Engineering of Spin Wave Dispersion in Ultrathin Films and Waveguides by a Software-Controlled Micromagnetic Framework

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Abstract

The research area of magnonics deals with the fundamental and application-based aspect of the physics of spin waves, the fundamental excitation of the magnetization in magnetic solids. Due to their outstanding features, such as their nanometric wavelengths and frequencies in the GHz and THz range and their propagation in magnetic insulators, which allows to envision spin-waves logic without the need of charge currents, magnons are of large interest to the research area of spintronics, which by itself exploits the spin degree of freedom to provide a next generation of efficient data processing. In the context of magnonics, micromagnetic simulations have become an indispensable tool to predict spin-wave phenomena. With the increasing complexity of the spin-wave devices to be simulated, the demand for a possibility to automatize entire series of simulations to optimize the design of spin-wave based devices or to reproduce experimental data. This would allow to use an automatized analysis in order to extract optimum parameters. Such a software package is the central aim of this Thesis. During its course, a python package has been developed which, after being supplied with the parameter space to be investigated, schedules, performs and evaluates entire simulation series. By some case studies, the usefulness of such a simulation framework will be presented. This provides the foundation to analyze arbitrary problems by means of simulation series in the future.
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CHAPTER 1

Introduction

The increasingly popular research area of magnonics \cite{1} \cite{2} \cite{3} \cite{4} \cite{5} \cite{6} \cite{7} covers the physics and applications of spin waves, the fundamental excitation of a magnetic solid. It constitutes a part of spintronics \cite{8} \cite{9}, a research direction that aims to harvest the spin degree of freedom in addition to the charge of electrons in order to create a new generation of power-efficient and high-performance devices. Spin waves show a tremendous potential for data processing, as they exhibit nanometric wavelengths in the highly application-relevant GHz to THz frequency range, intrinsic nonlinearities that can be triggered without the need for large powers, and the prospect of insulator-based spin-wave logic which is intrinsically energy efficient as it circumvents ohmic losses. As the understanding of linear and nonlinear magnon physics on the micro- and nanoscale improves \cite{10} \cite{11} \cite{12} \cite{13} and ever smaller structures with decent quality become accessible \cite{13}, magnonic experiments are becoming more and more complex and magnonic circuits and devices come into reach \cite{14}.

For such more involved layouts, micromagnetic simulations \cite{15} \cite{16} \cite{17} \cite{18} \cite{19} \cite{20} which grasp most features of magnon physics in a satisfactory manner, are becoming increasingly significant in order to study and optimize the performance of a potential device. Since, for instance, the magnon frequencies and nonlinearities depend very sensitively on geometric parameters, it makes much more sense to predict proper feature sizes by a micromagnetic simulation than in an experiment, which would require to fabricate a large set of structures and then selecting the proper ones in a time-consuming series of experiments. Nonetheless, the use of micromagnetic simulations to predict device performance comes along with large demands regarding the simulation machines and the working time of the operating person. Setting up and running simulation series is a tedious task that can easily overflow the resources of the simulation PC and their analysis requires a significant manpower. However, large parts of this working routine can potentially be optimized and automatized. The main aim of this thesis is the provision of a framework that helps to ease these problems. The framework is intended to schedule and perform parameter sweeps, i.e., to perform a series of simulations with a variation of an $n$-dimensional parameter space where parameters like the applied magnetic field, material parameters or geometric parameters are varied. It allocates the simulation within such a simulation series to the available computers in a (local) network and
keeps track of their status. By a graphical user interface, the user can have a visualization of the profile. In addition, the framework performs a basic data analysis, i.e., it gathers the data and processes them into a memory saving and easily accessible format on the hard disk of the simulation machines. Moreover, it can perform a more sophisticated data analysis which can be adapted by the user to fit a certain problem which is addressed in the simulation series, such as the extraction of the dispersion relation and the consequent fitting of the dispersion relation to experimental data in order to extract material parameters, or the evaluation of more complex quantities such as the spin wave decay length or the excitation spectrum of spin-wave sources. Within this thesis, the framework is applied to two physical problems in order to demonstrate its power and general functionality. The first problem concerns the extraction of material parameters extracted from Brillouin Light Scattering Spectroscopy data [21] measured on ultrathin films featuring structural inversion asymmetry [22] and a strong perpendicular magnetic anisotropy [23] [24]. The second problem concerns an array of waveguides which is transversely magnetized [25] and the excitation spectrum therein for its application in a magnonic on-chip spectrum analyzer. While these are just exemplary tasks for the framework, they already give a good overview over its functionality and assets.

