} \sigma\omega\mu \frac{\sin(\omega \Delta_t)}{\omega \Delta_t} &= 2\alpha_\star\beta_\star \frac{\sinh(\alpha \Delta_x)}{\alpha \Delta_x} \frac{\sin(\beta \Delta_x)}{\beta \Delta_x} \\ \downarrow \Delta_t \rightarrow 0 & \quad \downarrow \Delta_x \rightarrow 0 \\ \sigma\omega\mu & \quad 2\alpha_\star\beta_\star \\ \Leftrightarrow \sigma\omega\mu &= 2\alpha_\star\beta_\star \end{aligned}$$

Now, in 3D both α and β are vectors, and need *not* point in the same direction. This would mean that while the wave propagates in one direction, the exponential decay of the amplitude is at its strongest in another direction, and only a fraction of that (given by the angle between the two vectors) happens in the direction of propagation.

Let us assume that propagation happens along a diagonal in several dimensions (where $\Delta_x = \Delta_y = \Delta_z$), and that $(\alpha_x, \alpha_y, \alpha_z) = \left(\frac{\alpha}{\sqrt{d}}, \frac{\alpha}{\sqrt{d}}, \frac{\alpha}{\sqrt{d}} \right) =: \alpha \parallel \beta := \left(\frac{\beta}{\sqrt{d}}, \frac{\beta}{\sqrt{d}}, \frac{\beta}{\sqrt{d}} \right) = (\beta_x, \beta_y, \beta_z)$. Then we can simply replace $\Delta_x \rightarrow \frac{\Delta_x}{\sqrt{d}}$ in equations (62) and (63) (where $d \in \{1, 2, 3\}$):

$$2\varepsilon\mu \sin^2 \left(\frac{\omega \Delta_t}{2} \right) = \frac{d\Delta_t^2}{\Delta_x^2} \left(1 - \cosh \left(\frac{\alpha \Delta_x}{\sqrt{d}} \right) \cos \left(\frac{\beta \Delta_x}{\sqrt{d}} \right) \right)$$

$$\sigma \sin(\omega \Delta_t) = \frac{2d\Delta_t}{\mu \Delta_x^2} \sinh \left(\frac{\alpha \Delta_x}{\sqrt{d}} \right) \sin \left(\frac{\beta \Delta_x}{\sqrt{d}} \right)$$

Or equivalently

$$\cosh\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)\cos\left(\frac{\beta\Delta_x}{\sqrt{d}}\right) = 1 - \frac{2\varepsilon\mu\Delta_x^2}{d\Delta_t^2}\sin^2\left(\frac{\omega\Delta_t}{2}\right) \quad (64)$$

$$\sinh\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)\sin\left(\frac{\beta\Delta_x}{\sqrt{d}}\right) = \frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t) \quad (65)$$

We shall expand upon (64) and (65) in order to solve for α and β separately:

$$\cosh^2\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)\cos^2\left(\frac{\beta\Delta_x}{\sqrt{d}}\right) = \left(1 - \frac{2\varepsilon\mu\Delta_x^2}{d\Delta_t^2}\sin^2\left(\frac{\omega\Delta_t}{2}\right)\right)^2 \quad (66)$$

$$\sinh^2\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)\sin^2\left(\frac{\beta\Delta_x}{\sqrt{d}}\right) = \left(\frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t)\right)^2 \quad (67)$$

$$\cos^2\left(\frac{\beta\Delta_x}{\sqrt{d}}\right) = \frac{\left(1 - \frac{2\varepsilon\mu\Delta_x^2}{d\Delta_t^2}\sin^2\left(\frac{\omega\Delta_t}{2}\right)\right)^2}{1 + \sinh^2\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)} \quad (68)$$

$$\sin^2\left(\frac{\beta\Delta_x}{\sqrt{d}}\right) = \frac{\left(\frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t)\right)^2}{\sinh^2\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)} \quad (69)$$

$$\Leftrightarrow 1 = \frac{\left(1 - \frac{2\varepsilon\mu\Delta_x^2}{d\Delta_t^2}\sin^2\left(\frac{\omega\Delta_t}{2}\right)\right)^2}{1 + \sinh^2\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)} + \frac{\left(\frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t)\right)^2}{\sinh^2\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)}$$

If we define $\mathcal{S} = \sinh\left(\frac{\alpha\Delta_x}{\sqrt{d}}\right)$, we obtain:

$$\mathcal{S}^4 + \mathcal{S}^2 \left(1 - \left(1 - \frac{2\varepsilon\mu\Delta_x^2}{d\Delta_t^2}\sin^2\left(\frac{\omega\Delta_t}{2}\right)\right)^2 - \left(\frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t)\right)^2\right) - \left(\frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t)\right)^2 = 0$$

Further using $c = \frac{1}{\sqrt{\mu\epsilon}}$, $s_c = \frac{c\Delta_t}{\Delta_x}$, we retrieve:

$$\Leftrightarrow \mathcal{S}^4 + \mathcal{S}^2 \left(1 - \left(1 - \frac{1 - \cos(\omega\Delta_t)}{ds_c^2}\right)^2 - \left(\frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t)\right)^2\right) - \left(\frac{\sigma\mu\Delta_x^2}{2d\Delta_t}\sin(\omega\Delta_t)\right)^2 = 0 \quad (70)$$

Keeping up with the usual quantities of interest on this subject, we define the following:

$$s_t = \frac{\sin\left(\frac{\omega\Delta_t}{2}\right)}{s_c\sqrt{d}} \quad (71)$$

$$\ell_{\tan\star} = \frac{\sigma}{\omega\varepsilon} \quad (72)$$

$$\ell_{\tan} = \frac{\left(\frac{\omega\Delta_t}{2}\right)}{\tan\left(\frac{\omega\Delta_t}{2}\right)} \ell_{\tan\star} \quad (73)$$

Here $\ell \tan_\star$ is referred to as the physical *loss tangent*, and $\ell \tan$ the discrete loss tangent. Using these newly defined terms, we rewrite (70) as follows:

$$\sinh^2 \left(\frac{\alpha \Delta_x}{\sqrt{d}} \right) = 2s_t^2 \left(s_t^2 - 1 + s_t^2 \ell \tan^2 \pm \sqrt{(1 + \ell \tan^2)(s_t^4 \ell \tan^2 + (1 - s_t^2)^2)} \right) \quad (74)$$

Similarly, one can obtain the expression for the numerical phase:

$$\sin^2 \left(\frac{\beta \Delta_x}{\sqrt{d}} \right) = 2s_t^2 \left(1 - s_t^2(1 + \ell \tan^2) \pm \sqrt{(1 + \ell \tan^2)(s_t^4 \ell \tan^2 + (1 - s_t^2)^2)} \right)$$

If we solve for the numerical loss, we choose the positive solution, and obtain:

$$\alpha = \frac{\sqrt{d}}{\Delta_x} \ln \left(\sqrt{2s_t^2 \left(s_t^2 - 1 + s_t^2 \ell \tan^2 + \sqrt{(1 + \ell \tan^2)(s_t^4 \ell \tan^2 + (1 - s_t^2)^2)} \right)} + \sqrt{1 + 2s_t^2 \left(s_t^2 - 1 + s_t^2 \ell \tan^2 + \sqrt{(1 + \ell \tan^2)(s_t^4 \ell \tan^2 + (1 - s_t^2)^2)} \right)} \right)$$

Now, a quantity of interest that is usually defined is the *penetration depth* δ of the electromagnetic waves into a lossy medium. This is defined as the depth at which the amplitude of the waves has decreased by $\frac{1}{e} \approx 0.368$, i.e.

$$\text{Find } \delta \text{ s.t. } \exp(-\alpha \delta) = \exp(-1) \Rightarrow \delta = \frac{1}{\alpha}$$

At this point, we have an expression for the discrete loss α , which depends on: the discretization parameters Δ_x, Δ_t , the frequency ω , the dimension d , and the tissue properties σ, ε , and μ (through the Courant number).

A relevant question to pose in this context is: How well is the penetration depth approximated discretely? In other words, how does the quantity below change with the discretization parameters, for example Δ_x ?

$$|\delta_\star - \delta| = \left| \frac{1}{\alpha_\star} - \frac{1}{\alpha} \right| \quad (75)$$

First of all, it is important to note that if one is to respect the Courant stability criterion, then when the spatial discretization becomes infinitely fine, so must the temporal one.

$$\Delta_x \rightarrow 0 \Rightarrow \Delta_t \rightarrow 0$$

For ease of notation, let us define

$$\mathcal{Q} := 2s_t^2 \left(s_t^2 - 1 + s_t^2 \ell \tan^2 + \sqrt{(1 + \ell \tan^2)(s_t^4 \ell \tan^2 + (1 - s_t^2)^2)} \right)$$

Then the following holds:

$$\alpha = \frac{\sqrt{d} \ln(\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1})}{\Delta_x}$$

With this we can rewrite (75) for 1D as

$$\left| \frac{1}{\alpha_\star} - \frac{1}{\alpha} \right| = \left| \frac{1}{\omega \sqrt{\frac{\varepsilon \mu}{2}} \sqrt{\sqrt{1 + \left(\frac{\sigma}{\varepsilon \omega}\right)^2} - 1}} - \frac{\Delta_x}{\ln(\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1})} \right| \quad (76)$$

Before we continue, using the fact that $\lim_{x \rightarrow 0} \frac{\tan(x)}{x} = \lim_{x \rightarrow 0} \frac{\sin(x)}{x} = 1$, and evaluating the limit $\frac{s_t}{\Delta_x} = \frac{\sin(\frac{\omega \Delta_t}{2})}{\frac{\omega \Delta_t}{2}} \cdot \frac{\frac{\omega \Delta_t}{2}}{\Delta_x \frac{c \Delta_t}{\Delta_x}} \xrightarrow{\Delta_x \rightarrow 0} \frac{\omega}{2c}$, we can analyze $\lim_{\Delta_x \rightarrow 0} \frac{\sqrt{\mathcal{Q}}}{\Delta_x}$:

$$\lim_{\Delta_x \rightarrow 0} \sqrt{2 \frac{s_t^2}{\Delta_x^2} \left(s_t^2 - 1 + s_t^2 \ell \tan^2 + \sqrt{(1 + \ell \tan^2)(s_t^4 \ell \tan^2 + (1 - s_t^2)^2)} \right)}$$

$\downarrow$
 $\frac{\omega^2}{2c^2}$

$\downarrow$
0

$\downarrow$
0

$\downarrow$
0

$\downarrow$
1

So what we are left with is:

$$\lim_{\Delta_x \rightarrow 0} \frac{\sqrt{\mathcal{Q}}}{\Delta_x} = \frac{\omega}{\sqrt{2c}} \sqrt{\sqrt{1 + \ell \tan_\star^2} - 1} = \frac{\omega}{\sqrt{2c}} \sqrt{\sqrt{1 + \frac{\sigma^2}{\omega^2 \varepsilon^2}} - 1} = \alpha_\star \quad (77)$$

Thus we have retrieved the physical value of α from Griffiths [15] as the limit of $\frac{\sqrt{\mathcal{Q}}}{\Delta_x}$. This yields information about $\lim_{\Delta_x \rightarrow 0} \alpha$. Returning to (74), let us apply the square root, divide by $\alpha \Delta_x$ on both sides, and take the limit w.r.t. Δ_x :

$$\lim_{\Delta_x \rightarrow 0} \frac{\sinh(\alpha \Delta_x)}{\alpha \Delta_x} = 1 = \lim_{\Delta_x \rightarrow 0} \frac{\sqrt{\mathcal{Q}}}{\alpha \Delta_x} \Leftrightarrow \lim_{\Delta_x \rightarrow 0} \frac{\alpha \Delta_x}{\sinh(\alpha \Delta_x)} = 1 = \lim_{\Delta_x \rightarrow 0} \frac{\alpha \Delta_x}{\sqrt{\mathcal{Q}}}$$

Which reveals the following:

$$\lim_{\Delta_x \rightarrow 0} \frac{\alpha \Delta_x}{\sqrt{\mathcal{Q}}} \cdot \lim_{\Delta_x \rightarrow 0} \frac{\sqrt{\mathcal{Q}}}{\Delta_x} = 1 \cdot \alpha_\star = \lim_{\Delta_x \rightarrow 0} \left(\frac{\alpha \Delta_x}{\sqrt{\mathcal{Q}}} \cdot \frac{\sqrt{\mathcal{Q}}}{\Delta_x} \right) = \lim_{\Delta_x \rightarrow 0} \alpha$$

Hence, as one would expect,

$$\lim_{\Delta_x \rightarrow 0} \alpha = \alpha_\star$$

Let us now go back to (76). We shall define $\tilde{\alpha} := \frac{\ln(\alpha_\star \Delta_x + \sqrt{\alpha_\star^2 \Delta_x^2 + 1})}{\Delta_x}$ and $\tilde{\delta} = 1/\tilde{\alpha}$.

$$\lim_{\Delta_x \rightarrow 0} \frac{1}{\Delta_x^2} (\tilde{\delta} - \delta_\star) = \lim_{\Delta_x \rightarrow 0} \frac{1}{\Delta_x^2} \left(\frac{\Delta_x}{\ln(\alpha_\star \Delta_x + \sqrt{\alpha_\star^2 \Delta_x^2 + 1})} - \frac{1}{\alpha_\star} \right) \quad (78)$$

At this point, due to (77), one might be tempted to claim that finding the limit above is our goal. However, even though $\sqrt{\mathcal{Q}} \sim \alpha_\star \Delta_x$ asymptotically, as we shall see soon,

$$\mathbb{R}_+^* \ni c_1 = \lim_{\Delta_x \rightarrow 0} \frac{1}{\Delta_x^2} (\tilde{\delta} - \delta_\star) \neq \lim_{\Delta_x \rightarrow 0} \frac{1}{\Delta_x^2} (\delta_\star - \delta) = c_2 \in \mathbb{R}_+^*$$

Thus both limits exist, but they are not the same. Let us now evaluate both of them.

Theorem 1 (Cazacu). *The asymptotic approximation of the numerical penetration depth $\tilde{\delta}(\Delta_x)$ converges to the physical penetration depth δ_* at the rate of Δ_x^2 , in particular:*

$$\lim_{\Delta_x \rightarrow 0} \frac{\tilde{\delta} - \delta_*}{\Delta_x^2} = \frac{\alpha_*}{6}$$

Proof. By our previous equation (78), we have:

$$\begin{aligned} \lim_{\Delta_x \rightarrow 0} \frac{\tilde{\delta} - \delta_*}{\Delta_x^2} &= \lim_{\Delta_x \rightarrow 0} \left(\frac{1}{\Delta_x \ln(\alpha_* \Delta_x + \sqrt{\alpha_*^2 \Delta_x^2 + 1})} - \frac{1}{\Delta_x^2 \alpha_*} \right) \\ \Leftrightarrow \lim_{\Delta_x \rightarrow 0} \frac{\tilde{\delta} - \delta_*}{\Delta_x^2} &= \lim_{\Delta_x \rightarrow 0} \frac{\alpha_* \Delta_x - \ln(\alpha_* \Delta_x + \sqrt{\alpha_*^2 \Delta_x^2 + 1})}{\alpha_* \Delta_x^2 \ln(\alpha_* \Delta_x + \sqrt{\alpha_*^2 \Delta_x^2 + 1})} \end{aligned}$$

And since $\lim_{x \rightarrow 0} \frac{\ln(x+1)}{x} = 1$, we can rewrite this as

$$\lim_{\Delta_x \rightarrow 0} \frac{\tilde{\delta} - \delta_*}{\Delta_x^2} = \lim_{\Delta_x \rightarrow 0} \frac{\alpha_* \Delta_x - \ln(\alpha_* \Delta_x + \sqrt{\alpha_*^2 \Delta_x^2 + 1})}{\alpha_* \Delta_x^2 (\alpha_* \Delta_x + \sqrt{\alpha_*^2 \Delta_x^2 + 1} - 1)}$$

If we now employ L'Hôpital's rule three times, we obtain:

$$\begin{aligned} \lim_{\Delta_x \rightarrow 0} \frac{\tilde{\delta} - \delta_*}{\Delta_x^2} &= \lim_{\Delta_x \rightarrow 0} \frac{\left(\frac{d}{d\Delta_x}\right)^3 (\alpha_* \Delta_x - \ln(\alpha_* \Delta_x + \sqrt{\alpha_*^2 \Delta_x^2 + 1}))}{\left(\frac{d}{d\Delta_x}\right)^3 (\alpha_* \Delta_x^2 (\alpha_* \Delta_x + \sqrt{\alpha_*^2 \Delta_x^2 + 1} - 1))} \\ \Leftrightarrow \lim_{\Delta_x \rightarrow 0} \frac{\tilde{\delta} - \delta_*}{\Delta_x^2} &= \lim_{\Delta_x \rightarrow 0} \frac{f(\Delta_x)}{g(\Delta_x)} \end{aligned}$$

where

$$\begin{aligned} f(\Delta_x) &:= \frac{\alpha_*^3 - 2\alpha_*^5 \Delta_x^2}{(\alpha_*^2 \Delta_x^2 + 1)^{5/2}} \\ g(\Delta_x) &:= 6\alpha_* \left(\alpha_* + \frac{\alpha_*^2 \Delta_x}{\sqrt{\alpha_*^2 \Delta_x^2 + 1}} \right) + 6\alpha_* \Delta_x \left(\frac{\alpha_*^2}{\sqrt{\alpha_*^2 \Delta_x^2 + 1}} - \frac{\alpha_*^4 \Delta_x^2}{(\alpha_*^2 \Delta_x^2 + 1)^{3/2}} \right) + \\ &\quad + \alpha_* \Delta_x^2 \left(\frac{3\alpha_*^6 \Delta_x^3}{\sqrt{\alpha_*^2 \Delta_x^2 + 1}} - \frac{3\alpha_*^4 \Delta_x}{(\alpha_*^2 \Delta_x^2 + 1)^{3/2}} \right) \end{aligned}$$

Let us note that neither f nor g have a singularity at 0, thus we can evaluate:

$$\Leftrightarrow \lim_{\Delta_x \rightarrow 0} \frac{\tilde{\delta} - \delta_*}{\Delta_x^2} = \lim_{\Delta_x \rightarrow 0} \frac{f(\Delta_x)}{g(\Delta_x)} = \frac{f(0)}{g(0)} = \frac{\alpha_*^3}{6\alpha_*^2} = \frac{\alpha_*}{6}$$

□

We can also evaluate the validity of this claim numerically. We shall use a short Python script that fits a linear function to the log-log data of $\tilde{\delta} - \delta_*$ versus $\Delta_x \in \{\frac{\lambda}{20} \cdot \frac{1}{2^i} | i \in \{0, 1, \dots, 12\}\}$, using NumPy's polyfit function [31]. Since we are computing the linear fit of $\ln(\tilde{\delta} - \delta_*)$ versus $\ln(\Delta_x)$, with slope m and constant c , the fit will have the form $\exp(m \ln(\Delta_x) + c)$. Thus, the slope m will yield the numerically computed convergence

rate, and $\exp(c)$ will be the numerically computed limit of $\frac{\tilde{\delta}-\delta_\star}{\Delta_x^m}$. The printout of the polyfit result is presented in Figure [26].

```
PS A:\Dropbox\PhD Thesis> python .\convergence_order.py
Order of convergence: 1.99880, constant: 1.42136
alpha_star/6: 4.18538, e^constant: 4.14277, error: 1.01806 %
```

Figure 26: Output of Python script which checks convergence rate numerically (with $\tilde{\delta}$).

We observe that the limit from Theorem 1 is reached within 1.02% relative error, computed as $\frac{\alpha_\star - \exp(c)}{\alpha_\star}$, and the convergence rate is approximated as 1.9988. Let us now check what happens in the case of δ .

Theorem 2 (Cazacu). *The numerical penetration depth $\delta(\Delta_x)$ converges to the physical penetration depth $\delta_\star$ at the rate of Δ_x^2 , in particular:*

$$\lim_{\Delta_x \rightarrow 0} \frac{\delta_\star - \delta}{\Delta_x^2} = \frac{\alpha_\star}{6} \left(1 - \frac{\alpha_\star^2 c^2 + \omega^2}{2\alpha_\star^2 c^2 + \omega^2} \right)$$

Proof.

$$\lim_{\Delta_x \rightarrow 0} \frac{\delta_\star - \delta}{\Delta_x^2} = \lim_{\Delta_x \rightarrow 0} \frac{\ln(\sqrt{Q} + \sqrt{Q+1}) - \alpha_\star \Delta_x}{\alpha_\star \Delta_x^2 \ln(\sqrt{Q} + \sqrt{Q+1})}$$

In order to proceed, let us find the (Taylor or Laurent) series expansion of $\sqrt{Q} + \sqrt{Q+1}$.

$$Q = 2s_t^2 \left(s_t^2 - 1 + s_t^2 \ell \tan^2 + \sqrt{(1 + \ell \tan^2)(s_t^4 \ell \tan^2 + (1 - s_t^2)^2)} \right)$$

We shall break this down into steps by rewriting:

$$Q = 2s_t^2 (\mathcal{A} + \sqrt{\mathcal{B}})$$

Now note that $\frac{\omega \Delta_x}{2} = \frac{\omega \Delta_x}{2c}$. Furthermore, since we expect second order convergence, we shall only list terms of up to order 3, and denote the power series by $\Sigma[\cdot]$.

$$\begin{aligned} \Sigma[\mathcal{B}] &= \left(1 + \ell \tan_\star^2 \Sigma \left[\frac{\left(\frac{\omega \Delta_x}{2c} \right)^2}{\tan^2 \left(\frac{\omega \Delta_x}{2c} \right)} \right] \right) \\ &\cdot \left(\ell \tan_\star^2 \Sigma \left[\left(\frac{\omega \Delta_x}{2c} \right)^2 \sin^2 \left(\frac{\omega \Delta_x}{2c} \right) \cos^2 \left(\frac{\omega \Delta_x}{2c} \right) \right] + \Sigma \left[\left(1 - \sin^2 \left(\frac{\omega \Delta_x}{2c} \right) \right)^2 \right] \right) \end{aligned}$$

For ease of notation, we shall rewrite the argument Δ_x as x in the following series expansions. After performing some coefficient matching, we obtain:

$$\Sigma[\mathcal{B}] = (\ell \tan_\star^2 + 1) - \frac{x^2 ((4\ell \tan_\star^2 + 3) \omega^2)}{6c^2} + \frac{x^4 \omega^4 (15\ell \tan_\star^4 + 61\ell \tan_\star^2 + 25)}{240c^4} + O(x^5)$$

$$\begin{aligned} \Sigma[\sqrt{\mathcal{B}}] &= \sqrt{\ell \tan_\star^2 + 1} - \frac{x^2 ((4\ell \tan_\star^2 + 3) \omega^2)}{12 (c^2 \sqrt{\ell \tan_\star^2 + 1})} + \\ &+ \frac{\omega^4 x^4 (45\ell \tan_\star^6 + 148\ell \tan_\star^4 + 138\ell \tan_\star^2 + 30)}{1440c^4 (\ell \tan_\star^2 + 1)^{3/2}} + O(x^5) \end{aligned}$$

$$\begin{aligned}\Sigma[\mathcal{A}] &= -1 + \frac{x^2 (\ell \tan_\star^2 \omega^2 + \omega^2)}{4c^2} - \frac{x^4 \omega^4 (3\ell \tan_\star^2 + 1)}{48c^4} + O(x^5) \\ \Rightarrow \Sigma[\mathcal{Q}] &= \frac{x^2 \left(\sqrt{\ell \tan_\star^2 + 1} \omega^2 - \omega^2 \right)}{2c^2} + \\ &\quad + \frac{\omega^4 x^4 \left(3\sqrt{\ell \tan_\star^2 + 1} \ell \tan_\star^2 - 5\ell \tan_\star^2 + 4\sqrt{\ell \tan_\star^2 + 1} - 4 \right)}{24c^4 \sqrt{\ell \tan_\star^2 + 1}} + O(x^5)\end{aligned}$$