The general structure of the thesis is as follows. In Chapter 2, a very brief overview over the relevant micromagnetic theory and the energy terms relevant for this work are given. Afterwards, Chapter 3 introduces the framework, giving an overview over the used simulation software MuMax3 [16], the framework architecture and the evaluation procedure. In Chapter 4, the two case studies are presented, starting with the thin-film simulations on Pt/CoFeB/MgO and W/CoFeB/MgO. Consequently, the device study of the magnonic spectrum analyzer is performed on two different material systems: Yttrium Iron Garnet (YIG), a ferrimagnetic insulator that excels due to lowest known spin-wave damping [26], and CoFeB, a ferromagnetic compound that is widely used in spintronics applications [24] [27] [28]. For the spectrum analyzer, these two materials are of large interest as their saturation magnetization, which is a highly important scaling factor for demagnetization effects, is different by an order of magnitude and the implications of this will be discussed. Ultimately, in Chapter 5, an overview over the results from this thesis and an outlook for future use of the framework will be given.
2.1. Magnetization and effective magnetic field

An externally applied magnetic field $\vec{H}$ aligns the magnetic moments of a solid body. This alignment of magnetic moments can be described by the magnetization $\vec{M}$, which is a term for the magnetic moment per volume of the solid body in question. For small strengths of the external field $\vec{H}$, the magnetization $\vec{M}$ scales linearly with $\vec{H}$

$$\vec{M} = \chi \vec{H}$$  \hspace{1cm} (2.1)

where $\chi$ is the magnetic susceptibility.

Together with the magnetic permeability $\mu = \mu_0 (1 + \chi)$, this yields the magnetic flux density $\vec{B}$:

$$\vec{B} = \mu_0 (\vec{H} + \vec{M}) = \mu_0 (\vec{H} + \chi \vec{M}) = \mu \vec{H}$$  \hspace{1cm} (2.2)

However, in reality the magnetic field is influenced by various different effects and, thus, one defines an effective magnetic field $\vec{H}_{\text{eff}}$ as a sum of the individual field contributions:

$$\vec{H}_{\text{eff}} = \vec{H}_{\text{ext}} + \vec{H}_{\text{ext(t)}} + \vec{H}_{\text{anis}} + \vec{H}_{\text{ex}} + \vec{H}_{\text{demag}} + \vec{H}_{\text{dmi}} + \vec{H}_{\text{therm}} \cdots$$  \hspace{1cm} (2.3)

- $\vec{H}_{\text{ext}}$: The applied external field.
- $\vec{H}_{\text{ext(t)}}$: The dynamical applied external field.
- $\vec{H}_{\text{demag}}$: The magneto-static field.
- $\vec{H}_{\text{ex}}$: The field created by the Heisenberg exchange interaction.
- $\vec{H}_{\text{dmi}}$: The field contribution by the Dzyaloshinskii-Moriya interaction.
- $\vec{H}_{\text{anis}}$: The magneto-crystalline anisotropy field.
- $\vec{H}_{\text{therm}}$: The field term due to thermal energy in the system.
2.2 Landau-Lifshitz Torque

The relevant individual contributions will be discussed in more detail in the following pages.

The effective field can be written as the variation of the magnetic energy densities $e$ with respect to the magnetization for each individual contribution.

$$H_{\text{eff},i} = -\frac{1}{\mu_0} \frac{\delta}{\delta \vec{M}} e_i$$

(2.4)

whereas the magnetic energy density is calculated from the integral over the local energy densities of the Volume $V$

$$e = \frac{dE}{dV}$$

(2.5)

The equilibrium magnetization state can be found by minimizing the total energy $e_{\text{total}}$ of the system. This comes into play later, when the ground state of the simulations is calculated (see section 3.1 for further details).

---

### 2.2. Landau-Lifshitz Torque

In the presence of an effective magnetic field $\mu_0 \vec{H}_{\text{eff}}$, a magnetic moment $\vec{\mu}_m$ and, analogously, the magnetization $\vec{M}$, constituting the volume average over all magnetic moments, for instance, in a micromagnetic cell, co-aligns with this field when it is in equilibrium position. When a magnetic moment $\vec{\mu}_m$ is out of line with the effective magnetic field $\mu_0 \vec{H}_{\text{eff}}$, a torque $\vec{\tau}$ acts on it:

$$\vec{\tau} = \vec{\mu}_m \times \mu_0 \vec{H}_{\text{eff}}$$

(2.6)

This leads to a precession with a frequency $f$ of the magnetic moment around the direction of the effective field. The resulting angular momentum $\vec{L}$ for an individual magnetic moment $\vec{\mu}_m$ has the following quantum mechanically relation:

$$\vec{\mu}_m = -g \frac{\mu_B}{\hbar} \vec{L} = -\gamma \vec{L}$$

(2.7)

As the angular momentum is the derivative in time of the torque, Equation 2.6 evaluates to:

$$\vec{\tau} = \frac{d\vec{L}}{dt} = -\frac{1}{\gamma} \frac{d\vec{\mu}_m}{dt} = \vec{\mu}_m \times \mu_0 \vec{H}_{\text{eff}}$$

(2.8)

Analogously, the volume average over all magnetic moments $\vec{M}$ can be considered and leads to the Landau-Lifshitz equation [29]:

$$\frac{d\vec{M}}{dt} = -\gamma (\vec{M} \times \mu_0 \vec{H}_{\text{eff}})$$

(2.9)

which describes a uniform precession with a constant opening angle $\epsilon$ in a translational invariant solid body. As there is no dissipation of energy included, this precession would continue until
2.2 Landau-Lifshitz Torque

Hence, the equation was extended by a damping term to the Landau-Lifshitz-Gilbert equation [30]:

$$\frac{d\vec{M}}{dt} = -\gamma (\vec{M} \times \vec{H}_\text{eff}) + \frac{\alpha}{M_s} \vec{M} \times \frac{d\vec{M}}{dt},$$

(2.10)

where $\alpha$ is the dimensionless Gilbert damping factor and $M_s$ the saturation magnetization. The precessional motion is described by the first term in Equation 2.10 and shown as the purple arrow in Figure 2.1, whereas the second term constitutes the damping contribution to the precession and is marked as the blue arrow.

The damping term leads to a parallel alignment of the magnetization $\vec{M}$ to the effective field $\vec{H}_\text{eff}$ and will become crucial for the numerical calculation of the ground state of a magnetic system in section 3.1.

Together, these terms describe the collective motion of spins in a magnetic body, known as spin waves. These distortions of the magnetic order can propagate through the magnetization landscape and convey information in form of their amplitude and phase. The effective field and, with it, the magnetization configuration in the ground state as well as the spin wave dynamics, are governed by the contributions presented in Equation 2.3. The correlation between the frequency of these spin waves and their wave vector is called the spin wave dispersion relation and is an essential tool to characterize these waves.
2.3. Heisenberg-Model

The Heisenberg-model is an important tool to facilitate the transition from the effects of individual magnetic moments to the collective phenomena of many magnetic moments. It is based on pure exchange interaction between spins coupled in pairs. The corresponding quantum mechanical Hamiltonian takes on the form

\[ \hat{H}_{ij} = -2J_{ij}\vec{S}_i \cdot \vec{S}_j \]  

(2.11)

whereas \( \vec{S}_i \) and \( \vec{S}_j \) correspond to the spin of particle \( i \) and \( j \) and \( J_{ij} \) is the exchange integral between the two particles and determines the magnetic order. The system is ferromagnetic if \( J \) is positive and will prefer parallel spins. Whereas, if \( J \) is negative, the system is antiferromagnetic and will prefer anti-parallel spins.

In order to use this formulation in practice, one can approximate the model to nearest-neighbor-interaction only and an equally strong exchange between each spin-pair. This yields the Hamiltonian

\[ H_i = -2J\sum_{j=1}^{NN} \vec{S}_j \]  

(2.12)

By including the definition of the gyromagnetic ratio, this gives us

\[ H_i = -2J\gamma \mu_0 \sum_{j=1}^{NN} \vec{S}_j = -\frac{\mu_0}{\gamma} \vec{M} \cdot \vec{H}_{\text{ex}}, \]  

(2.13)

where \( \sum_{j=1}^{NN} \vec{S}_j \) stands for the sum over the nearest neighboring spins. This allows us to describe the interaction of the spin of a particle in a lattice with a field term called the effective exchange field \( \vec{H}_{\text{ex}} \). Exchange is important for the spin wave dispersion particularly at large wave vectors. Its isotropy leads to the isotropic dispersion relation of exchange spin waves \[32\].

2.4. Zeeman energy

The Zeeman energy describes the energy of an external field \( \vec{H}_{\text{ex}} \) inside a magnetic body:

\[ \varepsilon_{\text{Zeeman}} = -\mu_0 \vec{M} \cdot \vec{H}_{\text{ext}}, \]  

(2.14)

where \( \varepsilon_{\text{Zeeman}} \) represents the magnetic energy density. This energy leads to a gapped spin wave spectrum starting from the frequency of the ferromagnetic resonance at \( f_{\text{FMR}} \)[33].
2.5. Demagnetization field

As a finite sized solid body is magnetized, magnetic surface charges will cause magnetic stray fields outside of the body and demagnetization fields inside the body. The latter will counteract the magnetization of the body and, thus, will lower the effective magnetic field. It can be derived from the stationary magneto-static Maxwell equation:

\[ \nabla \hat{B} = \nabla(\hat{H} + \hat{M}) = 0, \]
\[ \nabla \times \hat{H} = \vec{j}, \]

and can be split up into a curl field \( \hat{H}_{\text{ext}} \propto \vec{j} \) and a curl free field \( \hat{H}_{\text{demag}} \). Thus, the demagnetization field can be evaluated by a magneto-static potential \( \nabla \Phi = -\hat{H}_{\text{Demag}} \) to:

\[ \hat{H}_{\text{demag}} = -\nabla \Phi \propto \int \vec{N}(\vec{r} - \vec{r}')\vec{M}(\vec{r}')d\vec{r}', \]

with the demagnetization tensor \( \vec{N}(\vec{r} - \vec{r}') \):

\[ \vec{N}(\vec{r} - \vec{r}') = -\frac{1}{4\pi} \nabla \nabla' \frac{1}{|\vec{r} - \vec{r}'|}. \]

Since this includes a integral over the volume of the magnetic body, it follows that analytical solutions are usually restricted to simplified assumptions about the magnetization and geometry of the problem, as the field can become substantially complex for more complicated scenarios. As such, the local magnetization can vary by a great degree over the magnetic body and introduces an anisotropic effect on magnetization dynamics. Herein lies the strength of the numerical approach, as it can later be seen in subsection 4.2.3, since the magnetization can be easily calculated when using discretized magnetic moments in a finite difference approach. However, as magneto-static effects are of a long-ranged nature, its calculation takes the main part of processing time but can be accelerated when using finite difference discretization (see section 3.1 for further details).