Thus, we arrive at the following expression:

$$\begin{aligned}\Sigma[\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1}] &= 1 + \frac{x \sqrt{\frac{(\sqrt{\ell \tan_\star^2 + 1} - 1) \omega^2}{c^2}}}{\sqrt{2}} + \frac{x^2 \left(\sqrt{\ell \tan_\star^2 + 1} \omega^2 - \omega^2 \right)}{4c^2} + \\ &\quad + \frac{x^3 \omega^2 \left(3\sqrt{\ell \tan_\star^2 + 1} \ell \tan_\star^2 - 5\ell \tan_\star^2 + 4\sqrt{\ell \tan_\star^2 + 1} - 4 \right) \sqrt{\frac{(\sqrt{\ell \tan_\star^2 + 1} - 1) \omega^2}{c^2}}}{24\sqrt{2}c^2 \sqrt{\ell \tan_\star^2 + 1} \left(\sqrt{\ell \tan_\star^2 + 1} - 1 \right)} + \\ &\quad + \frac{x^4 \omega^4 \left(3\sqrt{\ell \tan_\star^2 + 1} \ell \tan_\star^2 - 4\ell \tan_\star^2 + 2\sqrt{\ell \tan_\star^2 + 1} - 2 \right)}{96c^4 \sqrt{\ell \tan_\star^2 + 1}} + O(x^5)\end{aligned}$$

To proceed, one can either apply L'Hôpital's rule once, or compute $\Sigma [\ln(\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1})]$:

$$\begin{aligned}\Sigma [\ln(\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1})] &= \frac{x \sqrt{\frac{(\sqrt{\ell \tan_\star^2 + 1} - 1) \omega^2}{c^2}}}{\sqrt{2}} + \\ &\quad + \frac{x^3 \omega^2 \ell \tan_\star^2 \sqrt{\frac{(\sqrt{\ell \tan_\star^2 + 1} - 1) \omega^2}{c^2}}}{24\sqrt{2}c^2 \sqrt{\ell \tan_\star^2 + 1}} + O(x^5)\end{aligned}$$

With this we can compute the following ratio:

$$\begin{aligned}\frac{\Sigma [\ln (\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1}) - \alpha_\star x]}{\Sigma [\alpha_\star x^2 \ln (\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1})]} &= \frac{\frac{\ell \tan_\star^2 \omega^2 x^3 \sqrt{\frac{(\sqrt{\ell \tan_\star^2 + 1} - 1) \omega^2}{c^2}}}{24\sqrt{2}c^2 \sqrt{\ell \tan_\star^2 + 1}} + O(x^5)}{\frac{x^3 (\sqrt{\ell \tan_\star^2 + 1} \omega^2 - \omega^2)}{2c^2} + O(x^5)} \\ \Rightarrow \Sigma \left[\frac{\ln (\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1}) - \alpha_\star x}{\alpha_\star x^2 \ln (\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1})} \right] &= \frac{\ell \tan_\star^2 \omega}{12\sqrt{2}c \sqrt{\ell \tan_\star^2 + 1} \sqrt{(\sqrt{\ell \tan_\star^2 + 1} - 1)}} + O(x^2) \\ \Leftrightarrow \Sigma \left[\frac{\ln (\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1}) - \alpha_\star x}{\alpha_\star x^2 \ln (\sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q} + 1})} \right] &= \frac{\alpha_\star}{6} \left(1 - \frac{\alpha_\star^2 c^2 + \omega^2}{2\alpha_\star^2 c^2 + \omega^2} \right) + O(x^2)\end{aligned}$$

Taking the limit of $x \rightarrow 0$ ($\Delta_x \rightarrow 0$), we obtain the result in the claim. $\square$

We can also indirectly test this claim numerically, by altering the Python script to perform the linear fit of $\ln(\delta_\star - \delta)$ versus $\ln(\Delta_x)$. The output is illustrated in Figure [27].

```
PS A:\Dropbox\PhD Thesis> python .\convergence_order.py
Order of convergence: 1.99992, constant: 1.39241
alpha_star/6*(1-ratio): 4.04583, e^constant: 4.02455, error: 0.52585 %
```

Figure 27: Output of Python script checking convergence for $\delta_\star - \delta$.

Thus, we observe that this limit is approximated within 0.53% by the numerical algorithm.

In order to conclude, we must highlight the fact that this discussion has been carried out for a plane wave traveling along an axis-aligned direction. In reality, microwave applicators produce fields that are (potentially significantly) closer to purely spherical waves (“elliptical” wavefronts), which cover the entire range of possible directions.

Furthermore, with spherical wavefronts, the so-called *energy isosurfaces*, or surfaces of constant integrated energy, are the surfaces of a sphere centered on the source. Their radius increases at the same speed as the electromagnetic wave propagation. This means that in the case of a point dipole in a lossy material, the amplitude of the fields also decays proportionally with $\frac{1}{r^3}$, in addition to the exponential decay due to σ . Hence, the numerical loss error would be further scaled according to this proportionality.

Chapter 4

Combined Workflow

In this chapter we shall discuss various challenges involved in combining the discrete workflow pieces together, while incorporating realistic input data. The main components are the electromagnetic simulation and the (bio)heat simulation.

4.1 Material parameters

In order to obtain a complete simulation workflow, from an electromagnetic solver leading up to temperature and damage influence on tissue, we need to take a closer look at how exactly this interaction between all computational components takes place.

As we mentioned before, the output from the electromagnetic (EM) solver is given as input into a bioheat equation solver. This is done roughly every 1 second, based on how often it is considered that “relevant changes in heat” occur, and based on simulation time considerations. To this end, we take the *stabilized* state of the EM solver as input for the next step.

After the bioheat solver is finished, the resulting output is a change in temperature. Ideally, and in order to obtain the most realistic result, this temperature change should result in a change in material parameters. It is well known in medical practice and in the electrical engineering community that tissue dielectric parameters change with temperature.

In an optimal scenario, for every type of material or tissue present in the simulation pipeline, there would be an available analytic expression giving all dielectric parameters of that tissue, for any given temperature. This is not the case however, and in the clinical world, there are active efforts to run sufficiently many experiments, in order to properly characterize all clinically relevant tissue types (for example [18]).

One major drawback is that many such experiments are conducted in scenarios that do not match the reality of medical electromagnetic interventions. A plethora of experiments are performed ex-vivo, in particular ignoring the influence of blood perfusion on the entire process. It is known that proper accounting of perfusion plays a major role in how well numerical experiments are able to replicate reality [13], [36]. In particular, not taking it into account leads to an underestimation of the required temperature needed to achieve a given coagulation state.

There have been advances in terms of emulating the influence of perfusion during ex-vivo dielectric experiments, with procedures that artificially pump liquids or even blood into resected organs (such as that performed in [41]). However, there are still difficulties in the way of performing such measurements in realistic scenarios. Ideally, in order to obtain representative clinical data, the measurements would have to be done at all given points of a particular organ or tissue, and at all temperature points that are within the clinically/numerically reached range. However, current experimental technology is not yet at this advanced stage, and most experimental dielectric tissue measurements are conducted with some type of one-ended coaxial probe, to be placed on a “half-space” of tissue [22].

There are several difficulties with this attempt to, in a manner of speaking, perform a 1D measurement of a 3D volume of tissue. In terms of results, there are significant differences reported ([22]) as taking place when only altering the geometric distribution of tissue sub-components (fat, water, etc.) while preserving their volumetric ratios.

4.2 Time scale discrepancy

One potential issue that arises in the final (combined) workflow, involving both an electromagnetic and a heat solver, is the discrepancy in time scales that one has to deal with. Within the EM solver, one works with frequencies in the range of $[0.915, 2.45]$ GHz. This means that if one is to satisfy the stability criteria, a time step in the range of $[10^{-12}, 10^{-9}]$ seconds is to be used. Meanwhile, for the heat deposition component, we wish to evaluate changes in temperature in significantly larger time steps, due to simulation time considerations.

As previously mentioned, we would have to simulate billions of time steps from of the EM solver for each ≈ 1 s of simulated heat change, which can be very costly in terms of simulation time. A viable way to circumvent this problem is, given the right conditions, to expect that the EM simulation reaches a steady or quasi-steady state sooner than after billions of time steps. One would then stop this simulation, and obtain some output based on the quasi-steady state, to pass on to the heat solver.

The natural question that now has to be answered is, in what conditions can we expect a quasi-steady state to be reached? We have seen before that one can use a PML for example to terminate the computational grid. Given a thick enough such layer, we can expect “negligible” (which should be quantified properly) fields to accumulate within the PML. Modulo the efficiency of this absorbing outer boundary, and when dealing with harmonic sources, one would intuitively expect that eventually, the electromagnetic field is periodic within the entire domain.

The caveat here is to define exactly if and when this periodicity will happen. The first question that arises (and whose answer may not be immediately obvious) is: given a source oscillating at a given frequency ω , say a hard electrical field source $\mathbf{E}(x, t) = \mathbf{E}_0 \exp(i\omega t)$, and a computational domain Ω_h containing various heterogeneous regions (in terms of material parameters), should we expect that the entire computational domain reaches a periodic (quasi) steady state, oscillating at the same frequency ω ?

That is to say, is it true that, for a given compact Ω :

$$\exists t_{\text{stabilized}} \text{ s.t. } \forall x \in \Omega, \forall t > t_{\text{stabilized}}, \mathbf{E}(x, t) = \mathbf{E}\left(x, t + \frac{2\pi}{\omega}\right), \mathbf{H}(x, t) = \mathbf{H}\left(x, t + \frac{2\pi}{\omega}\right)?$$

It is trivial to prove this for a domain filled with vacuum, or in fact any homogeneous tissue parameters. The only difficulty that can arise is due to heterogeneities. If there are heterogeneities, there are material interfaces. We know from the construct that was made in Section 2.3 that the tangential component of the electrical field has to be continuous across such an interface. Therefore, for any incoming wave on an interface, the incident, reflected and refracted wave vectors will all lie in the same plane.

Let us assume that we have an incident plane wave impinging on a material interface, given by $\mathbf{E}_i = \mathbf{E}_{i0} \exp(i(\omega_i t - k_i r))$ for some distance r from the point of origin. The refracted and transmitted waves can be written out as well: $\mathbf{E}_r = \mathbf{E}_{r0} \exp(i(\omega_r t - k_r r))$, $\mathbf{E}_t = \mathbf{E}_{t0} \exp(i(\omega_t t - k_t r))$. This refraction is visualized in Figure [28].

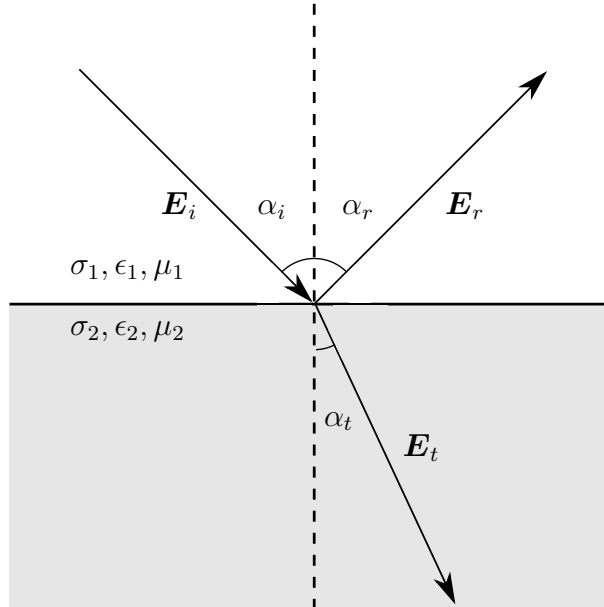


Figure 28: Refraction at an interface.

The point now is to ascertain whether during this process the frequency stays constant. In other words, is it true for this scenario that

$$\omega_i = \omega_r = \omega_t ?$$

Let us remark that for each one of the three waves the following holds:

$$\mathbf{E} = \mathbf{E}_{\parallel} + \mathbf{E}_{\perp}$$

Since the tangential components at the interface must be matched, and the total waves cannot oscillate at a different frequency from their tangential component, it must follow that the frequency stays constant throughout refraction. The important takeaway message is the following: given a finite “window” which is our computational grid, we can expect that with a source of energy of a given frequency ω , after a finite time, the electromagnetic field will be periodic at the same frequency.

The next step we have to consider is defining the output of the EM solver, and thus the input of the heat equation solver. The immediate idea is to stop the EM simulation after it has reached a quasi steady state, and use that instantaneous electromagnetic status as the input for the bioheat solver. The issue with this approach is that since the temperature changes much more slowly, the temperature spatial distribution will not capture the time variation of the electromagnetic field. Instead, it will represent a time-averaged version of the electromagnetic state. Hence, using the instantaneous version of the electromagnetic field as input would predictably produce undesirable results.

Instead, we should look to work with some averaged fields. In principle, averaging over an entire period would give us the best information, since then we would be using the envelope of the maximum amplitude of the field. However, since we are utilizing the norm of the electrical field as input for the heat solver, the complete information is actually already contained in one quarter of a period, due to:

$$\int_0^{2\pi} |\sin(t)| dt = \int_0^{\frac{\pi}{2}} |\sin(t)| dt$$

This fact has significant utility, because evaluating the average over past time steps involves saving the full 3D state of all twelve field components $(E_{x,y,z}, H_{x,y,z}, D_{x,y,z}, B_{x,y,z})$ and many other data structures, as many times over as the number of time points we wish to save. For example, let us assume we have a discretization with 160 points per period, which is quite realistic for real data. This number is inversely proportional to the smallest refractive index in the computational domain, which may very well be close to that of vacuum. This would mean the memory requirement is 160 times the above mentioned fields, versus 40 if we use a quarter of a period.

4.3 Time averaging errors

In this section we shall have a quick look at how we can quantify the difference in behavior of the heat solver input, depending on whether we average the electric field over the last period after the EM solver is finished.

First, in order to talk about continuous $L^p(\Omega, L^q[0, t_{\text{final}}])$ norms involving a modified (averaged) heat equation (HE) source term, we need to interpolate the results of the FDTD Maxwell solver E_h, H_h , which are only given pointwise at their respective grid vertices. If we define the grid Ω_h of size $N_h = N_x \times N_y \times N_z$, which discretizes the 3D space of extent $\Omega := [0, x_{\text{max}}] \times [0, y_{\text{max}}] \times [0, z_{\text{max}}]$.

We shall have to map the discrete fields to their continuous counterparts E_{hh}, H_{hh} :

$$\mathbb{R}^{N_h} \ni E_h \rightarrow \Pi_k E_h =: E_{hh} : \Omega \rightarrow \mathbb{R}^3$$

$$\mathbb{R}^{N_h} \ni H_h \rightarrow \Pi_k H_h =: H_{hh} : \Omega \rightarrow \mathbb{R}^3$$

where Π_k is some polynomial interpolant of order k . Now, the output E_{hh} becomes the input f_h for the heat equation. Here, we have at least the following two options for selecting a heat equation input f based on E_{hh} .

1. The final (instantaneous) state of the field: $f_{h1}(x, t) = \sigma_h(x, t)|E_{hh}(x, t)|^2$
2. The average of the field over the past period: $f_{h2}(x, t) = \sigma_h(x, t) \left(\oint_{t-T}^t |E_{hh}(x, t)| \right)^2$

Note that the conductivity is assumed constant throughout an EM simulation step, and thus can be pulled out of the integral. Now, most (apriori) error estimates involving the source term of the heat equation involve evaluating the input in some norm of the form

$$\|\cdot\|_{L^p L^q} := \|\cdot\|_{L^q(0, t_{\text{final}}; L^p(\Omega))} := \left(\int_0^{t_{\text{final}}} \|\cdot\|_{L^p(\Omega)}^q \right)^{\frac{1}{q}} = \left(\int_0^{t_{\text{final}}} \left(\int_{\Omega} \|\cdot\|^p \right)^{\frac{q}{p}} \right)^{\frac{1}{q}}$$

The argument that comes in deals with the difference $f - f_h$, where f is the analytical source term. In our case however, this would be the “analytical” output of the EM solver, i.e. the analytical solution, whose closed form is usually impossible to find for problems involving inhomogeneous media.

The best form one can hope to arrive at, is by using $L^1 L^1$ norms, comparing

$$I_1 := \int_0^t \int_{\Omega} f_{h1} \quad \text{vs.} \quad \int_0^t \int_{\Omega} f_{h2} := I_2$$

In this case, one can formulate a very concrete statement. Let us start with I_1 :

$$I_1 = \int_{\Omega} \int_0^t f_{h1} = \int_{\Omega} \int_0^t \sigma_h(x, t) |E_{hh}(x, t)|^2$$

Once more, assuming $\sigma_h(x, t)$ stays constant throughout an EM simulation, we have:

$$I_1 = \int_{\Omega} \sigma_h(x) \int_0^t |E_{hh}(x, t)|^2$$

For the integral which involves averaging over the last period I_2 the following holds:

$$I_2 = \int_0^t \int_{\Omega} \sigma_h(x) \left(\frac{2}{\pi} \|E_{hh}(x, t)\|_{L^\infty(t, t-T)} \right)^2$$

where we denote t_{final} by t for ease of notation. Since $[0, t]$ includes several periods, we can observe that $\|E_{hh}(x, t)\|_{L^\infty(t-T, t)} = \|E_{hh}(x, t)\|_{L^\infty(0, t)}$ due to periodicity.

$$I_2 = \int_0^t \int_{\Omega} \sigma_h(x) \frac{4}{\pi^2} \|E_{hh}(x, t)\|_{L^\infty(t, t-T)}^2$$

One further assumption that we can make now, which is easy to enforce, is that $t = kT$, for some $k \in \mathbb{N}$ (where T is the period of the source). We define the following two integrals, and check pointwise in space:

$$i_1(x) := \sigma_h(x) \int_0^t |E_{hh}(x, t)|^2 = \sigma_h(x) k \int_0^T |E_{hh}(x, t)|^2$$

$$i_2(x) := \sigma_h(x) \int_0^t \left(\oint_{t-T}^t |E_{hh}(x, t)| \right)^2 = \sigma_h(x) k \int_0^T \left(\oint_0^T |E_{hh}(x, t)| \right)^2$$

So what we are left to compare is:

$$\frac{i_1(x)}{\sigma_h(x)k} \quad \text{vs.} \quad \frac{i_1(x)}{\sigma_h(x)k} \Leftrightarrow \int_0^T |E_{hh}(x, t)|^2 \quad \text{vs.} \quad \int_0^T \left(\oint_0^T |E_{hh}(x, t)| \right)^2$$

Now using the fact that $|E_{hh}(x, t)|$ is of the form $\|E_{hh}(x, t)\|_{L^\infty(0, T)} |\sin(\omega t)|$, since we assumed a (stabilized) periodic behavior in the foreseeable past of the EM simulation, we are left to compare:

$$\begin{aligned} \|E_{hh}(x, t)\|_{L^\infty(0, T)} \int_0^{2\pi} |\sin(t)|^2 dt &\quad \text{vs.} \quad \|E_{hh}(x, t)\|_{L^\infty(0, T)} \int_0^{2\pi} \left(\oint_0^{2\pi} |\sin(t)| \right)^2 \\ \int_0^{2\pi} |\sin(t)|^2 dt &= \pi \quad \text{vs.} \quad \frac{8}{\pi} = \int_0^{2\pi} \left(\frac{2}{\pi} \right)^2 = \int_0^{2\pi} \left(\oint_0^{2\pi} |\sin(t)| \right)^2 \\ \pi^2 > 8 &\Leftrightarrow I_1 > I_2 \Leftrightarrow \int_0^t \int_\Omega f_{h1} > \int_0^t \int_\Omega f_{h2} \end{aligned}$$

So in conclusion, $\|f_{h1}\|_{L^1 L^1} > \|f_{h2}\|_{L^1 L^1}$, but this does not reveal much about terms of the form $\|f - f_{h1}\|_{L^p L^q}$. Let us have a look at an apriori error estimate for FDTD. Let $\mathbf{E}$ be the analytical solution of the FDTD Maxwell equations (in vacuum). Let $\mathbf{E}_h$ be the discrete (defined pointwise at grid points) solution.

Theorem 3 (Monk, Süli, 1992 [29]). *For $\mathbf{E}$ and $\mathbf{H}$ in C^3 , $\mathbf{H}_t \in C^2$, and all derivatives continuous in time, then $\forall T > 0, \exists C = C(T)$ s.t.*

$$\|E - E_h\|_E + \|H - H_h\|_H \leq C(T)h^2$$

The norms are defined in the case of evenly spaced grids as follows:

$$\begin{aligned} \|E - E_h\|_E^2 &:= \sum_i h^3 ((E_x(x_i) - E_{xh}(x_i))^2 + (E_y(x_i) - E_{yh}(x_i))^2 + (E_z(x_i) - E_{zh}(x_i))^2) \\ &\Leftrightarrow \left(\sum_i h^3 \|E_i - E_{hi}\|_{l^2}^2 \right)^{\frac{1}{2}} + \left(\sum_i h^3 \|H_i - H_{hi}\|_{l^2}^2 \right)^{\frac{1}{2}} \leq Ch^2 \end{aligned} \quad (79)$$

This result is presented in the discrete L^2 norm, but one would expect that it holds in all equivalent norms, for example any combination of $p, q \in \{1, 2, \infty\}$.

Note that the above is basically a statement about pointwise values of $\mathbf{E}$ and $\mathbf{E}_h$. In other words, the discrete L^2 error estimate is built by projecting on a finite dimensional space with locally constant basis functions $\varphi_i \equiv \frac{1}{8}$, such that integrating them over their support yields h^3 for a homogeneous grid.

With this in mind, if we want to look at “true” L^2 error estimates, we have to use the full information of $\mathbf{E}$ and interpolate somehow the pointwise values of $\mathbf{E}_h$, in order to be able to integrate the norm of the difference everywhere.