Demagnetization, or in general, the magneto-static interaction, is of substantial importance for the spin wave dynamics. It governs their dispersion at short wave vectors \( \vec{k} \) and is the origin of the anisotropic dispersion of the so called magneto-static spin waves [32].

2.6. Dzyaloshinskii-Moriya Interaction

The Dzyaloshinskii-Moriya Interaction (DMI) is a phenomenon resulting from spin-orbit coupling combined with broken symmetry [34], such as at the surface of a magnetic material [35]. This interaction is antisymmetric in nature and leads to a linear increase or decrease of the spin wave frequency depending on the direction of propagation perpendicular to the static magnetization.
2.7 Anisotropy field and Magneto-crystalline anisotropy

The experimental fingerprint of DMI will be further discussed with its manifestation in spin wave spectra in Section 4.1.

### 2.7. Anisotropy field and Magneto-crystalline anisotropy

The magnetic anisotropy leads to the energetic preference of specific directions of the magnetization. It is expressed as the anisotropy field \( \vec{H}_{\text{anis}} \).\[27\]\[23\] The direction which is energetically lower for the system is called easy axis and the energetically higher one hard axis. The effect has various origins with the form anisotropy and the magneto-crystalline anisotropy being the most prominent. The latter is caused by the spin-orbit-coupling in the solid body or at the interfaces of the magnetic layer, while the form anisotropy is caused by circumventing stray fields, which are energetically positive.

In this work, the uniaxial magneto-crystalline anisotropy of the first order, and the anisotropy resulting from the demagnetization, also known as the shape anisotropy field \( \vec{H}_s \), is used in the simulations.

An uniaxial magneto-crystalline anisotropy of the first order \( K_u \) exhibits the following effective field term:

\[
\mu_0 \vec{H}_{\text{anis}} = \frac{2K_u}{M_s} (\vec{u} \cdot \vec{m}) \vec{u}
\]

where \( \vec{u} \) is a unit vector which represents the direction of anisotropy.
CHAPTER 3

Framework Architecture

Micromagnetic Simulations have emerged as a potent alternative to analytical and experimental studies of the magnetization dynamics. Over the past decades, a large variety of software was developed with increasing accuracy and complexity. As analytical formulas are scarce and often limited by many boundary conditions in this domain of physics, the significance of numerical studies cannot be underestimated. With the advent of powerful GPU-based micromagnetic simulation programs like MuMax3, enormous amounts of numerical data about physical problems can be generated, even when using relatively affordable hardware. This imposes a new set of requirements to the modus operandi of a modern physicist and it becomes increasingly similar to the everyday life of a data scientist. Thus, it is not far-fetched to avail oneself of the methods and tools of the latter and introduce them as means to subdue the impending chaos which almost boundless amounts of simulation data bring. The framework is built for exactly this purpose. It embeds the simulation program and introduces tools to operate it in a larger frame, ranging from parametric sweeps to the organization and distribution of individual simulations across different workstations to the automated evaluation of all generated data. It comes with a graphical user interface, a database, and several small tools to examine the results, thus making the amount of simulations almost only dependent on the available hardware. Large-scale studies of parameter spaces are made possible and the foundation for investigations more intricate than simple parameter sweeps is laid.

This chapter will introduce the different building blocks, the flow and shape of the relevant data and will give an overview of MuMax3, the simulation program used in this work.

3.1. MuMax 3

Over the past decades, many micromagnetic simulation programs were developed, with the Object Oriented Micro Magnetic Framework (OOMMF) [15] developed by the National Institute for Standard and Technology (NIST) being the standard for more than a decade. MuMax3, developed by Arne Vansteenkiste at Ghent University, has a comparably young history but it possesses a strong asset which allowed it to prevail over its predecessors. Namely, it is the first open-access framework to utilize modern desktop graphic processing units (GPU), which allow for an increase
3.1 MuMax 3

in efficiency of an order of 140x compared to the CPU-based simulation programs with affordable hardware [16]. It is written in the programming language Go and CUDA (Compute Unified Device Architecture) and is developed as open-source software at [http://mumax.github.io](http://mumax.github.io). The program is built using finite-difference discretization, which divides the mesh into equally sized orthorhombic cells. This periodicity allows the application of the fast Fourier transform (FFT) to switch into the reciprocal space, where certain calculation steps can be processed significantly faster, with the drawback of lesser geometrical flexibility which finite-element micromagnetic software like NMag [20], TetraMag [19] or MagPar [18] offers. This becomes apparent when looking at the calculation of the demagnetization field:

\[
\vec{H}_{\text{demag}} = -\nabla \Phi = \int_V \vec{N}(\vec{r} - \vec{r}')\vec{M}(\vec{r}')d\vec{r}'
\]  

(3.1)

which can be interpreted as a convolution \(\vec{M} * \vec{N}\). The convolution theorem then gives us

\[
\mathcal{F}(\vec{M} * \vec{N}) = \mathcal{F}(\vec{M}) \circ \mathcal{F}(\vec{N})
\]  

(3.2)

where \(\circ\) stands for the component-wise multiplication. The term \(\mathcal{F}(\vec{N})\), which corresponds to the demagnetization kernel, does not vary in time. Hence, it has to be evaluated only once. Solely \(\mathcal{F}(\vec{M})\) will be calculated for each time step and convoluted with the demagnetization kernel. Afterwards, the result will be transformed back into real space by the inverse Fourier transform. Since the FFT computation time for \(n\) cells scales with \(O(n \log n)\) instead of \(O(n^2)\) for the case without the convolution, the advantage of the finite-difference discretization becomes apparent. Since the FFT is most efficient for \(2^n\) elements, the simulation area is always divided into \(2^n\) cells for each spatial direction in the course of this thesis.

The cell size in SI units is a decisive factor for the quality of the simulation. Typically, for micromagnetic simulations cell sizes corresponding to the smallest element of interest are chosen to be in the order of:

\[
l_{\text{ex}} = \sqrt{\frac{2A}{\mu_0 M_s^2}}
\]  

(3.3)

The width of the Néel wall has been used here to define the magneto-static exchange length \(l_{\text{ex}}\) [36], which is the relative strength of the exchange and magneto-static energy and gives a lower bound for reasonable cell sizes (along with the approximation conditions of the Heisenberg-Model, which fail for very small cells due to their nature as a small angle approximation). While running, MuMax3 calculates the magnetization as an individual magnetic moment for each grid cell. As every moment is influenced by its environment, the exchange and dipole interaction have to include the contributions from other cells. While the former is relatively short-ranged and, thus, only few cells have to be considered, the latter constitutes the bulk of computational effort due to its far-reaching nature. The resulting magnetization is then convoluted with the demagnetization kernel.
to yield the corresponding field $\vec{H}_{demag}$. This field term is then summed up to the effective field $\vec{H}_{eff}$ together with the various occurring static and dynamic fields, as mentioned in [2,3]

$$\vec{H}_{eff} = \vec{H}_{ext} + \vec{H}_{ext}(t) + \vec{H}_{anis} + \vec{H}_{ex} + \vec{H}_{demag} + \vec{H}_{dmi} + \vec{H}_{therm} \cdots .$$ (3.4)

Once the effective field is evaluated, the LLG-equation is solved for each cell and the next iteration of this procedure starts. MuMax3 provides a number of explicit Runge-Kutta methods for advancing the Landau-Lifshitz equation with RK45 (Dormand-Prince-Method) being set as the default solver. In addition to the solution, the solver also provides an error estimate. On that basis the time step is chosen in order to keep the error across the whole simulation time below a critical value.

The dynamical contributions included in the program, beside the Landau-Lifshitz torque, are the Zhang-Li spin-transfer and the Slonczewski spin-transfer torque. Also, thermal fluctuations are implemented via a stochastic Brownian field since the recent update 3.10.$\beta$.

The ground state can be found using the relax() function, which disables the precession terms (Landau-Lifshitz torque, Zhang-Li spin-transfer and Slonczewski spin-transfer torque). In this scenario, the effective field points towards decreasing energies. Hence, by advancing the damping term in Equation 2.10 in time until the total energy reaches the numerical noise floor, a state close to equilibrium is reached. Afterwards, the function tries to minimize the torque instead of the total energy, as the former tends to be less noisy and, thus, allows for a higher precision. The maximum error for the solver will then be lowered and the procedure is repeated until this error is reached.

It is important to note that the solver can be stuck in a saddle point, local minima or flat part of the energy landscape [16]. To counteract this issue, in all the applications presented in this work, the relax routine was extended by a simulation time with activated precession terms, minimizing residual torques. The information about the various internally used physical units, like the magnetization and effective field, can be saved for each cell. Typically, a time interval after which the quantity in question should be saved is defined. However, as the aforementioned internal time step of the solver is adaptive, the resulting save intervals can vary. This becomes important during the evaluation of the generated data which includes a fast Fourier transform (FFT) in time, therefore relying on equally spaced data points (see section 3.3 for further details).

The data generated is by default stored in a binary format created for the original micromagnetic simulation program OOMMF [15]. The format is used throughout this work. It contains information of the specified physical variable for each cell across the whole simulation area and a header which contains information about the mesh and time step and, thus, allows for various studies of the temporal course of the simulation.

The configuration of a simulation is done via a user written script file. Therein, one defines all the necessary parameters like the geometry, material parameters, the mentioned cell sizes, etc.. The syntax of these scripts is defined by a subset of the programming language Go, on which MuMax
3.2 Processing Pipeline

is built. It is practical to use separate scripts for ground state and dynamic simulations. The former is responsible to find the minimum of energy for a given geometry and set of fields, while the latter takes care of cases where the system behavior in time is of importance.