Let Π_k be an interpolation operator using basis functions of degree k , i.e.

$$\Pi_k : \mathbb{R}^N \rightarrow L^2(\Omega) \text{ (some } L^p \text{ space, when the values are bounded)}$$

Then what we want to make a statement about, or relate the error estimate (79) to, is:

$$\|E - \Pi_k E_h\|_{L^2(\Omega)} =: \|E - E_{hh}\|_{L^2(\Omega)}$$

$$\|E - E_{hh}\|_{L^2}^2 = \int_{\Omega} \|E - \Pi_k E + \Pi_k E - E_{hh}\|_{l^2}^2 \stackrel{\Delta \text{ ineq.}}{\leq}$$

$$\stackrel{\Delta \text{ ineq.}}{\leq} \int_{\Omega} (\|E - \Pi_k E\|_{l^2} + \|\Pi_k E - E_{hh}\|_{l^2})^2 \stackrel{\text{am-gm}}{\leq} \int_{\Omega} 2 (\|E - \Pi_k E\|_{l^2}^2 + \|\Pi_k E - E_{hh}\|_{l^2}^2)$$

We now denote by “ Π_k error” the (local) interpolation error given by $\|E - \Pi_k E\|_{l^2}^2$.

$$\begin{aligned} &= \int_{\Omega} 2 (\Pi_k \text{ error} + \|\Pi_k(E - E_h)\|_{l^2}^2) = \int_{\Omega} 2 (\Pi_k \text{ error} + \|\Pi_k(E - E_h)\|_{l^2}^2) \\ &= 2\|\Pi_k \text{ error}\|_{L^2}^2 + 2 \int_{\Omega} \|\Pi_k(E - E_h)\|_{l^2}^2 \end{aligned} \quad (80)$$

So the last term in equation (80) is what we are interested in.

$$\int_{\Omega} \|\Pi_k(E - E_h)\|_{l^2}^2 = \|\|\Pi_k(E - E_h)\|_{l^2}\|_{L^2}^2 = \int_{\Omega} \sum_i \varphi_i \|(E_i - E_{hi})\|_{l^2}^2$$

(If $\varphi_i \equiv \frac{1}{8}$ locally, such that $\forall i \int_{\Omega} \varphi_i = h^3$)

$$= \sum_i \int_{\Omega} \varphi_i \|(E - E_h)\|_{l^2}^2 = \sum_i \int_{\Omega} \varphi_i \|(E_i - E_{hi})\|_{l^2}^2 = \sum_i h^3 \|(E_i - E_{hi})\|_{l^2}^2$$

The right-hand side is exactly the term from the error estimate (79). So in summary,

$$\begin{aligned} \|E - E_{hh}\|_{L^2(\Omega)} &\leq (\Pi_k \text{ error}^2 + \|E - E_h\|_E^2)^{\frac{1}{2}} \\ \|E - E_{hh}\|_{L^2(\Omega)}^2 &\leq \Pi_k \text{ error}^2 + \|E - E_h\|_E^2 \stackrel{(16)}{\leq} \Pi_k \text{ error}^2 + Ch^4 \\ &\Leftrightarrow \|E - E_{hh}\|_{L^2(\Omega)}^2 \leq C_1 h^2 + C_2 h^4 \end{aligned}$$

since we expect a first order convergence rate for piecewise constant interpolants ([33] p. 346). Alternatively, if we choose piecewise *affine* φ'_i s that also integrate to h^3 , and such that the interpolation error is also second order, we obtain:

$$\Leftrightarrow \|E - E_{hh}\|_{L^2(\Omega)} \leq (C_1 + C_2)h^2$$

Therefore we observe that the number of degrees of freedom in choosing the interpolating functions only allow us accuracy of order up to 2, but the semidiscrete error is order 2 as well. So even if we could increase the accuracy of the interpolation, it would be dominated by the other term.

To conclude, there are two reasons why this error analysis cannot reveal meaningful error information or improved estimates in usual cases. Firstly, one needs to know the analytical solution of the EM problem. Secondly, information for this particular form of source term is not easily extractable in norms other than $L^1 L^1$. This is severely limiting because most heterogeneous electromagnetic problems do not have a closed form analytical solution, and most error estimates are done in norms belonging to Hilbert spaces, i.e. $L^2 L^2$.

Chapter 5

Numerical Experiments

In this chapter we will describe various discretized scenarios that should shed light on some numerical aspects which were discussed so far in the continuous context.

5.1 Truncation error

In the present section we will look at the convergence of the numerical scheme. In order to do this, we shall need a reference analytical solution. This can be most easily achieved by working in vacuum, or air, since there are readily available analytical solutions in quite a few sources (the clearest of which we consider [6]).

The simplest way to construct an error rate test is to try and replicate the field produced by a dipole. As we remember from Section 3.2.1, the simplest ways in which the field can be reproduced is with hard and soft point sources. Furthermore, since we will be working in vacuum, we would expect total reflection to take place within the computational domain, without any absorbing boundary condition.

To this end we shall use the UPML presented earlier. Now, the Yee scheme is quoted as having a second order convergence rate in space and in time, which is in 2D [12]:

$$\|E - E_h\| + \|H - H_h\| \leq C(\Delta_x^2 + \Delta_y^2 + \Delta_t^2) \quad (81)$$

where Δ_x is the spatial discretization step, and Δ_t is the temporal discretization step. The precise norm $\|\cdot\|$ is yet to be defined, but we expect that in theory all norms should be equivalent (for finite dimensional spaces of the same dimension). For example, we should obtain the same order of convergence in space in any of the following norms:

$$\begin{aligned} \|\cdot\|_{L^1(\Omega)} &:= \int_{\Omega} |E_{\text{analytic}} - \Pi_k E_{\text{discrete}}| \\ \|\cdot\|_{L^2(\Omega)} &:= \left(\int_{\Omega} |E_{\text{analytic}} - \Pi_k E_{\text{discrete}}|^2 \right)^{\frac{1}{2}} \\ \|\cdot\|_{L^\infty(\Omega)} &:= \max_{\Omega} |E_{\text{analytic}} - \Pi_k E_{\text{discrete}}| \end{aligned}$$

where we need to perform some interpolation process as in Section 4.3 to evaluate the discrete values at non-grid points. These spatial norms will of course have to be coupled with some method of incorporating behavior in time, such as:

$$\|\cdot\|_{L^p(\Omega)L^q(t_1,t_2)} := \left(\int_{t_1}^{t_2} \left(\left(\int_{\Omega} \|\cdot\|^p dx \right)^{\frac{1}{p}} \right)^q dt \right)^{\frac{1}{q}}$$

In order to quantify the truncation error in vacuum, we need to set up a source, say a point hard E_z source, with a dipole moment given by a function of our choice. Two of the most popular dipole moments are the sine, and the Gaussian pulse. Let us first discuss the case of a sine wave excitation.

There are several issues to be raised when trying to evaluate the truncation error with a sinusoidal wave:

1. If we initialize the domain to zero, then the turn-on discontinuity at $t = 0$ causes a nonphysical pulse (often called *transient*, since it is only temporary) that significantly deviates the numerical solution from the analytical one. We then have to wait for a few wavelengths to pass through until the behavior starts to align to the expected one. This however means that we require one of the following: an absorbing boundary condition to eliminate this transient, or a large enough computational domain such that the reflected transient does not return too early.
2. If we simulate an infinite domain, and evaluate the error within a finite volume around a periodic source, we would expect to eventually reach periodic behavior within this finite volume. This can be achieved by either a very large domain (in relative terms to the wavelength), or through an absorbing boundary condition, such as a PML. Otherwise, the reflection with the computational domain's outer walls would interfere with the fields we wish to quantify.
3. One way to mitigate this turn-on discontinuity is to smoothen the jump, with the aid of a Gaussian pulse for example. However, this introduces a quasi-static field that results in a larger final error after stability is reached. Similarly, using a soft point source or introducing the pulse via a TFSF boundary results in a smaller turn-on error than the hard source. However it also produces a larger final error in the periodic state.
4. Finally, one would wish to obtain a wave that is at least reasonably resolved by the grid; in most applications, this requires at least 20 spatial discretization points per wavelength. Since waiting several wavelengths without seeing reflections would imply an impractically large computational domain, most of the time one chooses to use a PML (or other absorbing boundary conditions). This allows for a significantly smaller domain, and a faster testing cycle. However, this also means that in reality, when one evaluates $\|E - E_{\text{analytic}}\|$ numerically, one is actually looking at the *combined error* of both the truncation and PML. Furthermore, one should note that these two error sources can interact constructively or destructively, also inhomogeneously so.

Since it would be practically impossible to completely separate these two error influences within a scenario containing a PML, the best one could hope for is to maintain one of the errors constant somehow while varying the other, when looking for convergence rates.

The common way to check for convergence rate with respect to some quantity, is to vary it while “keeping everything else constant”. This is usually fairly straightforward to define,

however it is important to note that for equations involving waves, the quantity of interest is not just the discretization step, but its ratio to an intrinsic physical parameter of the wave, namely its wavelength. In this context, one usually defines resolution in terms of *points per wavelength*. Hereon we abbreviate points per wavelength as *ppw*.

Thus, one way to check convergence with respect to spatial discretization refinements, is to take a wave of a given frequency and then refine the grid. Of course, one needs to take special care for maintaining certain physical invariants constant, such as the volume in which the error is evaluated, the distance from the source and the PML, and so on. However, one significant disadvantage of this straightforward approach is that computational time increases cubically with increasing refinements.

Since the invariant of interest is the number of points per wavelength, one could instead maintain a constant resolution, and just vary the wavelength of the source wave. This would also eliminate concerns about maintaining exact ratios of volumes when dealing with integer divisions and so on. Moreover, only varying the frequency of the source would in general reduce the overhead, in terms of defining and maintaining constant physical invariants in the problem. The issue that would have to be treated with care is evaluating the error norm over the same (absolute) time interval, and over the same relative (to the wavelength) volume regions.

The latter issue would however require us to adjust the absolute size of the grid, returning us to cubic size and time increases. In Figure [29], we qualitatively illustrate the geometric setting of our further experiments.

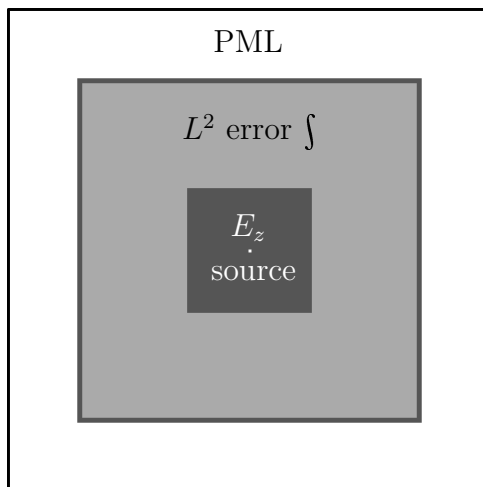


Figure 29: Partition of computational grid for hard point source scenario, 2D slice.

We shall initially run the simulations for ten periods of the sinusoidal source, in order to evaluate results over the same fixed amount of time. Afterwards, we will average the L^2 error in time over the final three periods, to iron out the oscillations caused by the source:

$$\text{Error}_{L^2}(\text{ppw}) := \int_{t_{\text{final}}-3T}^{t_{\text{final}}} \|\mathbf{E} - \mathbf{E}_{\text{analytic}}\|_{L^2(\Omega)}$$

where T is the period for a given sampling rate (ppw), and $\mathbf{E}_{\text{analytic}}$ is given by (32). Since the temporal discretization is not varied, evaluating the convergence in this norm should produce the same result as the non-averaged (in time) version.

We also have to adjust the final L^2 error by the square root of the integrated volumes' ratio (since the L^2 norm scales with $\sqrt{\text{integrated volume}}$), which varies slightly due to the integer divisions involved. Furthermore, as we can infer from the section on sources and currents (3.2), if we define a hard source in one Yee cell, the total current contained inside (and thus the amplitude of the produced fields) scales with $\Delta_x \Delta_y \Delta_z$. In order to account for this, one has to scale either the amplitude of the source, or the L^2 norms.

We shall run each simulation until the L^2 error has stabilized, and then use those final values. We will then assume that the final error values remain constant until the latest time point we are considering. Finally, we estimate the slope of the error decay with NumPy's polyfit function [31], which performs a linear fit within the log – log plot. In Table [1], we present the stabilized L^2 norms of the errors, together with all relevant parameters and a piecewise slope evaluation. In Figure [30] we present the evolution in time of the errors.

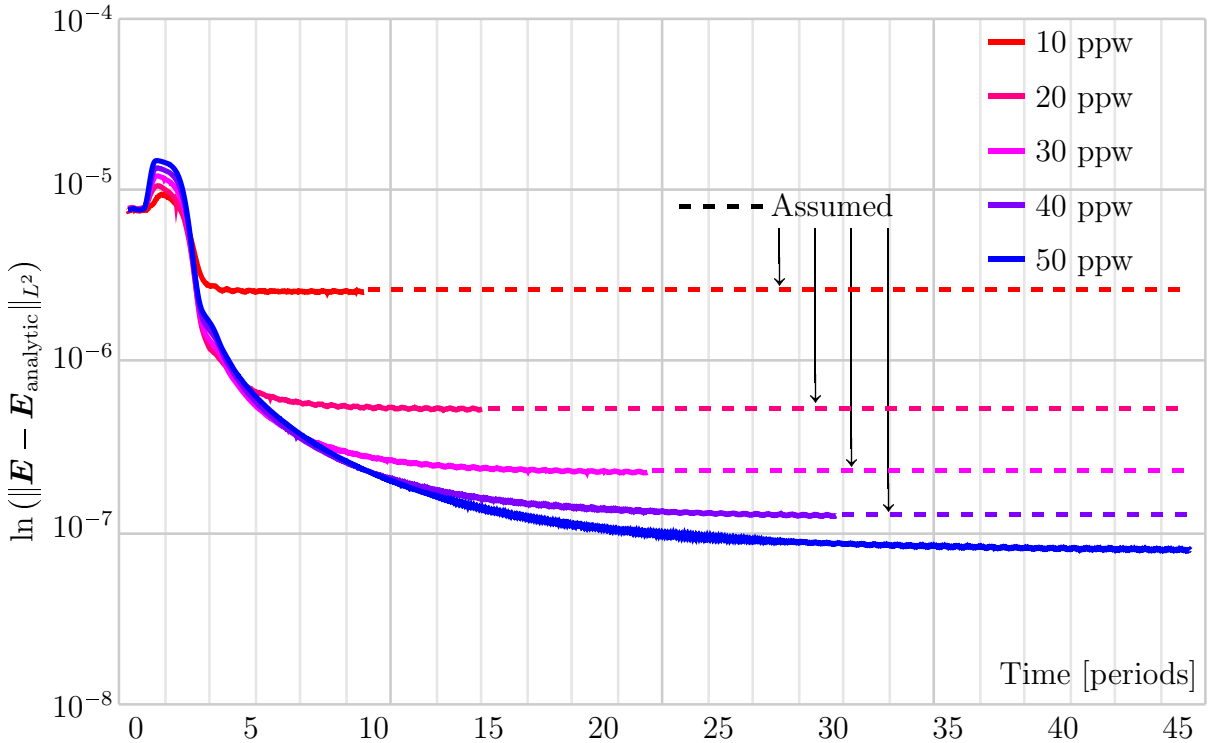
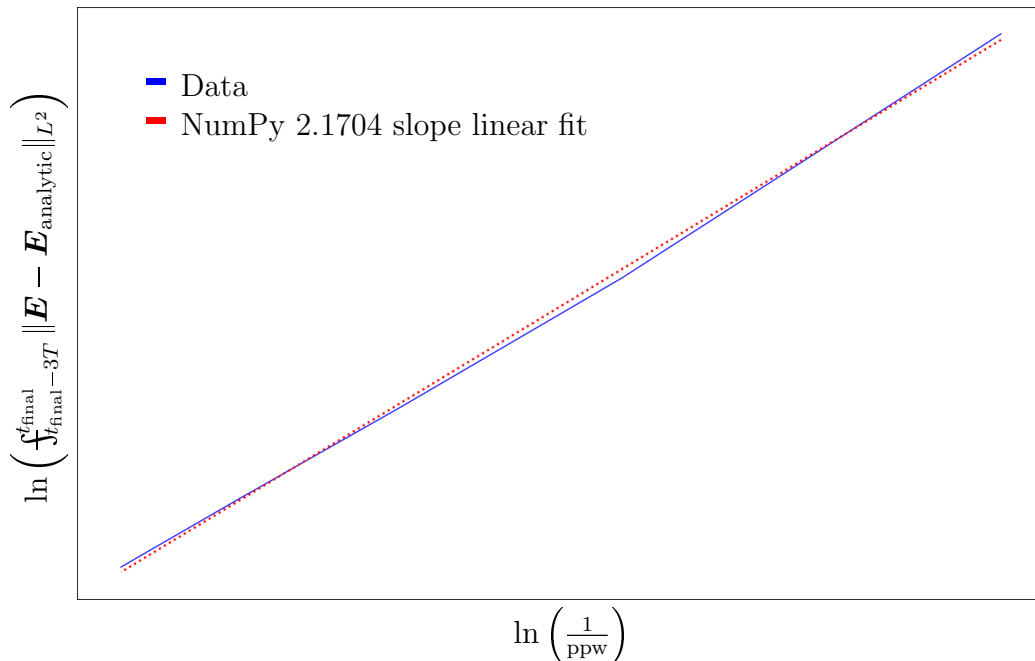


Figure 30: L_2 error over a volume and several resolutions, with predicted behavior.

In Figure [30], we display with a dashed line the assumed behavior past what is simulated in order to evaluate the $L^2 L^2$ norms over the same intervals in time. Since we were varying the spatial discretization but keeping the temporal one constant, Δ_x changes, but Δ_t does not. We specify the resulting Courant ratio $S_c = \frac{c\Delta_t}{\Delta_x}$ in Table [1], relative to the upper limit. The first column displays the volume $v(S_c/S_{c,\max})$ in which we integrate the error, and for the fourth column we adjust the error by $\sqrt{v(0.125)/v(S_c/S_{c,\max})}$. In the final column we evaluate the slope between the current error and the next, in a log – log scale.

Error $\int$ volume	$S_c/S_{c,\max}$	λ/Δ_h	(adjusted) Average L^2 error	Slope w.r.t. next
$2.70 \cdot 10^{-4}$	0.125	10	$2.610 \cdot 10^{-6}$	2.31
$2.85 \cdot 10^{-4}$	0.250	20	$5.259 \cdot 10^{-7}$	2.09
$2.88 \cdot 10^{-4}$	0.375	30	$2.249 \cdot 10^{-7}$	2.04
$2.89 \cdot 10^{-4}$	0.500	40	$1.252 \cdot 10^{-7}$	2.07
$2.90 \cdot 10^{-4}$	0.625	50	$7.885 \cdot 10^{-8}$	

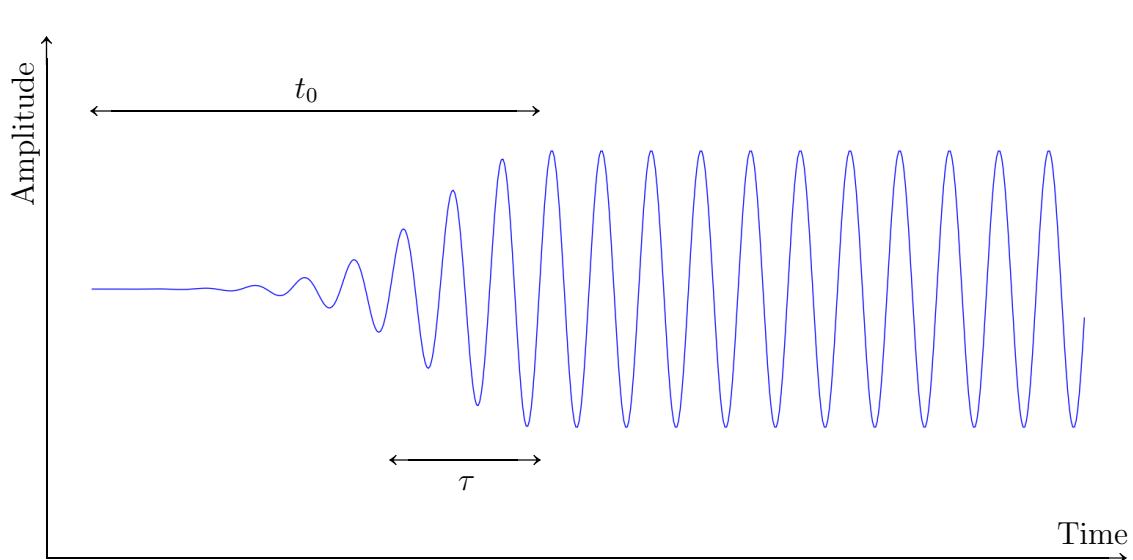
Table 1: Error produced by varying λ/Δ_h .

Figure 31: Convergence rate of L_2 error.

In Figure [31], we display *polyfit*'s [31] estimate of the slope in the log-log plot, which yields 2.17045. This fits our expectation of second-order convergence. We shall now discuss ways to mitigate the turn-on discontinuity, whose influence can be observed in Figure [30]. A first idea would be to ramp up the amplitude of the hard sine (of angular frequency $\omega = 2\pi f$) with a Gaussian pulse, until it reaches the full amplitude of unity. Consider the following hard source:

$$E_z(t) = \begin{cases} \sin(\omega t) \exp\left(-\left(\frac{t-t_0}{\tau}\right)^2\right), & t < t_0 \\ \sin(\omega t), & t \geq t_0 \end{cases}$$

One can define the so-called *width* τ and *delay* t_0 of the Gaussian in terms of the period of the sinusoidal source, for example as $t_0 = \frac{m}{f}$, $\tau = \frac{n}{f}$, for two arbitrary integers $m, n \in \mathbb{N}$ satisfying $m > n$. This ramping is illustrated in Figure [32].

Figure 32: Amplitude ramping for sine wave for $m = 9$, $n = 3$.

Let us check how this approach influences the evolution of the L^2 error versus the non-ramped version, for the 20 ppw scenario.

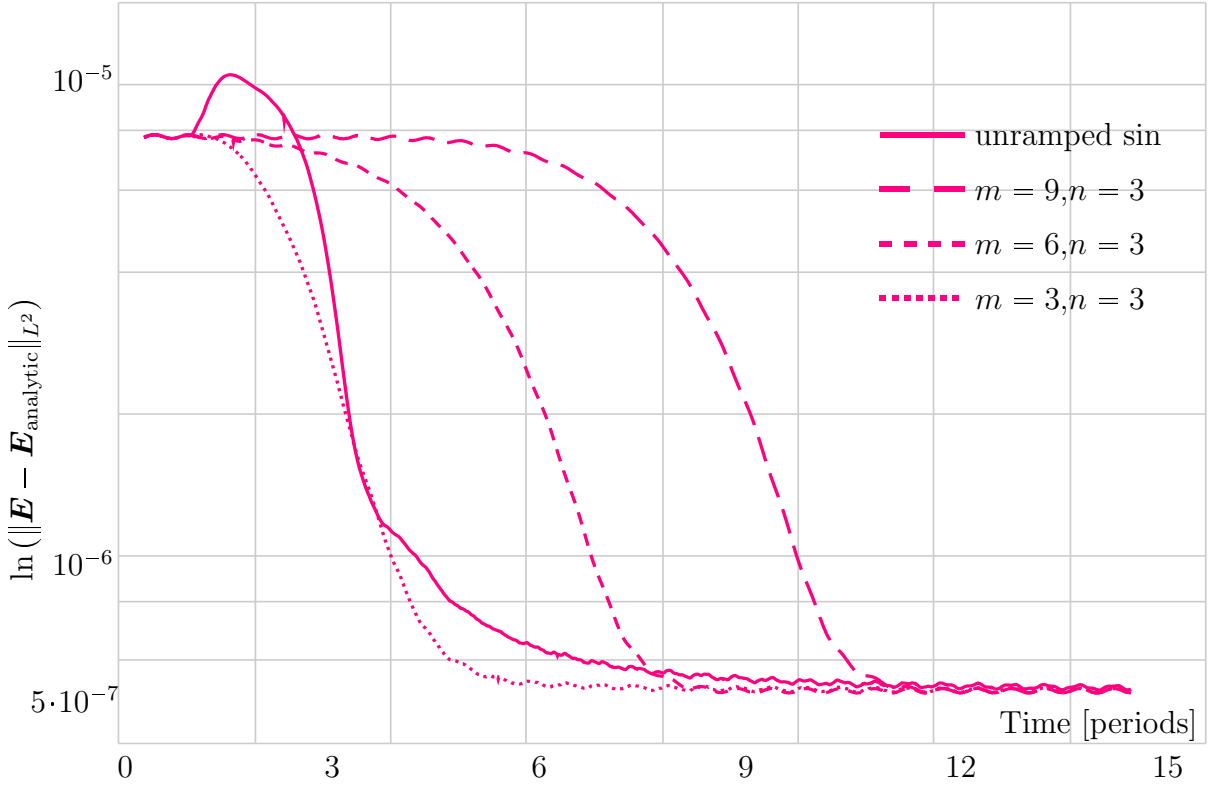


Figure 33: L_2 error evolution in time.

Figure [33] illustrates the expected behavior. Any turn-on discontinuities have a very small amplitude, thus they do not pollute the solution much. Figure [34] zooms in on the final three periods, and we observe that the error stabilizes at a very slightly lower error than the unramped scenario, since there is no large initial spike that has to be absorbed.

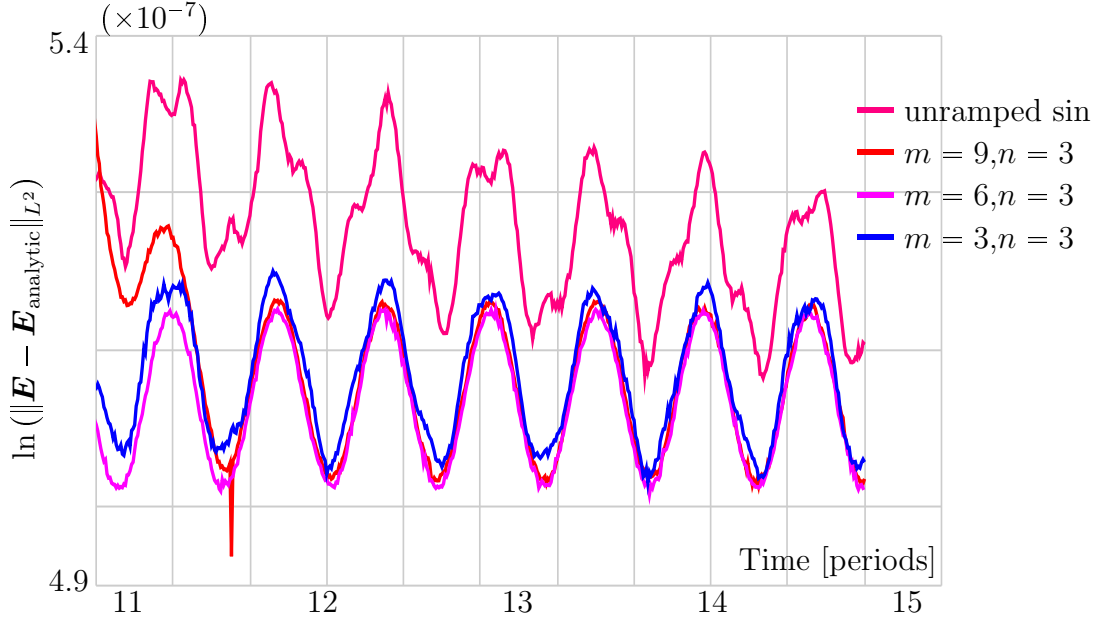


Figure 34: L_2 error evolution in time, last three periods.

Overall, this ramping can save us somewhere in the range of three to six periods worth of simulation time, before reaching (approximately) the same stabilized error.

Now, let us analyze convergence with respect to the temporal discretization. We use a spatial discretization of 20 ppw, and keep all quantities constant except Δ_t , or equivalently, the Courant number. In terms of physically relevant quantities, we are in essence varying the number of *points per period* (ppp), and discretely $\lceil \frac{T}{\Delta_t} \rceil$, where T is the period of the source. The resulting changes in $L^2 L^2$ error are displayed in Table [2].

$S_c/S_{c,\max}$	$\lceil \frac{T}{\Delta_t} \rceil$	λ/Δ_h	Average L^2 error	Slope w.r.t. next
1.00	35	20	$4.8819 \cdot 10^{-7}$	-0.18
0.75	47	20	$5.1483 \cdot 10^{-7}$	-0.12
0.50	70	20	$5.4092 \cdot 10^{-7}$	-0.03
0.25	139	20	$5.5305 \cdot 10^{-7}$	

Table 2: Error produced by varying T/Δ_t .

We see that the error does not decrease, and furthermore that it even increases when decreasing Δ_t . This is surprising, despite the known fact that certain errors actually increase with decreasing Courant number, such as the numerical dispersion error [43]. However, if we have a second look at (81), we note that this is a coarse estimation, and clearly so due to the discrepancy in units of the spatial and temporal discretization parameters. To be consistent with respect to units, it should read as:

$$\|E - E_h\| + \|H - H_h\| \leq C_1(\Delta_x^2 + \Delta_y^2 + \Delta_z^2) + C_2\Delta_t^2$$

We know that if we enforce the Courant condition in 3D, this would turn into

$$\|E - E_h\| + \|H - H_h\| \leq C_1(\Delta_x^2 + \Delta_y^2 + \Delta_z^2) + C_2\frac{\Delta_x^2}{3c^2}$$

where $c = 2.99792458 \cdot 10^8 \frac{m}{s}$ is the speed of light in vacuum. Let us find the exact constants in the error estimate, to get an idea of the orders of magnitude involved, and whether one coefficient is much larger than the other. We start by performing a Taylor series expansion with truncation for all derivatives involved in Ampère's Law (2b). Denote by $\partial_{t,h}$ the discrete finite difference operator

$$(\partial_{t,h}f)(t) := \frac{f(t + \frac{\Delta_t}{2}) - f(t - \frac{\Delta_t}{2})}{\Delta_t}$$

We also define the discrete curl operator $\nabla_h \times (\cdot)$ for a vector field $\mathbf{V} = (V_x, V_y, V_z)$:

$$(\nabla_h \times \mathbf{V}) := \begin{pmatrix} \frac{V_z(x, y + \frac{\Delta_y}{2}, z) - V_z(x, y - \frac{\Delta_y}{2}, z)}{\Delta_y} - \frac{V_y(x, y, z + \frac{\Delta_z}{2}) - V_y(x, y, z - \frac{\Delta_z}{2})}{\Delta_z} \\ \frac{V_x(x, y, z + \frac{\Delta_z}{2}) - V_x(x, y, z - \frac{\Delta_z}{2})}{\Delta_z} - \frac{V_z(x + \frac{\Delta_x}{2}, y, z) - V_z(x - \frac{\Delta_x}{2}, y, z)}{\Delta_x} \\ \frac{V_y(x + \frac{\Delta_x}{2}, y, z) - V_y(x - \frac{\Delta_x}{2}, y, z)}{\Delta_x} - \frac{V_x(x, y + \frac{\Delta_y}{2}, z) - V_x(x, y - \frac{\Delta_y}{2}, z)}{\Delta_y} \end{pmatrix}$$

We have suppressed the arguments on the LHS for typesetting purposes. We will also shorten $\mathbf{E}(x, y, z, t)$ as $\mathbf{E}_{x,y,z}^t$ in the following two equations. Using Taylor's Theorem with truncation at third order terms, and vector notation to show applicability to all three vector components, we obtain for some $\tau_1 \in [t, t + \frac{\Delta_t}{2}]$, $\tau_2 \in [t - \frac{\Delta_t}{2}, t]$:

$$\mathbf{E}\left(x, y, z, t + \frac{\Delta_t}{2}\right) = \mathbf{E}_{x,y,z}^t + \frac{\Delta_t}{2} \frac{\partial}{\partial t} \mathbf{E}_{x,y,z}^t + \frac{\Delta_t^2}{8} \frac{\partial^2}{\partial t^2} \mathbf{E}_{x,y,z}^t + \frac{\Delta_t^3}{48} \frac{\partial^3}{\partial t^3} \mathbf{E}(x, y, z, \tau_1)$$

$$\mathbf{E}\left(x, y, z, t - \frac{\Delta_t}{2}\right) = \mathbf{E}_{x,y,z}^t - \frac{\Delta_t}{2} \frac{\partial}{\partial t} \mathbf{E}_{x,y,z}^t + \frac{\Delta_t^2}{8} \frac{\partial^2}{\partial t^2} \mathbf{E}_{x,y,z}^t - \frac{\Delta_t^3}{48} \frac{\partial^3}{\partial t^3} \mathbf{E}(x, y, z, \tau_2)$$

Subtracting the last two equations, we obtain the truncation error of the centered stencil.

$$\frac{\mathbf{E}(x, y, z, t + \frac{\Delta_t}{2}) - \mathbf{E}(x, y, z, t - \frac{\Delta_t}{2})}{\Delta_t} = \frac{\partial}{\partial t} \mathbf{E} + \frac{\Delta_t^2}{48} \frac{\partial^3}{\partial t^3} (\mathbf{E}(x, y, z, \tau_1) + \mathbf{E}(x, y, z, \tau_2))$$

Similarly, we obtain the same estimate for the spatial derivatives. For $w \in \{x, y, z\}$, and some $\xi_{w1} \in [w, w + \frac{\Delta_w}{2}]$, $\xi_{w2} \in [w - \frac{\Delta_w}{2}, w]$, we obtain

$$\frac{\mathbf{H}(x + \frac{\Delta_x}{2}, y, z, t) - \mathbf{H}(x - \frac{\Delta_x}{2}, y, z, t)}{\Delta_x} = \frac{\partial}{\partial x} \mathbf{H} + \frac{\Delta_x^2}{48} \frac{\partial^3}{\partial x^3} (\mathbf{H}(\xi_{x1}, y, z, t) + \mathbf{H}(\xi_{x2}, y, z, t))$$

$$\frac{\mathbf{H}(x, y + \frac{\Delta_y}{2}, z, t) - \mathbf{H}(x, y - \frac{\Delta_y}{2}, z, t)}{\Delta_y} = \frac{\partial}{\partial y} \mathbf{H} + \frac{\Delta_y^2}{48} \frac{\partial^3}{\partial y^3} (\mathbf{H}(x, \xi_{y1}, z, t) + \mathbf{H}(x, \xi_{y2}, z, t))$$

$$\frac{\mathbf{H}(x, y, z + \frac{\Delta_z}{2}, t) - \mathbf{H}(x, y, z - \frac{\Delta_z}{2}, t)}{\Delta_z} = \frac{\partial}{\partial z} \mathbf{H} + \frac{\Delta_z^2}{48} \frac{\partial^3}{\partial z^3} (\mathbf{H}(x, y, \xi_{z1}, t) + \mathbf{H}(x, y, \xi_{z2}, t))$$

With this knowledge, let us plug in the Taylor expansions from above into Ampère's Law, and move all differential operators to the left-hand side. Let us also define the coefficients $\mathbf{C}_{\partial x H} := \frac{\partial^3}{\partial x^3} (\mathbf{H}(\xi_{x1}, y, z, t) + \mathbf{H}(\xi_{x2}, y, z, t))$, $\mathbf{C}_{\partial y H} := \frac{\partial^3}{\partial y^3} (\mathbf{H}(x, \xi_{y1}, z, t) + \mathbf{H}(x, \xi_{y2}, z, t))$, $\mathbf{C}_{\partial z H} := \frac{\partial^3}{\partial z^3} (\mathbf{H}(x, y, \xi_{z1}, t) + \mathbf{H}(x, y, \xi_{z2}, t))$, $\mathbf{C}_{\partial t E} := \frac{\partial^3}{\partial t^3} (\mathbf{E}(x, y, z, \tau_1) + \mathbf{E}(x, y, z, \tau_2))$.

$$\varepsilon \left(\frac{\partial}{\partial t} \mathbf{E} - \partial_{t,h} \mathbf{E} \right) - (\nabla \times \mathbf{H} - \nabla_h \times \mathbf{H}) = \frac{1}{48} \begin{pmatrix} \Delta_y^2 C_{\partial y H z} - \Delta_z^2 C_{\partial z H y} - \varepsilon \Delta_t^2 C_{\partial t E x} \\ \Delta_z^2 C_{\partial z H x} - \Delta_x^2 C_{\partial x H z} - \varepsilon \Delta_t^2 C_{\partial t E y} \\ \Delta_x^2 C_{\partial x H y} - \Delta_y^2 C_{\partial y H x} - \varepsilon \Delta_t^2 C_{\partial t E z} \end{pmatrix} \quad (82)$$

Putting this into words, what we have found is the *truncation error of Ampère's Law*. We can perform the same steps to obtain the analogue result for Faraday's Law.

$$\mu \left(\frac{\partial}{\partial t} \mathbf{H} - \partial_{t,h} \mathbf{H} \right) + (\nabla \times \mathbf{E} - \nabla_h \times \mathbf{E}) = \frac{1}{48} \begin{pmatrix} \Delta_z^2 C_{\partial z E y} - \Delta_y^2 C_{\partial y E z} - \mu \Delta_t^2 C_{\partial t H x} \\ \Delta_x^2 C_{\partial x E z} - \Delta_z^2 C_{\partial z E x} - \mu \Delta_t^2 C_{\partial t H y} \\ \Delta_y^2 C_{\partial y E x} - \Delta_x^2 C_{\partial x E y} - \mu \Delta_t^2 C_{\partial t H z} \end{pmatrix}$$

We need to take a few more steps in order to have an idea of the orders of magnitude. Let us assume that we are dealing with a plane wave in vacuum given by $\mathbf{E} = \mathbf{E}_0 \exp(\mathbf{k} \cdot \mathbf{r} - \omega t)$, $\mathbf{H} = \mathbf{H}_0 \exp(\mathbf{k} \cdot \mathbf{r} - \omega t)$, along the x -axis, such that $\mathbf{k} = (k_x, k_y, k_z) = (\frac{\omega}{c}, 0, 0)$. If we have a Courant number of $\frac{c \Delta_t}{\Delta_x} = \frac{1}{\sqrt{3}}$, and the electric field is polarized in the z -direction, and the magnetic field in the y -direction, we can rewrite (82) as follows:

$$\begin{aligned} \varepsilon_0 \left(\frac{\partial}{\partial t} \mathbf{E} - \partial_{t,h} \mathbf{E} \right) - (\nabla \times \mathbf{H} - \nabla_h \times \mathbf{H}) &= \frac{1}{48} \begin{pmatrix} 0 \\ 0 \\ \Delta_x^2 C_{\partial x H y} - \varepsilon_0 \Delta_t^2 C_{\partial t E z} \end{pmatrix} \\ \Leftrightarrow \text{LHS} &= \frac{1}{48} \begin{pmatrix} 0 \\ 0 \\ \Delta_x^2 (H_{y,xxx}(\xi_{x1}) + H_{y,xxx}(\xi_{x2})) - \varepsilon_0 \Delta_t^2 (E_{z,ttt}(\xi_{t1}) + E_{z,ttt}(\xi_{t2})) \end{pmatrix} \end{aligned}$$

Here we used a shortened notation where only the part of the argument differing from x, y, z, t was given, and f_{www} denotes the third partial derivative of f w.r.t. w . We now use the fact that in vacuum $|\mathbf{E}| = \eta_0 |\mathbf{H}|$, where $\eta_0 = \frac{1}{c\epsilon_0}$ is the impedance of free space.

$$\begin{aligned} \Leftrightarrow \text{LHS}_z &= \frac{1}{48} \left(\Delta_x^2 \frac{\omega^3}{c^3} (H_y(\xi_{x1}) + H_y(\xi_{x2})) - \epsilon_0 \frac{\Delta_x^2}{3c^2} (-\omega^3) (E_z(\xi_{t1}) + E_z(\xi_{t2})) \right) \\ \Leftrightarrow \text{LHS}_z &= \frac{1}{48} \left(\Delta_x^2 \frac{\omega^3}{c^3} (H_y(\xi_{x1}) + H_y(\xi_{x2})) - \epsilon_0 \frac{\Delta_x^2}{3c^2} (-\omega^3) \frac{1}{c\epsilon_0} (H_y(\xi_{t1}) + H_y(\xi_{t2})) \right) \\ \Leftrightarrow \text{LHS}_z &= \frac{\omega^3 \Delta_x^2}{48c^3} ((H_y(\xi_{x1}) + H_y(\xi_{x2})) + S_c^2 (H_y(\xi_{t1}) + H_y(\xi_{t2}))) \end{aligned}$$

We selected a Courant number $S_c = \frac{1}{\sqrt{3}}$ that ensures stability for arbitrary 3D propagation, however this scenario is essentially a 1D propagation, which means $S_c = 1$ would suffice. This implies that the truncation errors due to the spatial and temporal derivatives are in the same order of magnitude:

$$\Leftrightarrow \text{LHS}_z = \frac{\omega^3 \Delta_x^2}{48c^3} \left(\underbrace{H_y(\xi_{x1}) + H_y(\xi_{x2})}_{\partial x \text{ error}} + \underbrace{H_y(\xi_{t1}) + H_y(\xi_{t2})}_{\partial t \text{ error}} \right)$$

Let us now carry out the same process for Faraday's Law.

$$\begin{aligned} \mu_0 \left(\frac{\partial}{\partial t} \mathbf{H} - \partial_{t,h} \mathbf{H} \right) - (\nabla \times \mathbf{E} - \nabla_h \times \mathbf{E}) &= \frac{1}{48} \begin{pmatrix} \Delta_x^2 C_{\partial x E_z} & 0 \\ 0 & \mu_0 \Delta_t^2 C_{\partial t H_y} \end{pmatrix} \\ \Leftrightarrow \mathbf{LHS} &= \frac{1}{48} \begin{pmatrix} \Delta_x^2 (E_{z,xxx}(\xi_{x1}) + E_{z,xxx}(\xi_{x2})) & 0 \\ 0 & \mu_0 \Delta_t^2 (H_{y,ttt}(\xi_{t1}) + H_{y,ttt}(\xi_{t2})) \end{pmatrix} \\ \Leftrightarrow \text{LHS}_y &= \frac{1}{48} \left(\Delta_x^2 \frac{\omega^3}{c^3} \frac{1}{c\epsilon_0} (H_y(\xi_{x1}) + H_y(\xi_{x2})) - \mu_0 \frac{\Delta_x^2}{c^2} (-\omega^3) (H_y(\xi_{t1}) + H_y(\xi_{t2})) \right) \\ \Leftrightarrow \text{LHS}_y &= \frac{\omega^3 \Delta_x^2}{48c^2} \left(\frac{1}{c^2 \epsilon_0} (H_y(\xi_{x1}) + H_y(\xi_{x2})) + \mu_0 (H_y(\xi_{t1}) + H_y(\xi_{t2})) \right) \end{aligned}$$

However $c^2 = \frac{1}{\epsilon_0 \mu_0}$, thus:

$$\text{LHS}_y = \frac{\mu_0 \omega^3 \Delta_x^2}{48c^2} \left(\underbrace{H_y(\xi_{x1}) + H_y(\xi_{x2})}_{\partial x \text{ error}} + \underbrace{H_y(\xi_{t1}) + H_y(\xi_{t2})}_{\partial t \text{ error}} \right)$$

Once more, we find that the spatial and temporal truncation errors are also in the same order of magnitude for Faraday's Law. At this point, in order to advance further, one would need to translate these local equation-wide error estimates into global field error estimates. That is, to investigate the contribution of the spatial and temporal errors in $\|\mathbf{E} - \mathbf{E}_h\|$, $\|\mathbf{H} - \mathbf{H}_h\|$, or their sum. This was done using so-called *energy estimates* in the context of the semi-discrete equations by Monk and Süli [29]. However, Monk and Süli made use of the fact that the temporal derivative was not discretized. Due to time constraints, we shall depart from this topic and pronounce it as future work.

5.2 TFSF error

We now run a similar analysis to the one of the previous section, but this time with a TFSF surface, a cube, which introduces the energy into the grid. This TFSF surface will impose electric and magnetic currents J, M such that the fields produced by a point source at the middle of the grid are emanated. The grid is partitioned in two ways:

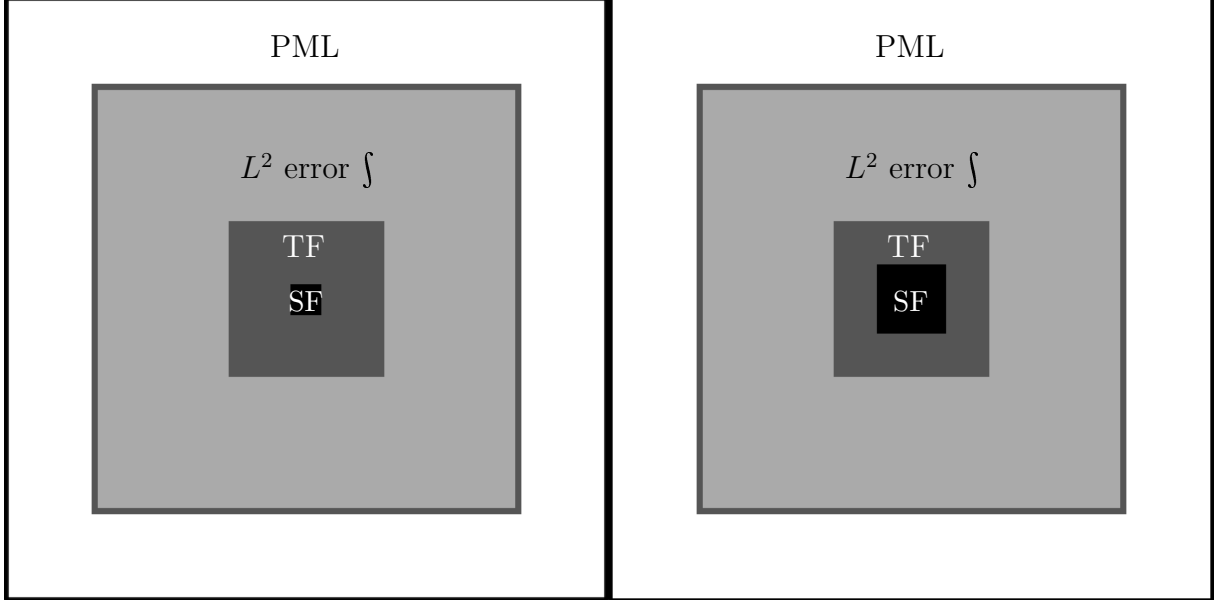


Figure 35: Partition of computational grid for TFSF source scenario, 2D slices.

where TF is the total-field region, and SF is the scattered-field region. In theory, the fields produced by the TFSF boundary currents cancel out inside the SF region, however in practice that is not true, as we will see in a moment. These fields pollute the solution and produce a higher final error. We will verify what happens when we increase the size of the SF region, and thus the TFSF interface on which we allocate currents. What is described in literature as *leakage* of the TFSF, namely the error introduced by this method, which in our case is the lack of cancellation inside the SF region, increases with the size of the SF region.