Since solving the LLG equation can be parallelized well, graphic cards can be used to boost the performance of micromagnetic simulations. Not only are Graphics cards specifically built to calculate in parallel, i.e. when rendering 3D objects to the pixel space, they also have a large and very quickly connected main memory which allows to store intermediate results in the GPU-RAM. Thus, the simulation program can quickly generate massive amounts of data on modern GPUs. The analyzation thereof can then easily become a non-trivial task and will be the main topic of the next section.

3.2. Processing Pipeline

As the main imperative of this software is to minimize manual input and, thus, making comparisons between measurement and simulation easily conductible, it is apparent to begin with a routine which will automatically queue the simulations. A real world example, where the benefits of such a routine becomes apparent is the excitation of spin waves via an oscillating external field. In real-world experiments, it is often the case that the external fields are varied for a constant excitation frequency. However, as a different external field can strongly alter the energy minimum of the spin configuration in a solid body, a new ground state has to be calculated. Thus, for every different field, a new set of ground state and dynamic simulation has to be created. Hence, it is of importance to find suitable solutions for creating the respective scripts with a given set of parameters and distributing them to the available computing resources.

Once this step is done, the automatically running simulation series can quickly generate large amounts of data. As such, the evaluation thereof can’t be done without additional automation in a humanly possible way. Firstly, however, it is necessary to know which evaluation tasks are needed. For acquiring insights about the properties of a system, it is typical to analyze the dispersion relation or to look at the behavior of specific frequency-wave vector combinations as a function of field. A typical example is ferromagnetic resonance spectroscopy, where the position of the uniform excitation is mapped as a function of the magnetic field. This can deliver material constants like the saturation magnetization $M_{\text{sat}}$ and the Gilbert damping factor $\alpha$ by observing the dependence of the excited resonance frequency under the change of the static external field. Hence, the automatic extraction of the dispersion relation from the dynamic simulation data becomes of high priority. However, as diverse as micromagnetic simulations are it is evident that the evaluation thereof varies to a similar degree. Therefore, the design of the analyzation process of the numerical data should be as generic as practicable. The idea is to create the possibility to tailor the
post-processing of finished simulations to each individual problem. When a basic procedure to gain interpretable results is developed, tasks like fitting a multitude of parameters, such as the anisotropy, exchange, DMI or other constants to an experimentally measured data set concurrently, become possible. Consequently, steps have to be taken to ensure a humanly readable representation of the generated results. The development of a database with metainformation about each simulation, like the parameters used, the storage location, etc., and a rudimentary user interface to keep track of the simulation queue and results, is therefore an important step along the way to thorough automatization. Especially as the database can also help tremendously at the task of distributing simulation jobs. To ensure that available computing resources are used to their full extent, ample details have to be taken care of, like distributing the workload between the different GPUs in one computer and the available machines in the network, where the database comes into play. Also, as the size on the hard disk of the simulation data can reach significant levels, methods for post-processing which eliminate unnecessary data have to be implemented.

The simulation framework is built in Python as the main programming language, which connects all the individual components together. The language was chosen as it offers a clear and readable syntax and powerful libraries. Python is a dynamically typed language and, thus, has a lot of overhead computational work for all operations. However, the evaluation of simulations is quite expensive as the data quickly reaches sizes of several GB. As such, this language is not expected to do well in this domain. Nevertheless, it serves as the connecting piece to all the different high-performance languages, allowing us to wrap everything we need into one common framework. Expansive data analysis and mathematical Python libraries, mainly NumPy and SciPy, have emerged over the past years, which wrap their Python functions around an implementation in C or even Fortran. Thus, one gains the clear and readable syntax and interoperability of Python with the high performance and optimization opportunities of static typed languages like the ones mentioned before. Prototyping, experimenting and automated analysis with large amounts of data is, thus, very approachable. The MuMax3 simulation itself is powered by Go and is merely called with the required arguments by the Python framework.

3.2.1 Job Creation

Firstly, one has to define the starting parameters and constants of new simulations, like the world size, cell size, material properties, etc. Then, it is often advisable to split the calculation of the ground state and the dynamic part into separated files as it will save a lot of computation and storage resources, since one ground state can be used for a multitude of dynamical simulations. The framework can handle these cases and offers various optimizations. The raw ground state and
3.2 Processing Pipeline

Figure 3.1: Schematic structure of the framework. Firstly, all required scripts and parameters are packed and loaded to the database. Afterwards, the computation nodes receive this data and start to run the simulations and post-processing. The created results can then be gathered and analyzed and a new simulation series, based on the previous results, can be started.

dynamic script are then provided as a template to the program. Afterwards, the parameter space has to be provided in the format of a .csv file. Two strategies for creating the individual parameter sets are available at the time of writing this thesis:

**Combinatory** - create a simulation for every possible combination of available different parameters;

**Single line** - Supply sets of defined combinations.

The program then replaces the provided parameters in the template scripts and packages them to an entry in the database along with some meta-information, for example the creation time. They are saved along a corresponding entry of a "simulation series object", which possesses information about all the jobs. Additionally, it can contain scripts for the post-processing of finished ground
state and dynamic simulation. When initializing the MuMax3 ground state scripts on the local computer, the program searches for the most similar, already calculated, ground states of the same series and replaces the initial magnetization with the one obtained from the old state. This can save significant amounts of calculation time, as, for example, a slightly different external field will shift the energy minimum in question also only slightly. Thus, the simulation is already in a state close to the desired one. However, care has to be taken when using this option, as in certain cases the direction of the effective field can change dramatically, e.g., when the intervals between the provided external field parameters are relatively large, and hence could introduce unwanted domain walls.