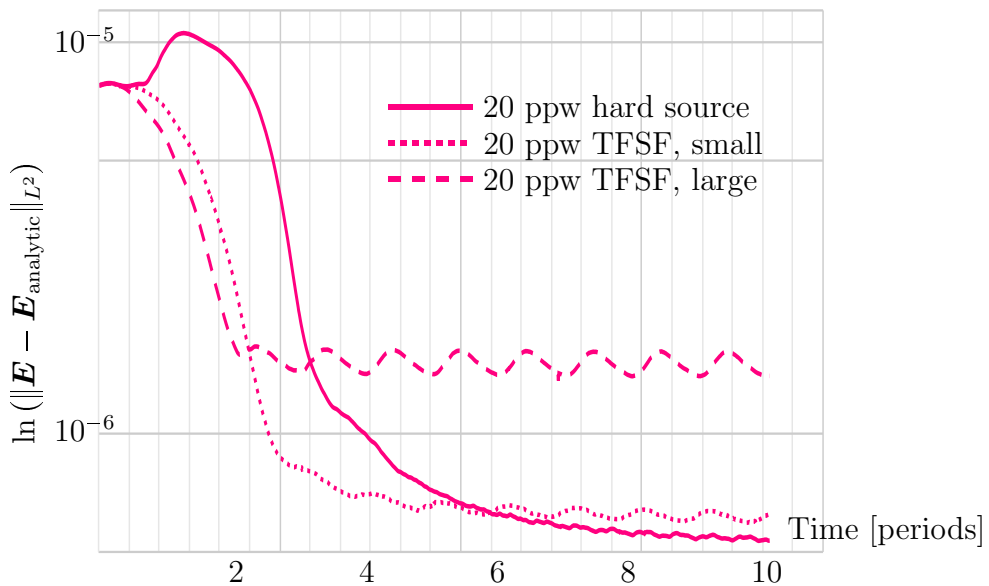


Figure 36: TFSF vs. hard point source errors.

5.3 TFSF plane wave

In this section we shall present an example scenario of the plane wave introduced by a TFSF surface, as illustrated in Figure [37]. We use a grid of size $97 \times 97 \times 97$, where an outer layer of thickness $N_{\text{PML}} = 14$ is defined as a UPML. The innermost cube inside is designed as the total field (TF) volume.

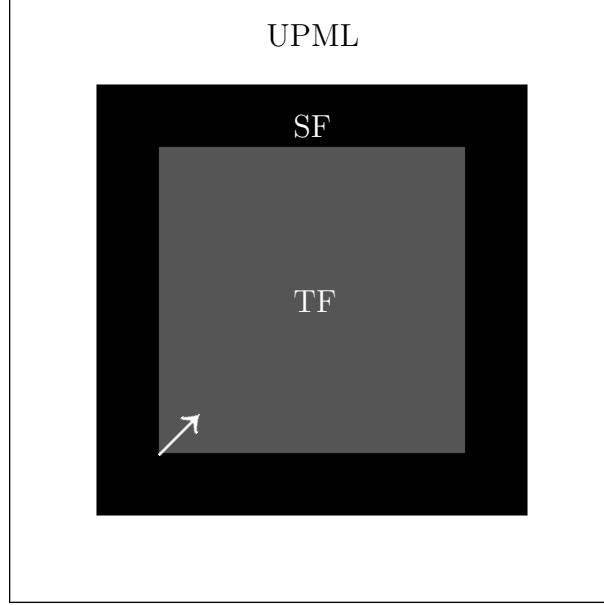


Figure 37: TFSF plane wave setup, 2D slice.

A Gaussian pulse is inserted from the bottom left corner of the TF zone, in the diagonal direction, as shown by the white arrow in Figure [37]. We shall present the visualization from this corner, and note that the contrast of the images is scaled to the range of values (hence the variation). In Figure [38], we plot the maximum value of the norm over time, with the note that the wave has exited the TF zone by time step 200, and higher values are shown in darker colors, due to printing considerations. In Figure [39] we shall visualize the norm of the electric field through a 2D slice in the domain.

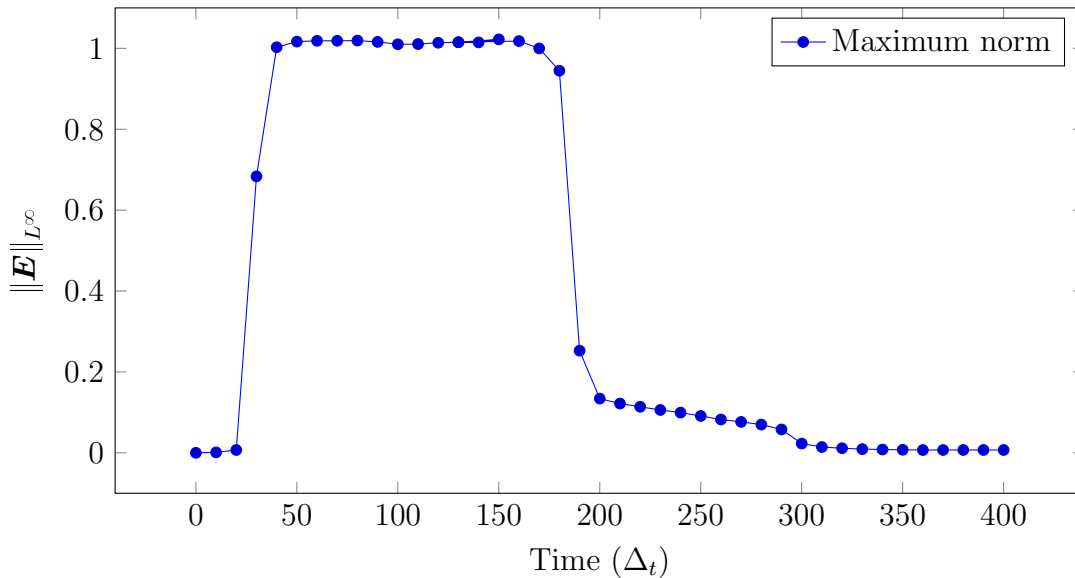


Figure 38: Time evolution of $\|\mathbf{E}\|_{L^\infty}$ within the entire domain.

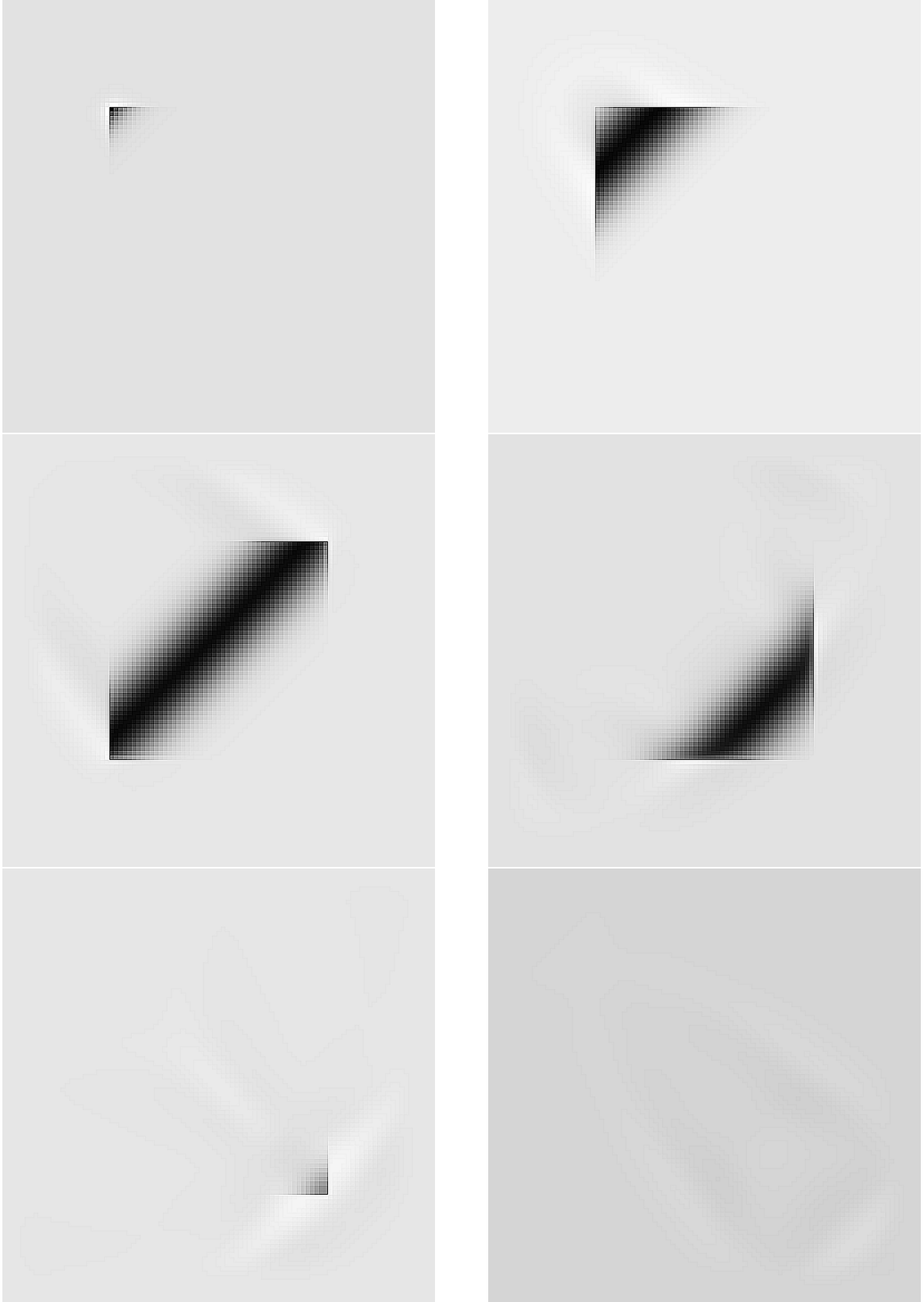


Figure 39: Diagonal propagation of plane wave in 3D, $\|\mathbf{E}\|$ (2D slices).

As we see both in the maximum value of the norm, and in the figures above, the error produced by the TFSF, which is slowly absorbed by the UPML. Let us now also observe what happens when we introduce a perfect electric conductor in the center of the grid by enforcing zero electric fields, to scatter our plane wave. This is illustrated in Figure [40].

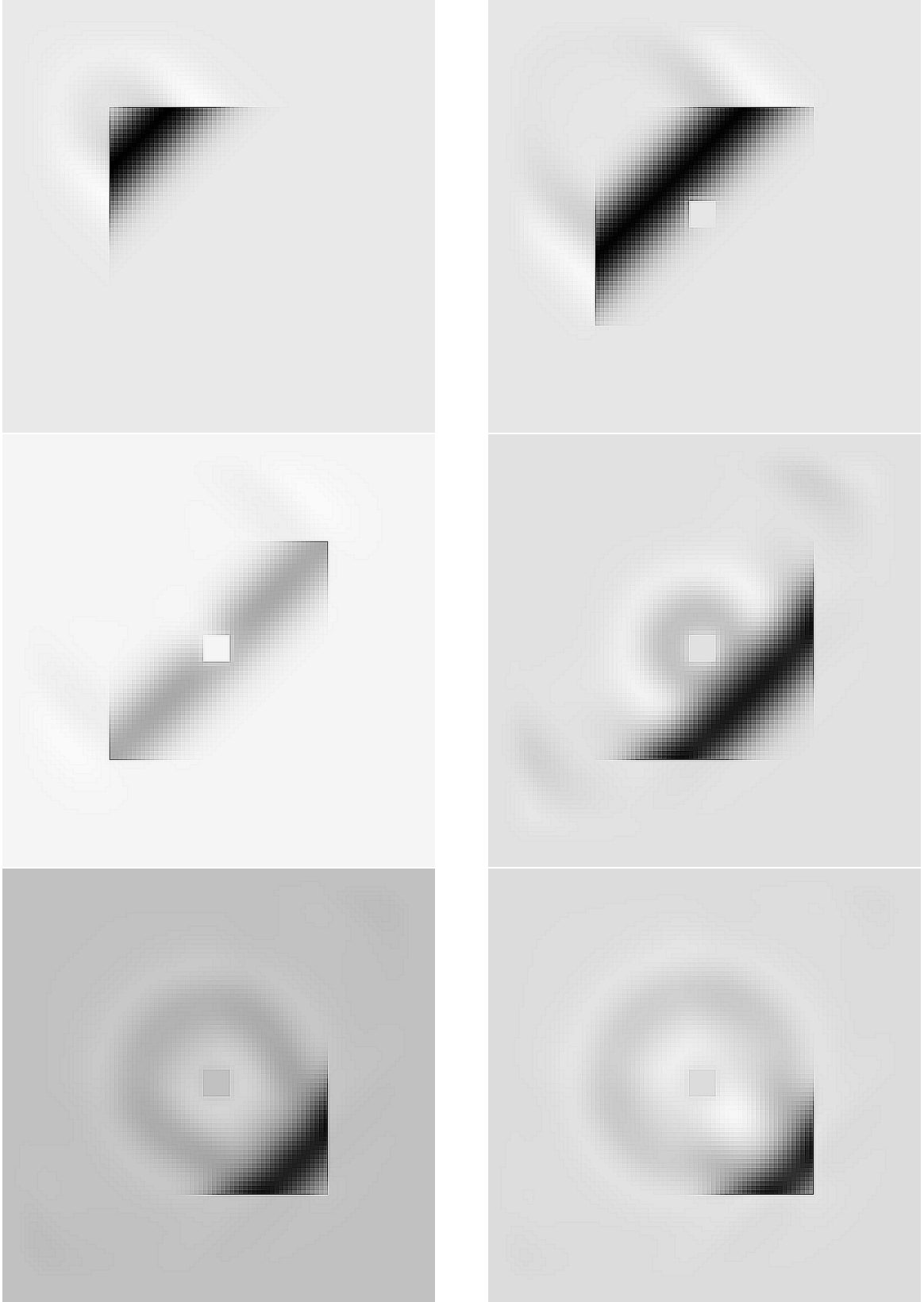


Figure 40: PEC cube scattering by plane wave, $\|\mathbf{E}\|$ (2D slices).

We can observe the quasi-spherical wavefront generated from the scattering, and with this we conclude the exposition of the TFSF plane wave implementation example.

5.4 PML error

As we have mentioned in the previous sections, the two main ways in which the PML introduces errors are through the (remainder of the) reflected wave, and the numerical artifacts that arise from the staircasing of the PML parameters. In the continuous setting, if we have a conductivity grading given by $\sigma_x(x)$ along the x -coordinate, the theoretical reflection for a wave impinging on a PML of thickness d at the angle of φ is given by Equation (50). In particular, for a polynomial grading of order three of σ_w we obtain:

$$R(\varphi) = \exp\left(-2\eta \cos \varphi \frac{\sigma_{x,\max}}{4}\right)$$

Particularly, in the case of what is referred to in literature as the “optimal” $\sigma_{w,\max}$, for which an attenuation of e^{-16} for 10-cell thick PML takes place, we obtain:

$$R(\varphi) = \exp\left(-1.6 \frac{\cos \varphi}{\Delta_h}\right)$$

where Δ_h is the spatial discretization step size. We now wish to check the sensitivity of the two error types introduced by the PML. We shall do this within the following scenario: we use a hard sinusoidal

$$E_z\left(\frac{N_x}{2}, \frac{N_y}{2}, \frac{N_z}{2}, n\Delta_t\right) = \sin(\omega n\Delta_t)$$

point source at the center of our computational domain of size $N_x \times N_y \times N_z$, use a UPML of thickness N_{PML} , and vary $\sigma_{w,\max}$ (initially $= \sigma_{w,\text{optimal}}$) and N_{PML} slightly. We evaluate the discrete L^2 norm in space, and the discrete L^2 norm in time over the last three periods. We also run the simulation for ten periods, enough that the initial transients due to the source turn-on discontinuity are absorbed by the PML. Space is discretized at 10 ppw.

In order to define quantities in physically relevant terms, the thickness will be given in relative terms to the size of the wavelength λ , taking values in the set $N_{\text{PML}}\Delta_x \in \{\delta\lambda \mid \delta \in \{0.3, 0.5, 0.7, 1, 1.3, 1.6, 1.9, 2.2\}\}$. What we expect to see is that the error slightly increases when going either left or right of the optimal maximum σ , and furthermore that the error increases when we decrease the size of N_{PML} (due to the shorter distance). We illustrate the evolution of the errors in Figure [41].

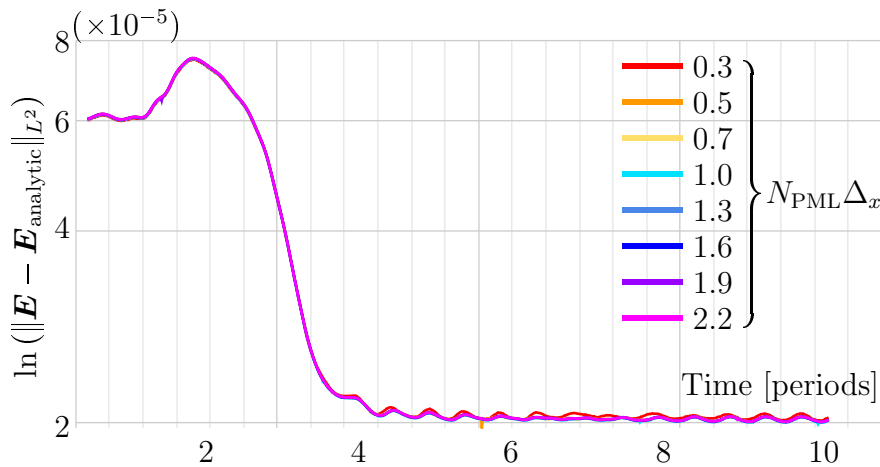


Figure 41: PML thickness errors.

If we zoom in on the last three periods from Figure [41], we observe the following:

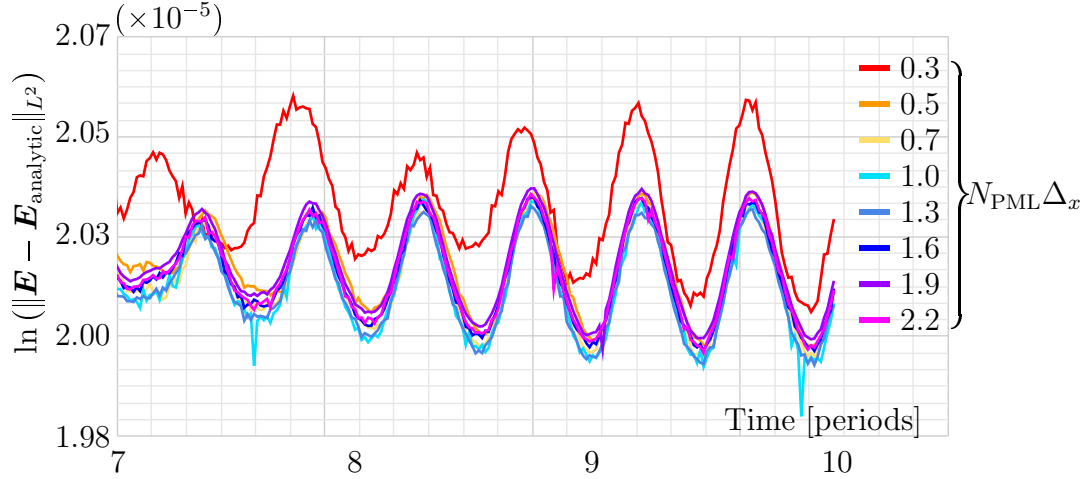


Figure 42: PML thickness errors.

We notice that the outlier is the lowest thickness value. However, there is not much difference between the rest of the thicknesses, although most of their errors stay mainly above that of the thickness $N_{\text{PML}} = \frac{\lambda}{\Delta_x}$. Throughout these tests the sigma profile was unchanged. Let us now keep the PML thickness fixed, and slightly vary σ_{max} away from the optimal value. We illustrate the behavior of the errors in Figure [43].

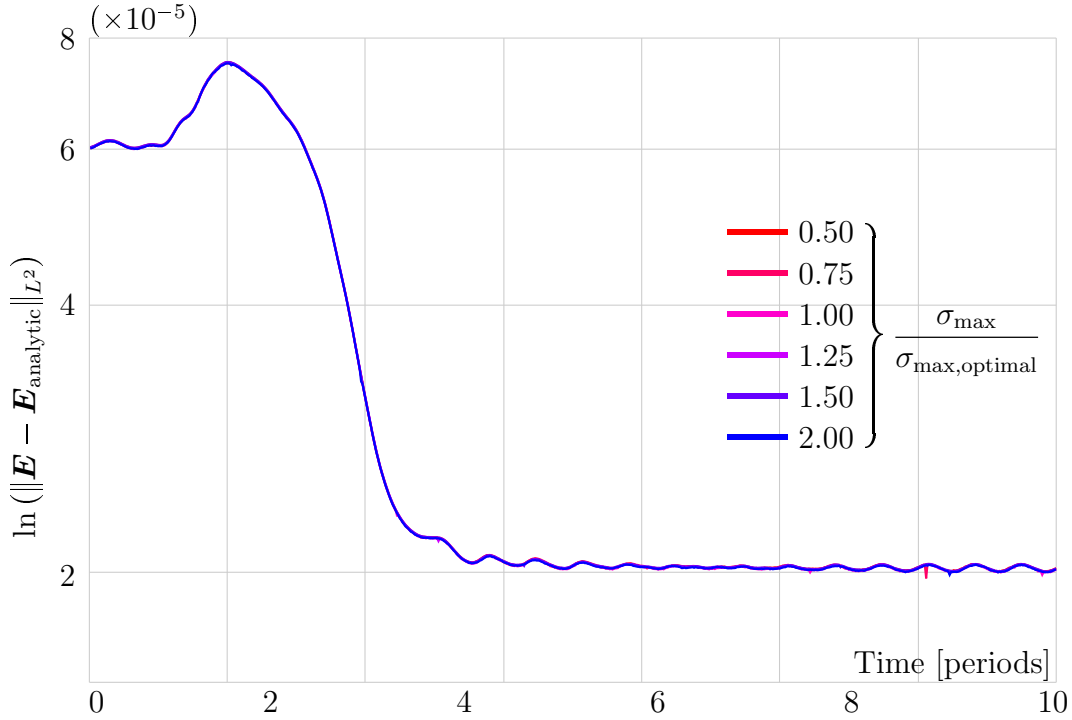
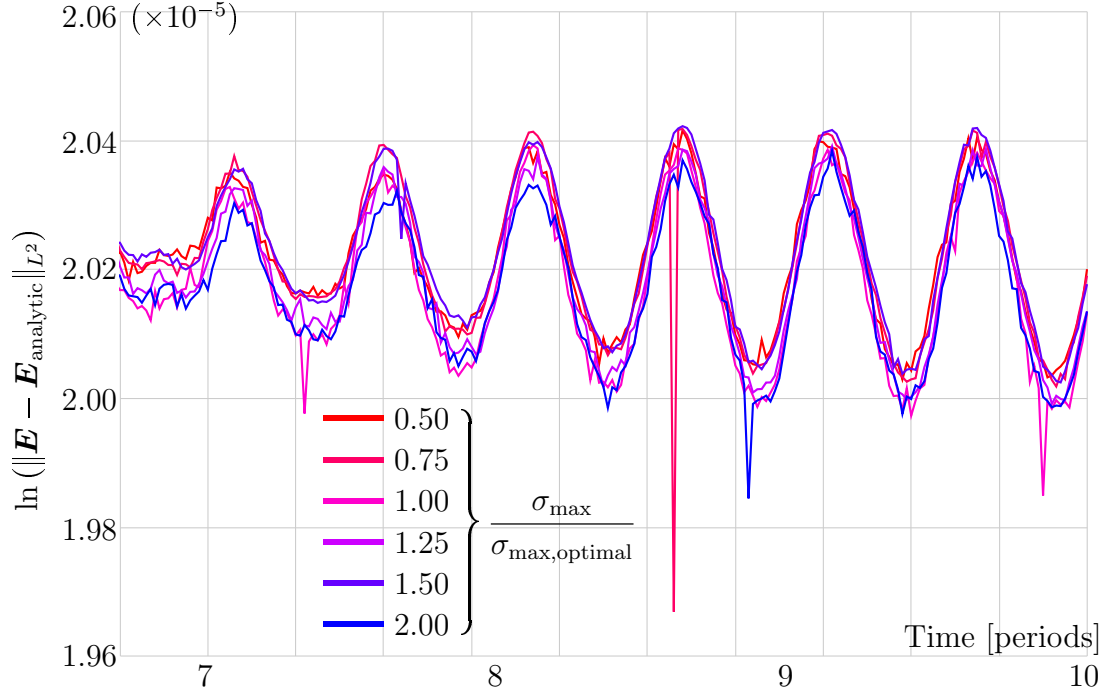


Figure 43: Error variation due to σ_{max} .

Once again, we cannot distinguish any differences at this scale. We shall proceed by examining the behavior over the last three periods from Figure [43], illustrated (and zoomed in) in Figure [44].

Figure 44: Error variation due to $\sigma_{\max}$.

Below in Table [3] we list the average error over the last three periods:

$\frac{\sigma_{\max}}{\sigma_{\text{opt}}}$	Stabilized L^2 error
0.50	$2.021869 \cdot 10^{-5}$
0.75	$2.022178 \cdot 10^{-5}$
1.00	$2.017653 \cdot 10^{-5}$
1.25	$2.018924 \cdot 10^{-5}$
1.50	$2.022861 \cdot 10^{-5}$
2.00	$2.017115 \cdot 10^{-5}$

Table 3: Error produced by varying σ_{opt} .

And we note that a local minimum is attained at the optimal value. However, since the error decreases past this point for doubling the optimal value of σ , one can assume one of the following: either the floating point accuracy is comparable to the error introduced by increasing σ , or there is some destructive interference going on, artificially lowering the error. In Table [4], we reference the stabilized L^2 error rates for the PML thickness variation.

Resolution	$N_{\text{PML}} \Delta_x / \lambda$	Average L^2 error
41^3	0.3	$2.0380 \cdot 10^{-5}$
45^3	0.5	$2.0224 \cdot 10^{-5}$
49^3	0.7	$2.0193 \cdot 10^{-5}$
55^3	1.0	$2.0177 \cdot 10^{-5}$
61^3	1.3	$2.0176 \cdot 10^{-5}$
67^3	1.6	$2.0205 \cdot 10^{-5}$
73^3	1.9	$2.0230 \cdot 10^{-5}$
79^3	2.2	$2.0209 \cdot 10^{-5}$

Table 4: Error produced by varying N_{PML} .

Once more, the value of σ_{opt} indeed seems to satisfy a local minimum in terms of introduced errors. With this we conclude Chapter 5, and move on to the centerpiece simulation.

Chapter 6

Simulation with Patient Data

In this chapter we shall test a complete heat-coupled EM simulation on a set of patient data. The data was provided by Christian Rieder of Fraunhofer MEVIS [39], and rendered in color with an in-house planning tool for catheter-based interventions named SAFIR [34]. The data set was produced with the help of Rheinisch-Westfälische Technische Hochschule Aachen, and it consists of a computer tomography (CT) scan of the abdominal area of a patient. The data also provides a so-called *segmentation* of the CT scan, formatted as a mask that delimits and labels (with integers) all tissue types.

Hereon, in order to visualize 3D data, we shall most often use an *orthogonal* view, split into three or four parts, where we render 2D slices **perpendicular** to the x -, y - and z -axes respectively. The correspondence between these slices and our two most common ways of rendering data are labeled in Figure [45]. If displayed, the (yellow or otherwise) orthogonal lines denote where the other two slices are evaluated.

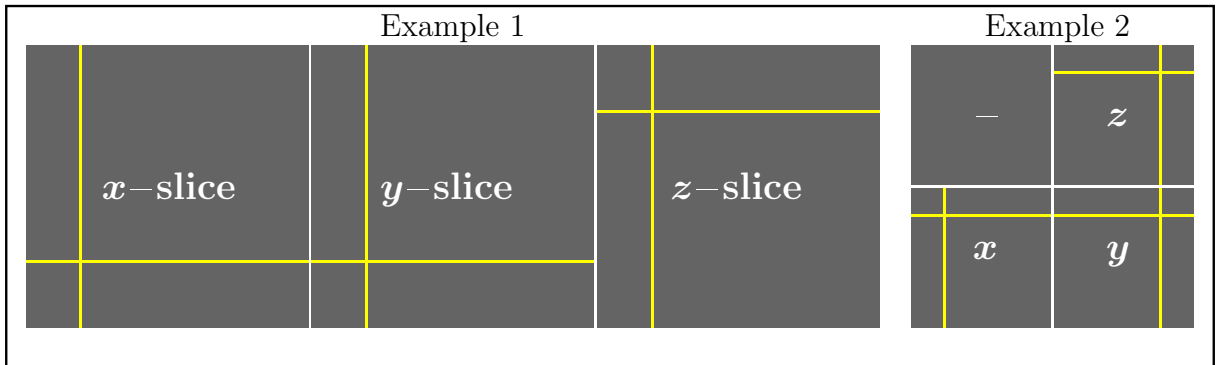


Figure 45: Visualization interpretation guideline.

We shall often refer to such (scalar) data as images, since they are stored and loaded as scalar-valued 3D images. Once interpreted as images, we utilize MeVisLab [35], a software tool that has significant visualization and data manipulation capabilities. Given this short introduction, we first present a visualization of the full abdominal data set within SAFIR.

The top left image from Figure [46] is a render in which different segmented organs are colored, where the ribs, liver and lungs are visible. In the remaining three images, we render the slices according to the legend in Figure [45], Example 2. We also highlight the liver tumor segmentation with an orange boundary. The integer labeling is visualized in Figure [47].

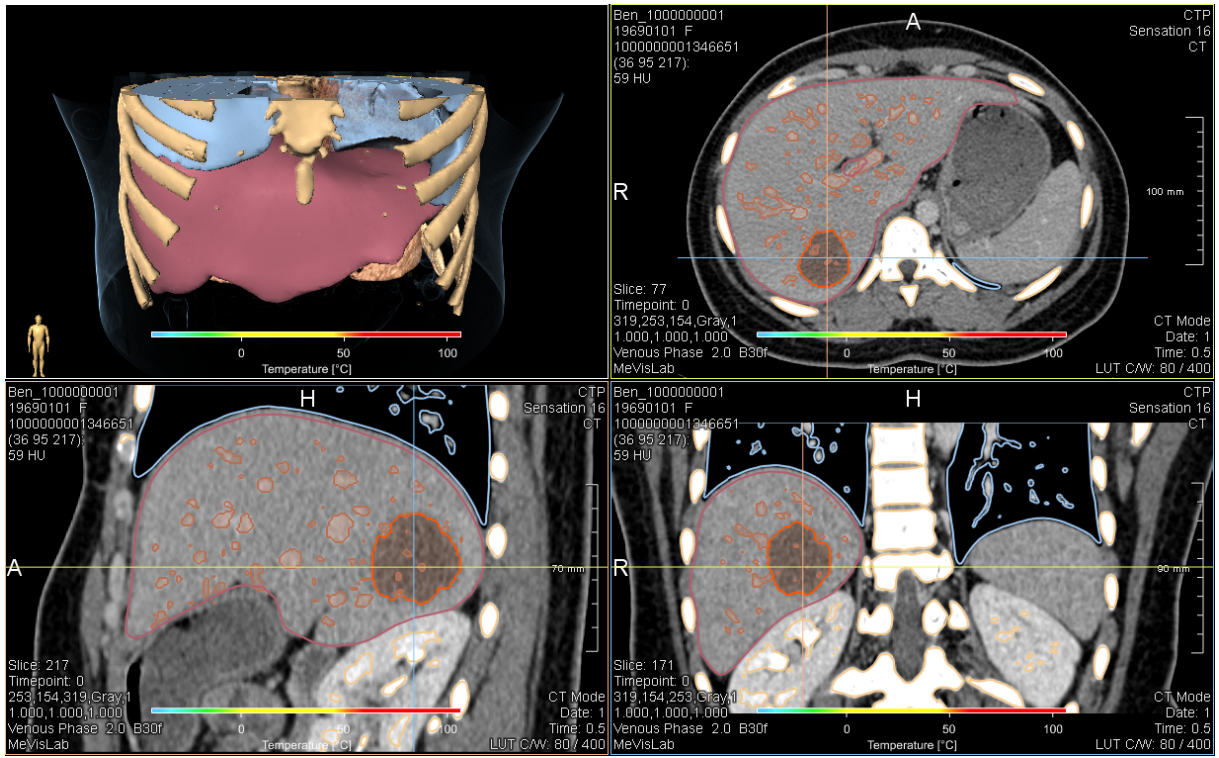


Figure 46: Visualization of patient data within SAFIR [34].

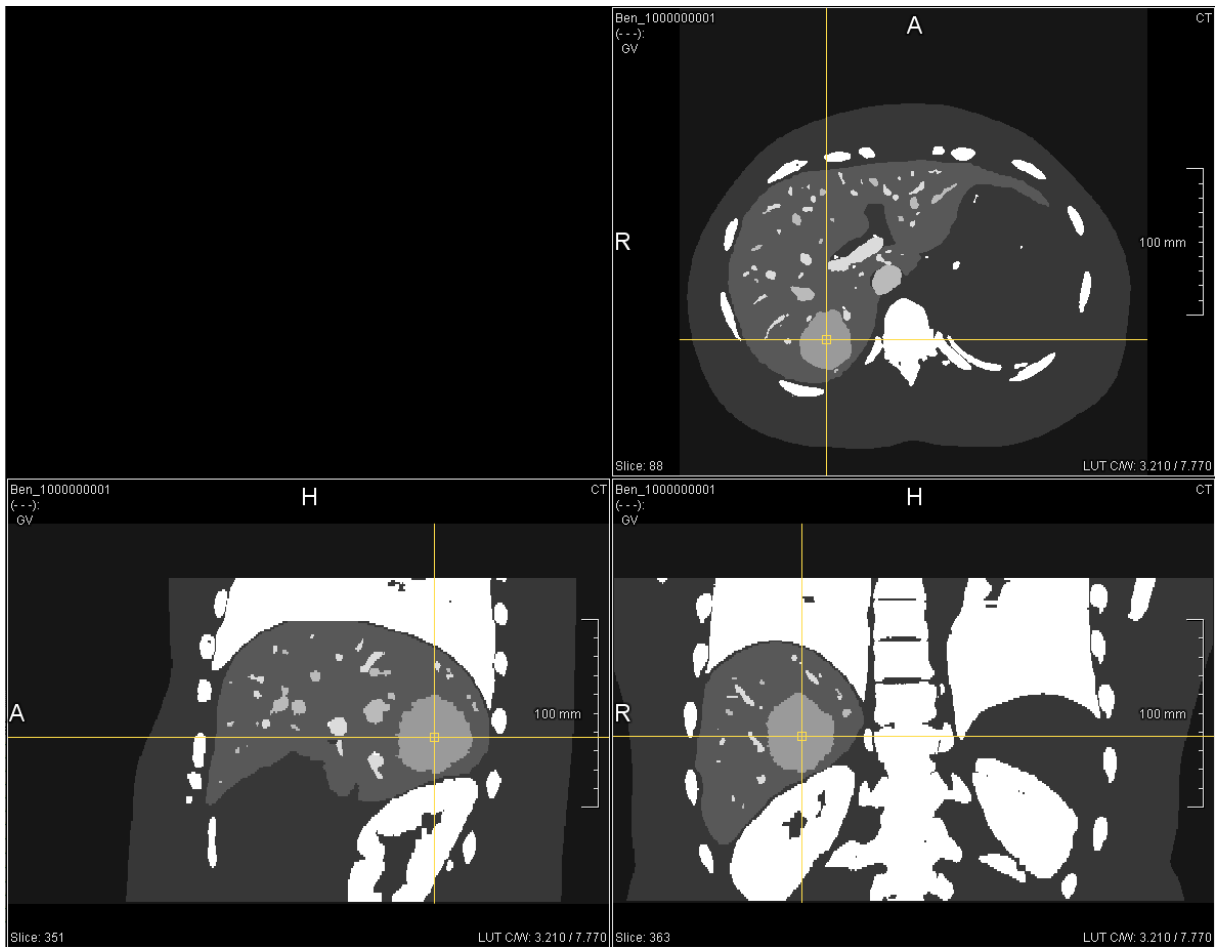


Figure 47: Segmentation mask of the patient data, visualized in MeVisLab [35].

The tissue types from the grayscale mask in Figure [47] are listed in Table [5], parametrized according to: electric conductivity σ , thermal conductivity λ , heat capacity κ , mass density ρ_{kg} , relative electric permittivity ε_{rel} . The label image is used as input for our simulation. We allocate different dielectric and thermal parameters to each labeled material. Most parameter values are taken from the database of The Foundation for Research on Information Technologies in Society (Zürich, Switzerland) [10].

The tissues whose values are not provided in the database are the following: *HV*, *PV* and *HA*, which denote the hepatic vein, portal vein, and hepatic artery, respectively. Furthermore, we shall label as *Patient* any remaining volume that does not fall into the other 11 categories from Table [5]. We estimate the parameter values of these four tissue types based on their similarity (as interpreted by the author) to the tissues with known values.

Label	Tissue type	$\sigma \left[\frac{\text{S}}{\text{m}} \right]$	$\varepsilon_{\text{rel}}[1]$	λ	κ	$\rho_{\text{kg}} \left[\frac{\text{kg}}{\text{m}^3} \right]$	Water content
0	Air	0.000	1.00	0.0260	1005	1.13	0.0000
1	Patient	0.500	30.00	0.5000	3800	1050	0.6431
2	Liver	0.860	46.70	0.5947	3577	1050	0.7146
4	Tumors	1.118	52.77	0.4194	3600	1050	0.7503
5	HV	1.540	61.30	0.5169	3617	1050	0.4950
6	PV	1.540	61.30	0.5169	3617	1050	0.4950
7	HA	1.540	61.30	0.5169	3617	1050	0.4950
8	Kidneys	1.400	58.60	0.5500	3763	1066	0.7947
9	Cartilage	0.789	42.60	0.4900	3568	1100	0.7500
10	Bones	0.145	12.44	0.3200	1313	1908	0.3181
11	Lung	0.460	22.00	0.3874	3886	722	0.8000

Table 5: Patient data registered tissue labels.

From the data in Figure [47], we select a subset containing a large liver tumor. This is done in order to (significantly) reduce the computational time and memory requirements. Furthermore, we expect that the amplitude of the electromagnetic waves will fall off considerably within a short distance from the tumor. This intuition is motivated by the lossy nature of the materials ($\sigma_{\text{tumor}} = 1.118 \frac{\text{S}}{\text{m}}, \sigma_{\text{liver}} = 0.860 \frac{\text{S}}{\text{m}}$), but also by the spherical nature of the wavefronts emanated by our energy source. However, the influence of these two factors is not equal. One could deduce from Section 2.1.1 that the field amplitude decays by approximately 1% per voxel (thus, per mm). This is nowhere near as influential as the $\frac{1}{r^3}$ decay of amplitude due to the spherical shape of the wavefront.

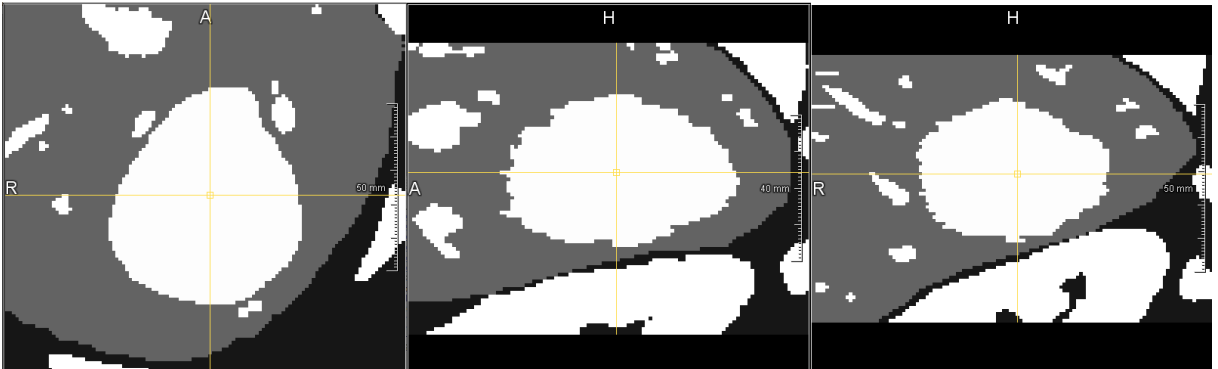


Figure 48: Subset of registered liver tumor patient data, centered on tumor.

In Figure [49] we also render the data from Figure [47] in 3D. The darker volume region in the center of the image is the segmented tumor. The vascular system and ribs are also shown, however the liver is not rendered in order to observe the tumor.

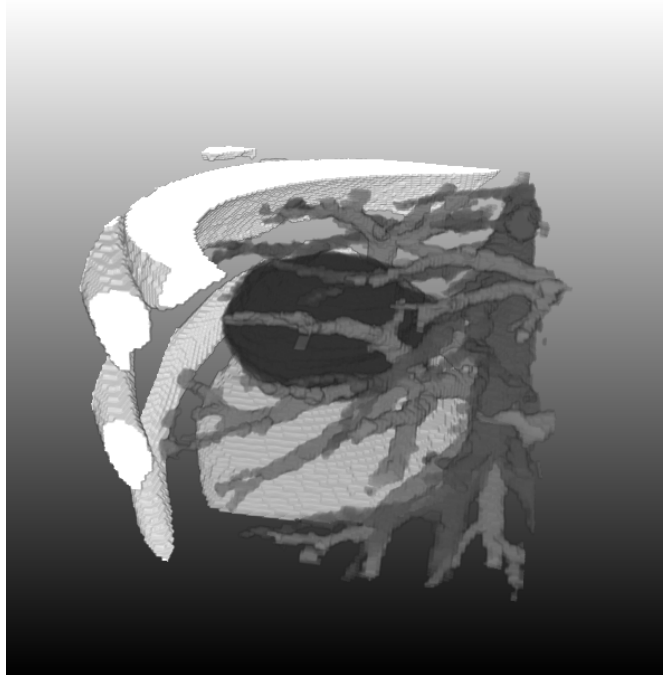


Figure 49: Subset of registered liver tumor patient data, 3D render.

The data subset has a resolution of $120 \times 110 \times 80$, with a voxel size of $1\text{mm} \times 1\text{mm} \times 1\text{mm}$. We shall note however that due to memory limitations, we will not be able to evaluate stability in terms of whether the computational domain has reached a quasi-periodic state. However, as we will see shortly, the electromagnetic waves are heavily dampened by the time they leave the tumor, which also means that a UPML grid termination is unnecessary.

In terms of how we shall model the antenna, there are mainly two options. The first is to use the TFSF method, and define the physical surface of the antenna as the TFSF interface. In this case, one would need to impose some currents that recreate a given electromagnetic field. An intuitive choice is to use the field produced by one or more point dipoles. While the resulting field inside a lossy medium will obviously be nonphysical, since we only have the vacuum analytical formula available, it will however be symmetric and smooth. We shall rescale $\sigma \|\mathbf{E}\|^2$ to have a fixed power of 40W (which is on the lower end of power achievable by MWA, but it will suffice for our qualitative analysis) over the entire domain, which means the amplitudes themselves do not matter, only the spatial distribution.

There are some practical issues with this approach however. Firstly, the TFSF error and internal reflections from the SF zone (which would be vacuum) would pollute the solution, and accumulate in time. Secondly, using the vacuum analytical formula to define the TFSF fields in a lossy medium would quickly lead to nonphysical currents. This is clearly the case since the vacuum fields do not satisfy Maxwell's equations in a tumor. A workaround could be to define the TFSF surface completely within vacuum, inside the antenna. However, in this case, the (physically meaningful) refractions and reflections arising at the vacuum-tumor interface would pollute the solution.

Thus, we have to rely on other ways of introducing electromagnetic energy. The most desirable option is to simulate a physical antenna, with all of its geometry. While some antennas have a simple enough structure, if we wish to simulate a realistically large antenna (2–5mm in diameter), the grid resolution we have available would not be sufficient. Furthermore, modern MWA applicators are significantly geometrically complex, often involving liquid cooling systems. The scope of the research at hand did not include physical antenna modeling, and this area deserves a lengthy investigation of its own.

Thus, we have one possible energy source left at our disposal: infinitesimal dipoles. It has long been the case that electrical engineers superimpose such point sources in order to recreate more complex fields. We shall stack, within the center of the active zone of the antenna, a line of z -polarized hard sources. Their position is illustrated with white in Figure [50], and the antenna geometry is rendered in orange. In Figure [51] we visualize the underlying electrical conductivities, and color blood vessels in blue.

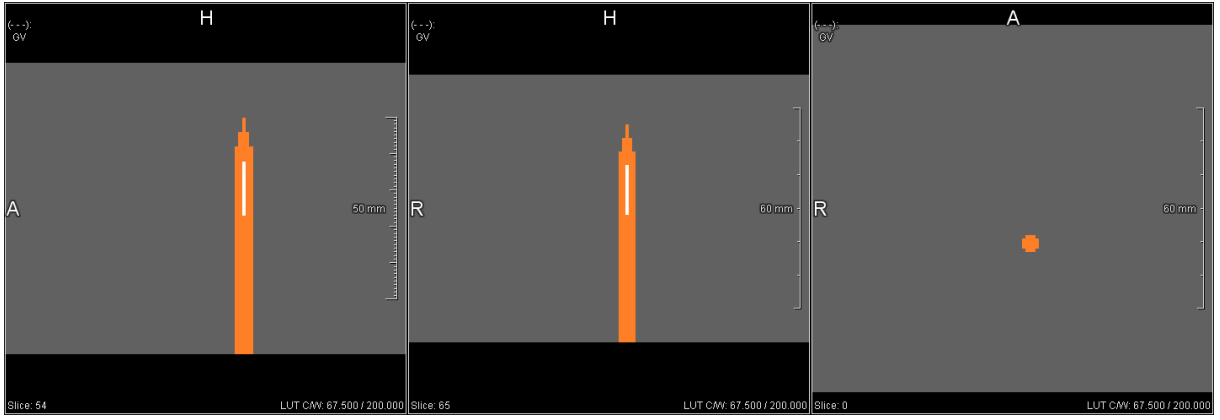


Figure 50: Placement of E_z point dipoles inside antenna.