While operating the program, a folder for demagnetization kernels can be set. MuMax3 will then be given the respective commands to either save the calculated demagnetization kernel or use it, if its already available for the respective geometry. When creating the dynamic scripts, the initial magnetization is replaced by the corresponding ground state calculation on the local machine or, when it was processed on another computer, requested over the network. With all the optimization methods mentioned above and with the fact that several dynamic jobs can share one ground state, the speed and efficiency of the computation of a multitude of simulations increased significantly compared to the manual standard.

### 3.2.2 Distribution

All information needed for the computation of the simulation series is loaded onto a database. In the time of writing in this thesis the database runs with PostgreSQL [postgresql.org] and the interactions are handled using the Python framework Django [djangoproject.com]. Computation nodes which run the framework, typically a workstation or a dedicated GPU-server, will periodically check the database for available jobs to compute. Once new jobs are available, a node will fetch all needed information, e.g. the MuMax3 script, a possible required ground state simulation and post-processing tasks for the results. During that process, the job entry is blocked from access by other nodes and will subsequently be marked as running, to prevent multiple nodes from running the same job. As of now, no priorities are assigned for individual nodes, but this could easily be implemented within the current pipeline, for example, by assigning weights based on the computing complexity of the simulation and an internal factor for each machine which represents its computing power.

### 3.2.3 Computation and Post-Processing

Once all necessary files are downloaded, the program will check if all requirements are met, like having the correct ground state locally available and enough free GPU resources available. If the ground state was computed by a different node, the program will look up the network address in
the database and fetch all necessary files via a Peer-to-Peer network integrated in the framework. If all conditions are met, it will call the MuMax3 program with the corresponding parameters. The program will start as many simulations as GPUs are available, however it will not load multiple jobs onto one GPU at the same time, as it was shown that this is very likely to slow down the computation due to the overhead created from context switching. As the simulations will only use up marginal CPU resources, the framework will start the specified post-processing of available simulation results in parallel to the running simulations. After a job is finished, the corresponding database entry is updated and marked as complete or erroneous. The machine which finished the job then looks up the post-processing scripts defined for the respective series and executes them. This typically entails the conversion into NumPy arrays and subsequent deletion of the OVF data in order to save disc space and to easily access the data within Python.

For the interpretation of the data, it is possible to look at the individual time steps. From this, information such as the wavelength of the excited modes can be extracted. For the interpretation of the temporal course of the simulation, however, this representation is unsuitable. Therefore, the benefits of the construction of a matrix which encompasses all time steps is apparent. For this work, all raw data is read-in as a 4-dimensional matrix for each step individually with the axes \([z, y, x, n]\), whereby \(z, y, x\) are the cell indices in the respective direction and \(n\) being the selected physical component, which is typically the magnetization vector. In the case of time resolved data, a 5-dimensional matrix with an additional time axis \(t\) is constructed, leading to the format \([t, z, y, x, n]\). Extensive care has to be taken when reading in the data, as one simulation can quickly grow to several tens of GB. If done inappropriately, the import and analyzation of data can be significantly slower than its creation or could potentially bring the computer to a complete halt when the working memory is flooded with too much data. For larger simulated systems, the working memory limit could very well be exceeded and would then force sequential processing of the data. In this work, the simulation size was small enough to fit inside the working memory of the utilized computers (32GB) and the NumPy package delivered enough performance to keep the time spent analyzing in a reasonable frame, as it resorts to heavily optimized functions in C and Fortran. As such, all the evaluation programs used in the framework are using the NumPy/SciPy stack.

Another recurring task is to fast Fourier transform the data from the space-time into the frequency-wave vector domain to acquire the dispersion relation of a dynamic simulation (see section 3.3 for further details).

### 3.2.4 Gathering

In order to get the whole set of post-processed results, a storage server can request all the nodes to send their computed results over the network. The IP address of the corresponding nodes is saved
3.3 Evaluation

in the database. All nodes have a mirrored folder structure to enable quick access to relevant files. The directory path for each job is saved in the database, starting from the root folder. As all the relevant data is now available on one machine, it is now ready to be interpreted.