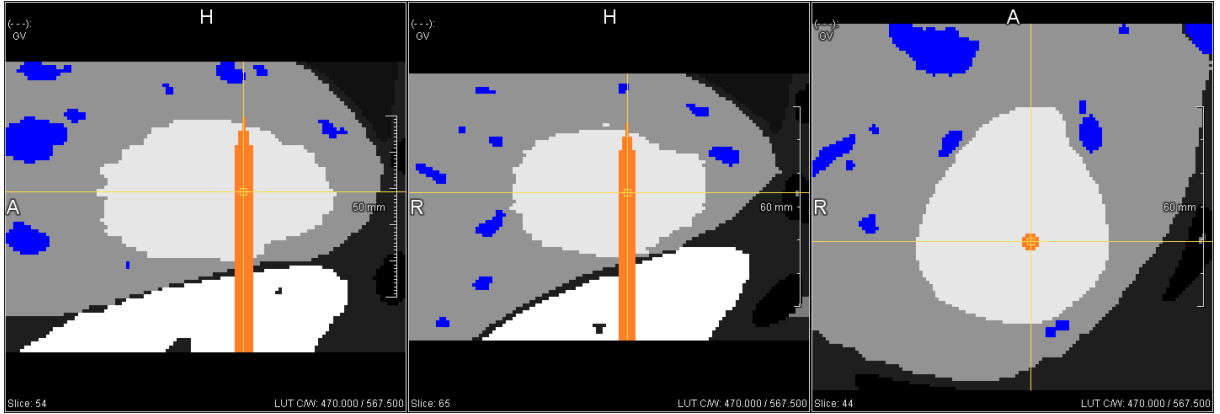


Figure 51: Placement of the antenna, background given (qualitatively) by σ .

We shall then assume that the interior of the antenna is parametrized by the underlying physical parameters (thus mostly tumor tissue). For example, in Figure [51] we display the antenna together with the underlying values of σ . We shall run each FDTD simulation for three periods of the 915MHz source, to obtain the EM fields inside the domain. This time interval has been visually determined to be sufficient to reach (global) periodic behavior. We then pass on the average (over the last quarter of a period) $\sigma \|E\|^2$ to the bioheat solver. This power is assumed to be zero within the antenna, and rescaled outside of it to have a total power of 40W within the domain. The bioheat solver then performs

one explicit time-step of 1s, computes the temperature, adapts the tissue parameters (this step will be detailed immediately), and feeds them back to the FDTD solver. The EM solver then resets the fields to zero, and restarts another simulation with the adapted parameters. We repeat this cycle for 60 steps, or seconds.

We know from medical practice that both RFA and MWA procedures last anywhere between 3 and 30 minutes, so clearly one minute is not a realistic liver ablation procedure length. This restriction was imposed due to time constraints, since the FDTD code is not completely optimized or parallelized on a GPU. In our case, 60 steps worth of three periods each takes approximately 8 hours on the present data. However, for an initial proof-of-concept, this one minute runtime already yields sufficient results for interpretation.

With this being said, let us turn to the temperature dependence of materials. While most of the material parameters presented in Table [5] do in fact vary with temperature, it is not within the scope of the work at hand to investigate this aspect exhaustively. We will, for a proof-of-concept, evaluate the conductivity at different temperatures, due to it being the most electromagnetically-impactful parameter.

We start by using the conductivity of (healthy) liver tissue as a reference point. Since the conductivity of different tissue types varies in different ways with temperature, we shall make a simplifying assumption, relying on the water content. While it is certain that a multitude of factors influence this parameter, we shall use water content to change the temperature profiling of the involved materials. We illustrate in Figure [53] how we assume the liver's conductivity varies, based on the data presented in Cristopher Brace's *Temperature-dependent dielectric properties of liver tissue measured during thermal ablation: Toward an improved numerical model* [5]. For reference, the data used is presented in Figure [52].

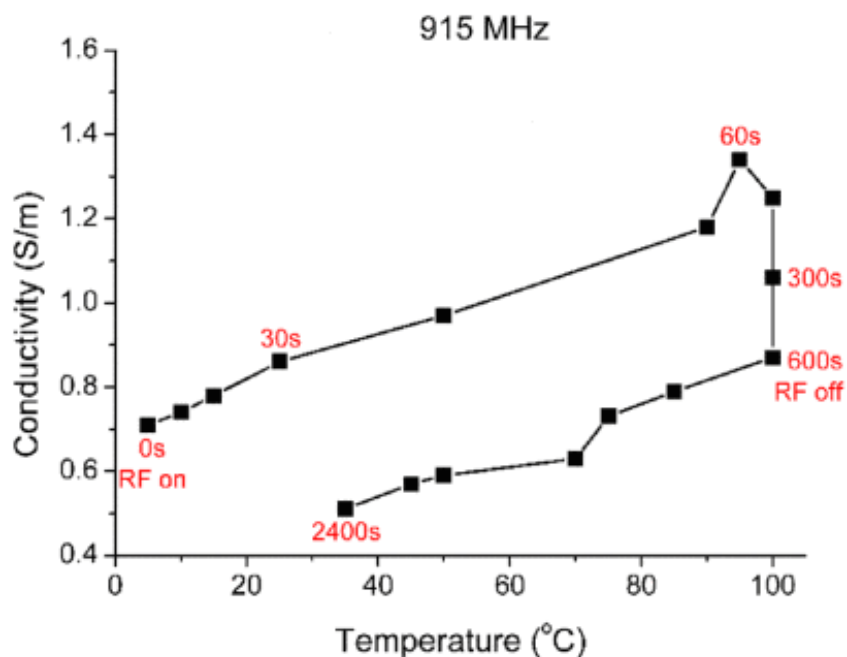


Figure 52: Temperature curve of σ at 915 MHz, taken from [5], p. 232, ©2008 IEEE.

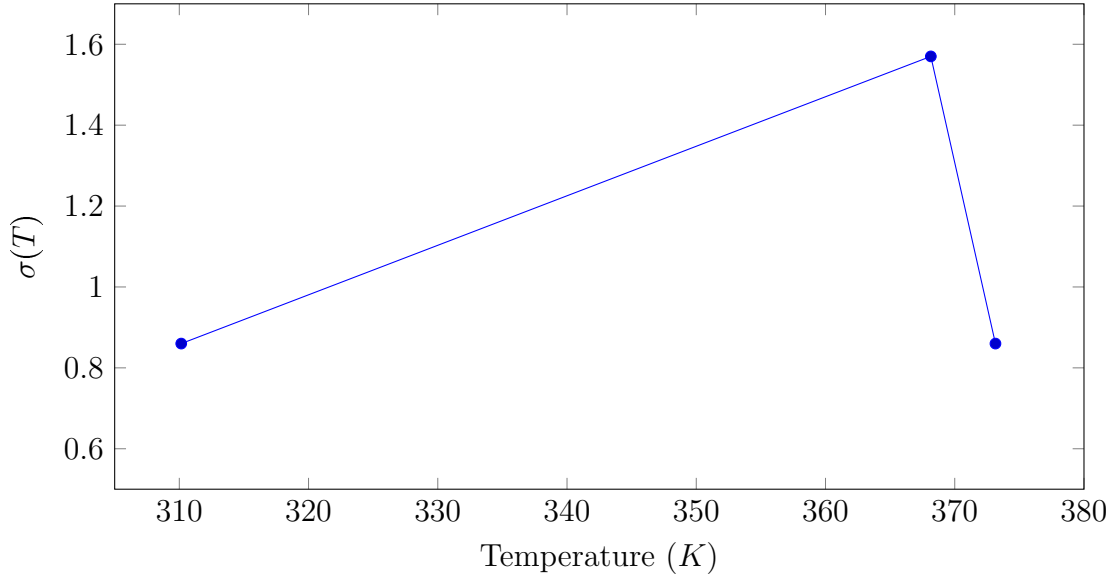


Figure 53: Assumed temperature dependence of σ , based on water content.

The closed form of our simplified curve from Figure [53] is:

$$\sigma(T) = \begin{cases} 0.86\left(\frac{1.57}{0.86} - 1\right)\frac{T}{58} + 0.86\left(1 - 310.15 \cdot \frac{\frac{1.57}{0.86} - 1}{58}\right) & \text{if } T \in [310.15, 368.15] \\ -0.86\left(\frac{1.57}{0.86} - 1\right)\frac{T}{5} + 0.86\left(1 + 373.15 \cdot \frac{\frac{1.57}{0.86} - 1}{5}\right) & \text{if } T \in [368.15, 373.15] \end{cases}$$

The starting conductivity at body temperature $310.15K$ is $0.86\frac{S}{m}$, which then increases to $1.57\frac{S}{m}$ five degrees below the boiling point ($368.15K$), and then decreases due to vaporization close to the original value. We shall clamp this final value to exactly the original value. Based on this curve, we shall approximate the conductivity profiles (dependence on temperature) based on the relative water content to that of healthy liver.

Using H.H. Mitchell's paper [28] as a reference, we claim that the water content of healthy liver tissue is 71.46%. For a given ratio of water content of another tissue, r , we shall scale the difference between the maximum achieved σ and the minimal one $\sigma_{\min}$ ($=0.86\frac{S}{m}$ for healthy liver) linearly, according to the water content ratio, as follows:

$$\sigma(T) = \begin{cases} 0.83\frac{r}{0.7146} \cdot \sigma_{\min}\frac{T}{58} + \sigma_{\min}\left(1 - \frac{r}{0.7146}310.15 \cdot \frac{0.83}{58}\right) & \text{if } T \in [310.15, 368.15] \\ -0.83\frac{r}{0.7146} \cdot \sigma_{\min}\frac{T}{5} + \sigma_{\min}\left(1 + \frac{r}{0.7146}373.15 \cdot \frac{0.83}{5}\right) & \text{if } T \in [368.15, 373.15] \end{cases}$$

While this model is clearly an oversimplification, we employ it as a proof of concept of how temperature dependent parameters, in particular σ , are incorporated into our complete MWA solver. In Figure [54] we illustrate the conductivity map before and after some heat was applied through the simulation of one EM solver cycle. This heat is highest around the active zone of the antenna, and as expected, that is also where our conductivity has increased, as highlighted with red circles. The brighter shades of gray represent higher values.

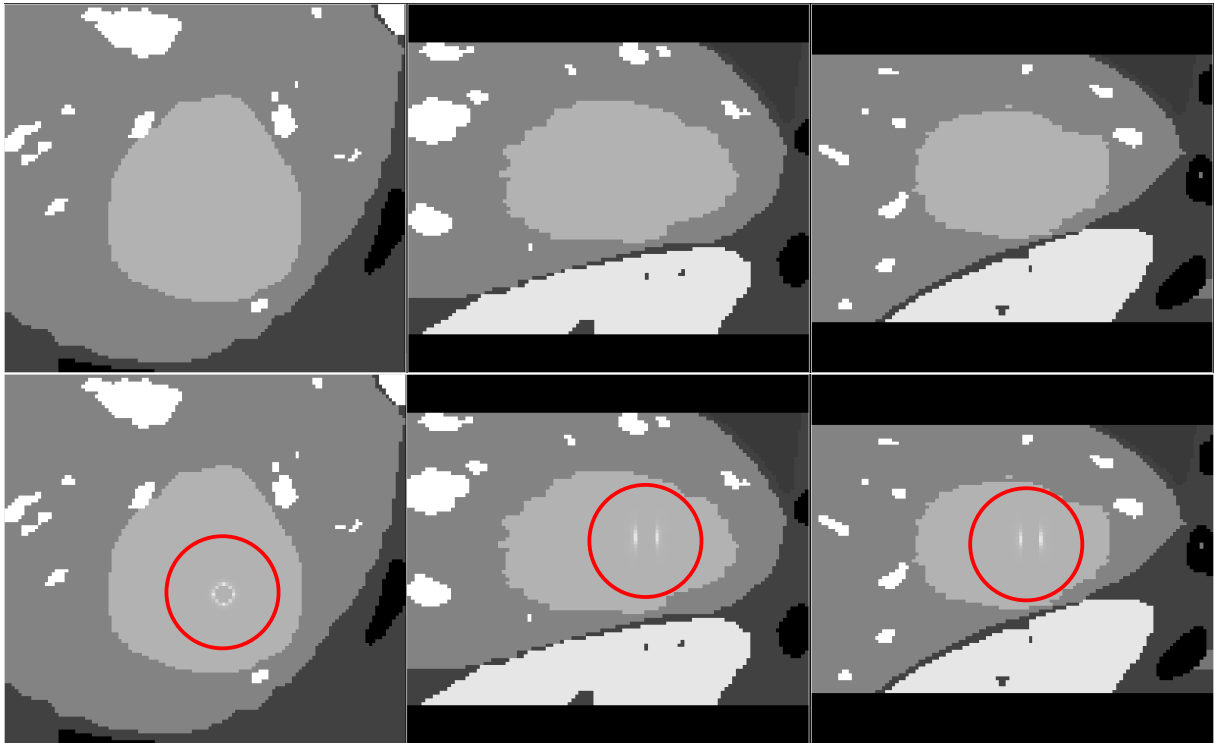


Figure 54: Electrical conductivity before (top) and after (bottom) a temperature increase.

Let us now describe the reference simulation that we shall compare our combined FDTD/heat solver to. We shall hereon refer to this in-house thermal ablation solver by “Thermal Ablation Simulation” or **TAS**¹ [14]. TAS consists of an electrostatic simulation, coupled with a heat solver. In Figure [55] we present a qualitative image of the output of the electrostatic solver, and thus the input for the TAS heat solver. The instrument created has a cross section of $4\text{mm} \times 4\text{mm}$, where one voxel has dimensions of $1\text{mm} \times 1\text{mm} \times 1\text{mm}$.

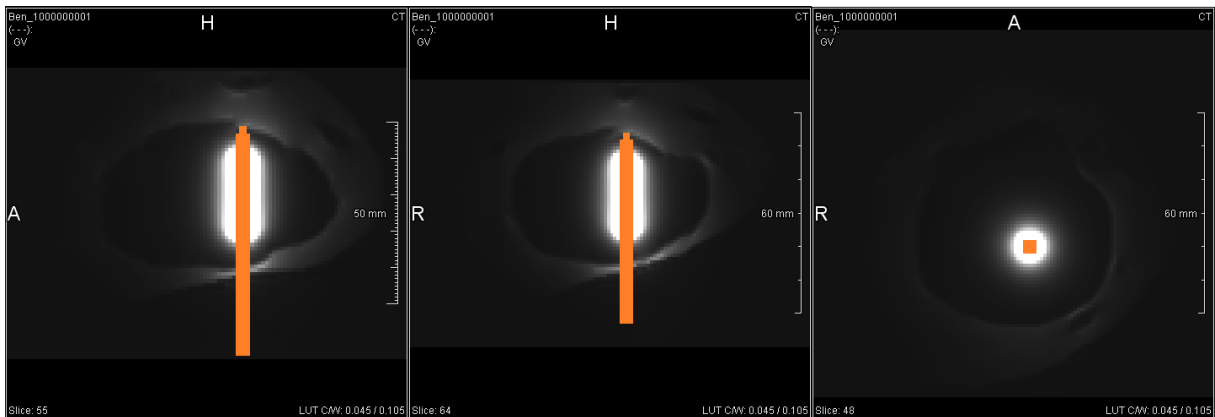


Figure 55: Input power for TAS solver.

The instrument is illustrated in orange, and inserted within the tumor in the same position as for our simulation. We shall run this simulation with an input power of $40W$, for one minute, and present the temperature values within an x -aligned line segment.

¹ThermalAblationSimulation module in MeVisLab

This particular position of the line segment is selected in order to have it intersect the highest achieved temperature points, as displayed in Figure [56]. We will then render in Figure [57] the temperature curve through this x -aligned segment, within a 30mm portion centered on the antenna (thus 25% of the total x -extent of the image).

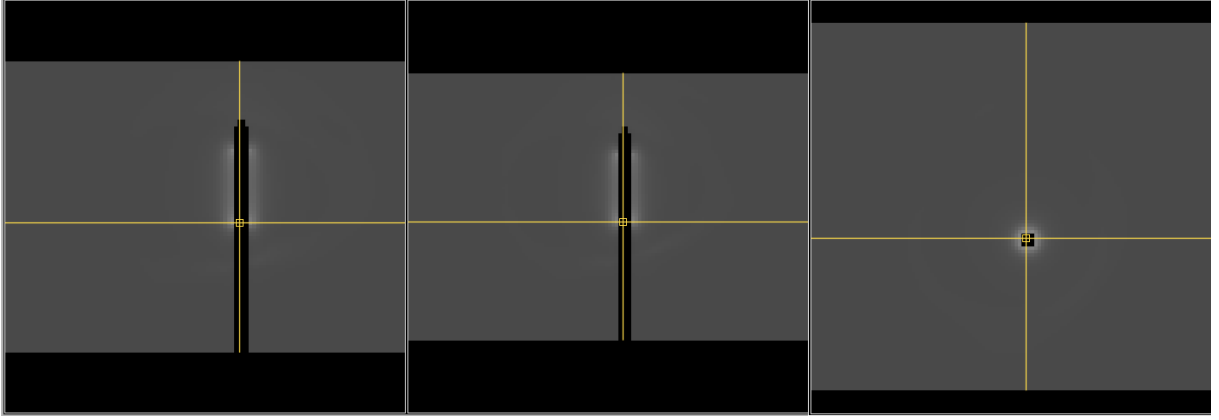


Figure 56: Temperature evaluation position for TAS solver.

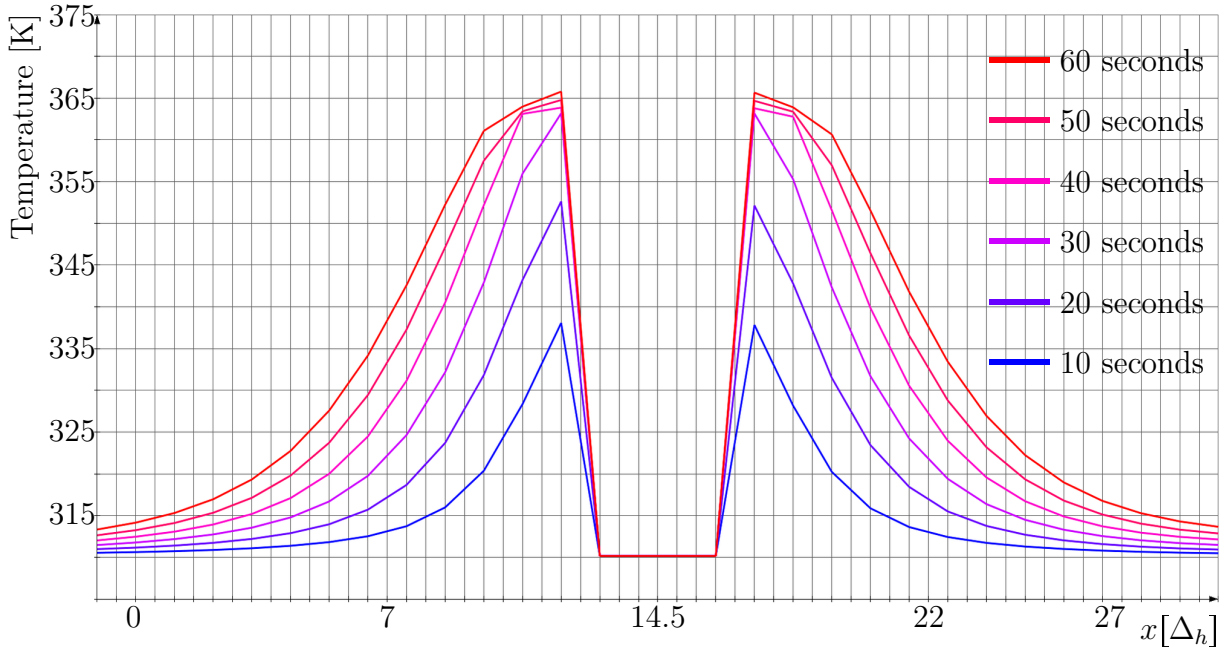


Figure 57: Temperature evolution resulting from TAS over 60 seconds.

Figure [57] illustrates how the maximum temperature achieved is 365.958 Kelvin, or 92.808° Celsius. Let us also observe that the peak steadily increases throughout the simulation, which matches the experimental results presented in the introduction. In figure [58] we visualize the status of the temperature produced by TAS for a simulation runtime of 60 seconds. We will note that this solver accounts for the nonlinear characteristics of the generator. Thus, we need to scale the power by a constant to ensure that the energy actually deposited into the tissue is 2400J (resulting from 40W over 60s). In the figures to follow, brighter gray values represent higher temperatures.

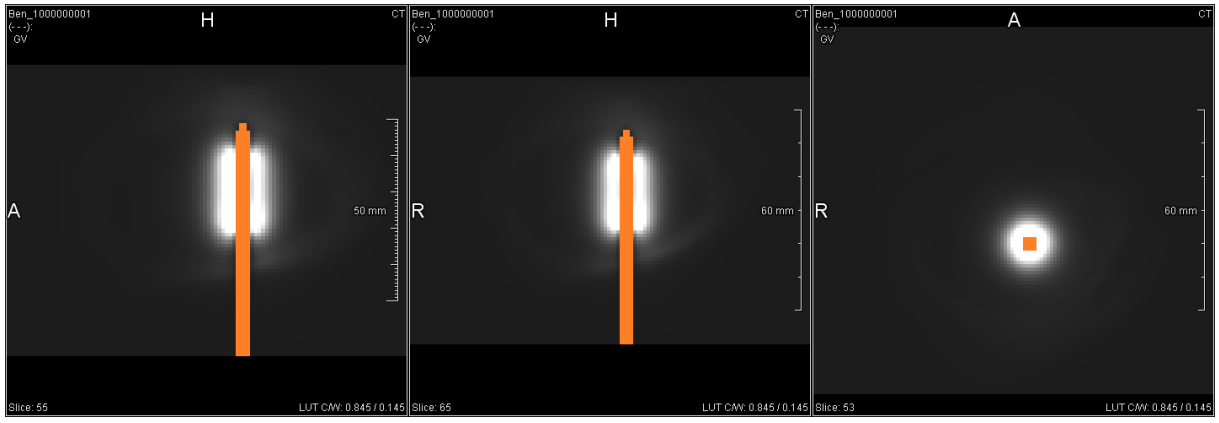
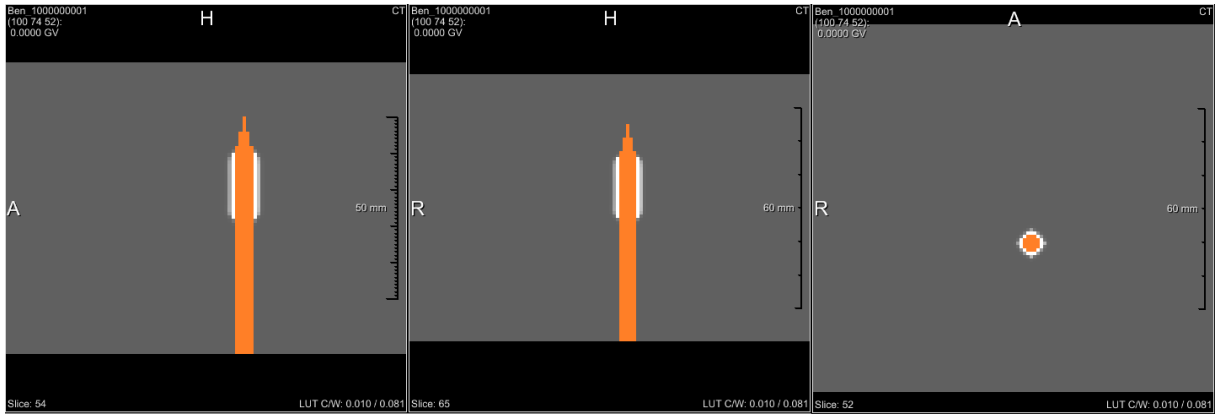
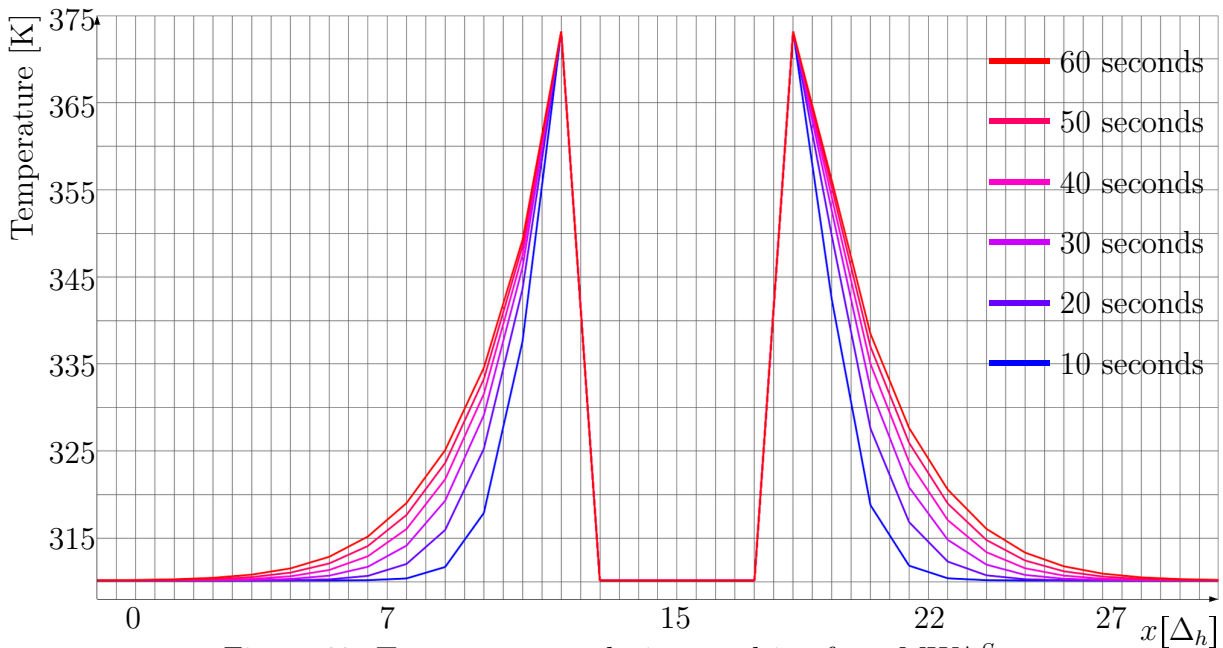


Figure 58: Temperature profile given by TAS after 1 minute.

Now we shall turn to the result given by our FDTD solver, coupled with the explicit bioheat solver, hereon referred to as *MWA simulation* or simply MWA^S . We first visualize the (electrodynamical) power yielded in the last second in Figure [59]. The power produced in previous seconds (0 – 59) is qualitatively the same, but scaled down slightly due to the smaller σ . Finally, in Figure [60] we illustrate the evolution of the temperature through the center of the active zone of the antenna (along a segment as done for Figure [57]).

Figure 59: Power input after 60seconds provided by MWA^S .Figure 60: Temperature evolution resulting from MWA^S .

We shall remark that for both MWA^S and TAS, the heat solver has employed a tissue dehydration model. Broadly speaking, this ramps up the required heating power to obtain a temperature increase, depending on how much water the tissue lost due to the higher (or boiling) temperature. We should acknowledge that our MWA^S has an arguably unrealistically high power gradient, due to the usage of point dipoles as sources. As a result, a lot of the power is concentrated into very few voxels. Without a dehydration model in place, this would result in a blow-up of the temperature field (at least without making any drastic changes to our heat equation modeling). This does mean that we somewhat underestimate the true heating performed by our MWA^S model. However, this cannot be avoided when using (point) dipoles. In Figure [61] we illustrate the final temperature field qualitatively.

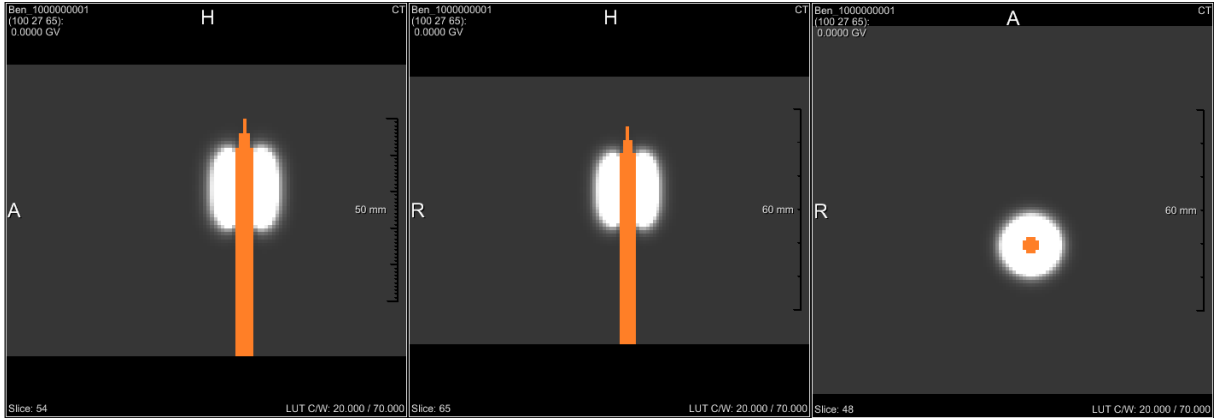


Figure 61: Resulting temperature from MWA^S after 60 seconds.

Let us scale down the contrast in the final temperature image, such that the lowest distinguishable value is 355.8K. We display the zoomed-in result in Figure [62]. We notice that there are large differences in the values across the surface of the applicator, and temperature is not radially symmetric. This fact is due to the poor geometric discretization of the probe, and to a lesser extent, due to the fact that information does not travel radially in this rectangular grid. One could counteract this aspect by using a larger probe, which will be (relatively speaking) better discretized by the grid. However, one would need to scale up the size of the domain, in order to maintain accurate size ratios of the other structures, which would be computationally restrictive in our case.

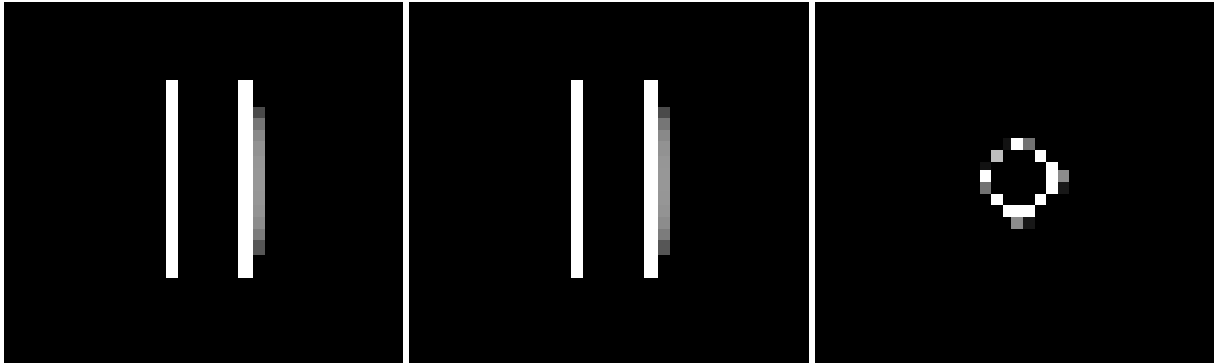


Figure 62: Scaled resulting temperature from MWA^S after 60 seconds, zoomed in.

Having interpreted both MWA^S and TAS results independently, let us finally turn to their comparison. Firstly, let us compare the temperature along the x -aligned line segment.

In Figure [63] we illustrate the final (60-second) temperatures of MWA^S and TAS. One should note that between the two models there is a discrepancy of one voxel in the discretization of the probe, leading to a slight shift.

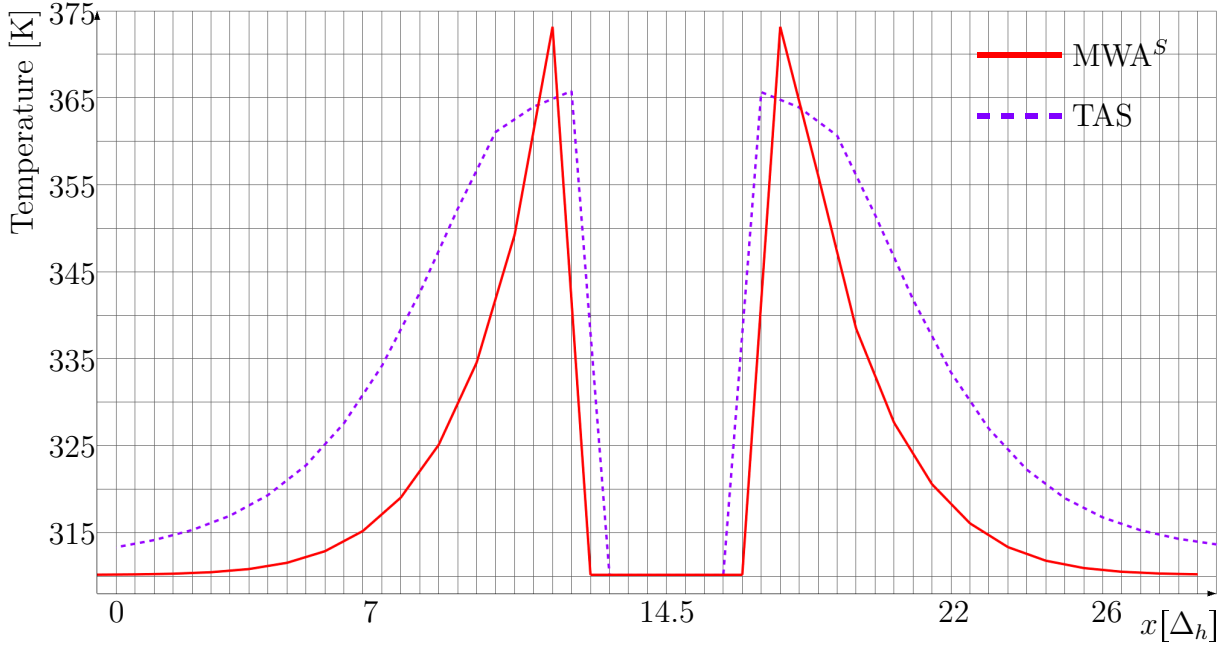


Figure 63: Comparison of final temperature between TAS and MWA^S .

Secondly, to mitigate the influence of the dehydration, and the low running time, we shall threshold the final temperature fields at 60°C . This should be easily reachable by both models, within a reasonably sized volume. We then refer to any tissue volume that has reached this temperature as “ablated”, or coagulated. As one can infer from Figure [63], at this lower temperature point, TAS does cover a larger volume. Let us denote by $\mathcal{V}_{\text{TAS}}^A$ the total ablated TAS volume, and by $\mathcal{V}_{\text{MWA}}^A$ the total MWA^S ablated volume. We also define $\mathcal{A}_{\text{MWA}}$ as the volume occupied by our MWA^S antenna, and the TAS analogue $\mathcal{A}_{\text{TAS}}$. In order to account for the discrepancy in discretization of the antennas, we shall ignore $\mathcal{A}_{\text{MWA}} \cup \mathcal{A}_{\text{TAS}}$ from the discussion ahead. We illustrate the difference in ablated volume in Figure [64].

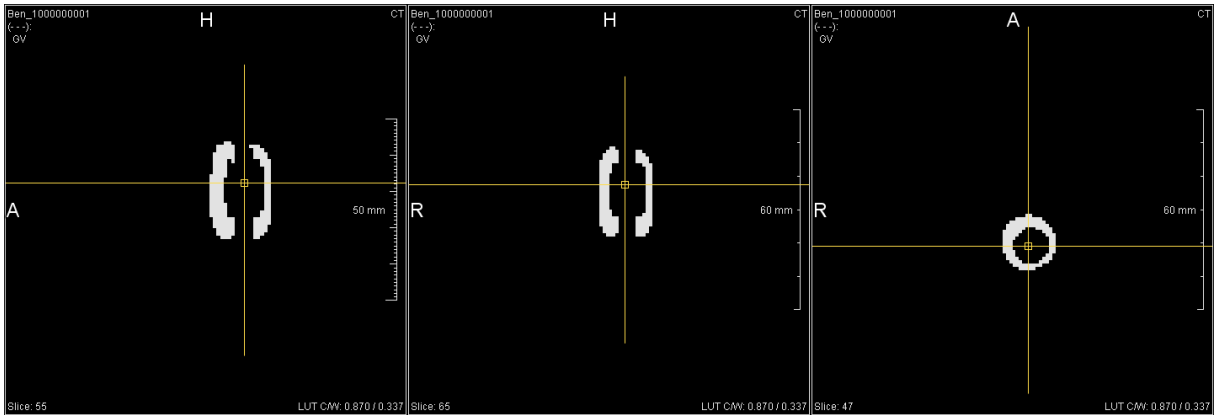


Figure 64: Visualization of the set difference $\mathcal{V}_{\text{TAS}}^A \setminus \mathcal{V}_{\text{MWA}}^A$.

In terms of distance from the applicator, TAS achieved an average ablated radius of six voxels, while MWA^S reached an average of three. Thus, the radius of the ablated volume

at the center of the active zone was doubled by TAS. The total volume ablated by TAS is $|\mathcal{V}_{\text{TAS}}^A| = 4.422 \cdot 10^{-6} \text{m}^3$, while TAS reports the smaller volume $|\mathcal{V}_{\text{TAS}}^A| = 0.911 \cdot 10^{-6} \text{m}^3$. Thus, the difference in ablated volume has the size $|\mathcal{V}_{\text{TAS}}^A \setminus \mathcal{V}_{\text{MWA}}^A| = 3.511 \cdot 10^{-6} \text{m}^3$. For reference, the total volume of the grid is 0.001056m^3 . In relative terms,

$$\frac{|\mathcal{V}_{\text{TAS}}^A|}{|\mathcal{V}_{\text{MWA}}^A|} \approx 4.85$$

This significant discrepancy is to be expected for a threshold under 100°C . Medical practice often mentions the ability to reach more than 100°C as a main motivation to use MWA instead of RFA. To a limited extent, we have witnessed our MWA simulation's ability to reach higher temperatures faster, however the (volumetric) impact is limited by the large gradient of the electrical field norm. One consequence is that no significant heating reaches the blood vessels, and we have no estimate on how well their cooling effect is counteracted. When employing various antennas as sources, one would expect that more of the heating is produced by electromagnetic energy transport due to their ability to guide the energy. In the results at hand, it is apparent that MWA^S mostly relied on the thermal diffusion to spread the heat.

Finally, let us provide some concluding remarks based on the results above. The MWA^S simulation presented in the present research is expectedly orders of magnitude slower than an electrostatic simulation. The property that counteracts this disadvantage is the physical accuracy of the model. In order to exploit the dynamic capabilities of such FDTD solvers, we should provide a proper source of electromagnetic energy, such as guiding antennas. These would provide more heating through electromagnetic energy transport, rather than relying on thermal diffusion. However, the MWA^S simulation we have developed already provides promising results even when powered by simplistic point dipoles.

Additionally, a proper optimization of the data structures used, and a switch to GPU parallelization (as opposed to CPU), would bring down the runtime to the order of minutes (instead of hours). This would suffice for the goal application of liver microwave ablation planning. Such medical interventions do not require real-time adaptations of the model, since no significant changes appear between the pre-operative imaging procedures (CT, MRI, etc.) and the ablation procedure.

Chapter 7

Conclusions and Discussion

The main motivation for the research within the present thesis, and the MICROPLAN project, has been to improve the clinical status quo of liver cancer treatment. In section 7.1, we shall first summarize how the research at hand can augment the microwave ablation intervention, and facilitate the work of medical practitioners. We will also highlight the questions left unanswered by this thesis, and offer some concluding remarks based on our initial goals. Finally, in section 7.2 we shall discuss some possibilities for improvement and ideas for future research in this area.

7.1 Summary and open problems

We have built an electrodynamic FDTD solver in order to dynamically solve Maxwell's equations, employing Kane S. Yee's algorithm. Some aspects of basic electromagnetic sources were introduced, together with certain usual discretization tools, such as the Perfectly Matched Layer and the Total-Field Scattered-Field techniques. The influence of the discretization on dielectric loss and phase velocity was also quantified, in the context of plane waves traveling along axis-aligned directions.

An overview of the difficulties involved in coupling electromagnetic and bioheat equations was showcased, also providing some initial insight into how certain aspects can be properly quantified. Furthermore, several numerical experiments were investigated, mainly in order to quantitatively assess the influence of particular components on the FDTD error.

Finally, the FDTD solver we have developed was coupled to an available bioheat equation solver available in-house at Fraunhofer MEVIS [21]. This heat solver discretized space with hexahedral Finite Elements, and time with explicit time-stepping. The final result of the combined solver was then compared to the results produced by an electrostatic in-house solver, that was also coupled to a heat solver.

The main difficulties that arise in such a process are the implementation of the antenna, and matching the output of an electromagnetic solver with any following building blocks in the microwave ablation simulation. We have seen that in spite of their widespread usage, point dipoles do not provide a satisfactory match to the ablation pattern produced by MWA^S applicators. It is clear that more time would need to be invested into the research at hand in order to incorporate more realistic energy sources. Furthermore, certain simplifications have to be made in order to streamline the interaction of the heat and electromagnetic simulation components. These are mostly related to initial conditions in

FDTD, but do not pose significant physically meaningful difficulties, since we are solving for harmonic states.

While it is readily apparent that electrostatic solvers are orders of magnitude faster than fully dynamic EM solvers, this comes at a cost. The physical accuracy in modeling complex dynamic processes is lost, and this translates into an inability to properly predict patient-specific results. In principle, the larger the volume of homogeneous lossy tissue that surrounds the energy source in the domain, the more accurate the prediction of an electrostatic solver should be. However, as we have seen in the previous chapter, this quasi-homogeneity is an unrealistic assumption in medical practice.

One clear shortcoming of the numerical model presented in the current work is the incomplete characterization of dielectric and thermal material parameters. This of course is an experimental electrical engineering endeavor, rather than a mathematical one. However, there are several (physically) qualitative changes that arise in (dielectric and thermal) tissue characterization. Reversible and irreversible phase transitions take place, tissues become cauterized, and complex thermodynamic and electromagnetic interactions take place. Furthermore, the effect of many of these processes is spread across various scales, and often requires microscopic analysis in order to reach macroscopic claims. In this regard, a proper physical analysis would be necessary, in order to grant thoroughness.

In the pursuit of providing a rigorous and accurate MWA prediction result, complete parametric characterizations of all involved materials are needed. Their dependence on frequency, temperature, blood perfusion, medical conditions, coagulation state, and many other factors would have to be properly quantified. Only then could one be confident in the accuracy of the numerical result.

With all of the above aspects in mind, let us see to what extent we have achieved the goals set out in the introduction. Firstly, we have incorporated three of the four components that were planned. The tissue damage model was not used, due to unavailability of a comparable result. However, the simulation of Maxwell's equations was connected to the bioheat equation to a sufficient degree. The tissue parameter model used was heavily simplified, and only varied one of the dielectric properties. Nonetheless, there would be no conceptual difficulty in implementing modified parameter curves.

We have presented one possible solution to the discrepancy in time scales, which does not introduce additional modeling difficulties, and allows us to retain acceptable simulation times. A sturdy UPML implementation was presented, which allowed us to handle long-time vacuum simulations. An extension of this model would be necessary though, in order to handle fully heterogeneous materials. The ability to integrate our numerical solver with image-based data was achieved, and allowed for straightforward input of clinical data.

We have not reached an experimental validation phase of the simulation at hand. However we have provided numerical substantiation of our FDTD solver's accuracy, both through numerical experiments and tests using realistic data. In its current state, the MWA^S numerical model requires: a dehydration model that is better adapted to microwave ablation, an expanded antenna model, and a simulated intervention time longer than one minute. Only when these prerequisites are satisfied could one hypothesize on the increased electromagnetic accuracy.

7.2 Future work

A clear direction in which this work can be extended is the section on numerical loss and dispersion. The extendability of those results for any arbitrary direction can be investigated, instead of just diagonals and axis directions. Furthermore, the analysis can be extended to spherical wavefronts, and not just plane waves. This could allow for an analogue closed form of discrete penetration depth, in the context of near-field applications using dipole-like sources. In order to move forward, one would need to pick up the thread at the beginning of the Section 3.6. Let us rewrite the plane wave equations.

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 \exp(i(\mathbf{k} \cdot \mathbf{r} - \omega t)), \quad \mathbf{H}(\mathbf{r}, t) = \mathbf{H}_0 \exp(i(\mathbf{k} \cdot \mathbf{r} - \omega t))$$

Taking the curl of Faraday's Law, using the zero divergence property, and then plugging in a plane wave solution, we obtain:

$$\Delta \mathbf{E} = \mu\epsilon \frac{\partial^2}{\partial t^2} \mathbf{E} + \mu\sigma \frac{\partial}{\partial t} \mathbf{E} \Rightarrow (k_x^2 + k_y^2 + k_z^2) = \mu\epsilon\omega^2 + i\mu\sigma\omega$$

For a general complex vector $\mathbf{k} = \boldsymbol{\beta} + i\boldsymbol{\alpha}$, this yields the system of equations

$$\begin{cases} |\boldsymbol{\beta}|^2 - |\boldsymbol{\alpha}|^2 = \mu\epsilon\omega^2 \\ \boldsymbol{\beta} \cdot \boldsymbol{\alpha} = \frac{\mu\sigma\omega}{2} \end{cases}$$

After investing some time, one would expect to reach a closed form of the numerical loss and dispersion, parametrized according to the wave vector. The final step will then be to incorporate the influence of the non-planar isosurfaces on the amplitude. With this, discrete dispersion and loss would be completely characterized for the types of materials we have considered in the present thesis.

On another note, geometrically modeling the applicator will undeniably provide more accurate numerical results. This of course involves the difficulty of demanding a higher resolution, in order to resolve all fine structures. Such a step might require some type of grid adaptivity, and (sub-voxel) interface matching of the fields. This should incorporate the fact that a large number of MWA applicators nowadays are cooled by liquid.

Finally, after tying up the loose ends presented in the current and previous sections, one could move on to the experimental validation phase. Ideally, one would test the predicted numerical results against the medical intervention results, within the scope of a large-scale clinical trial. Covering a wide range of physiologies (fatty liver disease, cirrhosis, etc.) and geometries would be required in order to yield robust results.

While effortless for us to list, most of these improvements will require a (continued) significant interdisciplinary effort. A thorough further collaboration between research scientists, medical practitioners and electrical engineers will be vital, in order to achieve the desired experimental accuracy. However, given sufficient academic initiative, there is no doubt that applied mathematics will continue to strengthen not only microwave liver ablation, but medical practice as a whole.

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