3.2.5 Analyzation

Potent scripts can be quickly created, which can iterate over all the simulations of a series. This is enabled by having easy access to the database, which contains all the meta information about the jobs regarding changed parameters, the data folder, the script, the corresponding ground state, etc. Examples of the results of those scripts can be found in chapter 4, e.g., phasemaps of a parameter sweep with two variables, the width and field of a waveguide. After evaluation, one can either manually create new adapted parameter lists / script files or automate the process of job creation with optimization algorithms providing the new input parameters. This is of special interest as many motives for numerical simulations of a physical system can be reformulated as an error function, e.g., when one tries to excite spin waves in a waveguide at a certain efficiency for a given field and antenna configuration. With the difference to the desired efficiency as the error function, it is conceivable to vary the free parameters via machine learning algorithms like an evolutionary strategy algorithm and, thus, explore a potentially highly non-linear solution space with proven methods for these types of problems.

3.3. Evaluation

In this chapter, relevant evaluation methods are discussed with the calculation of the dispersion relation from the simulation data as the most important one.

3.3.1 Calculation of the dispersion relation

In order to obtain the dispersion relation from the simulation data, several steps have to be taken, with the discrete fast Fourier transformation (FFT) being the most important one. This transforms the data from the space-time domain into the frequency-wave vector domain. In general, one first applies the FFT on the real space simulation area. This yields the wave vector amplitude over time. Finally, the FFT is performed on the time axis and delivers the frequency-wave vector Fourier signal. However, as this data has, in a general case, still four dimensions ($t, k_x, k_y$, and $k_z$), it is typical to reduce the problem to only the relevant dimensions, e.g., the wave vector of the spin wave in propagation direction. Here, the amplitude of the dynamic magnetization component is summed in real space over the in-plane axis, where the excitation happens mostly homogeneously. Afterwards, a FFT is performed along the axis where the spin waves propagate. Finally, the FFT in time is performed like in the general case. From the resulting data, points above the Nyquist frequency are removed and only the absolute value of the real and imaginary part is taken, as only
3.3 Evaluation

the amplitude and not the phase, which is included in the imaginary part of the transformed data, is relevant for this work. Typically, the absolute value is also squared in order to receive the intensity. The dispersion relation can then be extracted from the 2D intensity map of the frequency and wave vector. Exemplary, this process is shown in Figure 3.2 for a Yttrium Iron Garnet (YIG) waveguide simulation under excitation with a co-planar waveguide (CPW) antenna, which is later investigated in section 4.2. In the case of only one relevant mode, the dispersion relation consists of the points with maximum amplitude. For multi-mode dispersion relations, special algorithms have to be used to find the peaks. A derivation of the Canny Edge Detection was experimented with and delivered promising results. Ultimately, multi-mode dispersion relations were not relevant for the applications discussed in this work and, thus, no extraction method was fully developed.

According to the Nyquist–Shannon sampling theorem, the time interval between the saving of magnetization $T$ and the cell size $C_i$ determine the maximum resolvable frequency $f_{\text{max}}$ and wave vector $k_{\text{max}}$ with $T = \frac{1}{2f_{\text{max}}}$ and $k = \frac{1}{2k_{\text{max}}}$ respectively. Furthermore, from the characteristics of the FFT follows, that the frequency and wave vector resolution is dependent on the run time and world size.

It is to be noted that since MuMax3 uses an adaptive time step derived from the calculated error at each step, the save intervals are not equidistant to one another, which, however, is a prerequisite for the correct evaluation of the FFT. Thus, the data has to be interpolated to equidistant points along the time axis. As one is interested in the magnetization dynamics, it can be often beneficial to subtract the ground state before calculating the FFT.

Figure 3.2: Schematic of the transformation process from real space to the frequency-wave vector space for an exemplary waveguide simulation.
3.3.2 Script library

Over the course of the thesis, various scripts, which either analyze the data of an individual simulation or of a whole simulation series were developed. They are typically of short length, as they can make use of more generic functions, for the example the one mentioned above, which transforms the data into the frequency-wave vector space. Additionally, plots of the results of those routines will be created with the help of the open-source package Matplotlib [matplotlib.org]. Other scripts contained in the framework help with the organization and management of raw and processed data and plots or serve to keep the overview of the state of simulation series and their results. A list of the most used routines is presented here:

**Evaluation scripts:**

- Plot of frequency-space map and time-space map with interactive sliders to change the selected time step, frequency, z-layer and magnetization component.
- Frequency spectra over integrated wave vectors and maximum intensity frequency and full-width-half-maximum extraction of these peaks.
- Plot of ground states, effective field, cutlines at arbitrary positions thereof and direction of magnetization/effective field vector.
- Phasemaps of arbitrary variables from a simulation series.
- Modeprofiles of selectable frequencies.
- Intensities of selectable frequencies over an axis and determination of their decay length.
- Best fit finder which compares the results of simulations in a series to experimental data.
- Extract frequency at a fixed wave vector over externally applied field.
- Skyrmion classification and lifetime analysis based on their winding number.

**Organization scripts:**

- Automated report generation of simulation series in latex.
- Automated deletion of unneeded series data.
- Update running scripts.
- Messenger bot in the instant messenger Telegram, which updates about the state of simulation series.
3.3 Evaluation

- Automated installation of the framework.
In this chapter several applications of the framework are discussed. It will be shown, that the dispersion of singlelayer structures can be engineered via parametric sweeps and automatic evaluation of the gathered simulation data.

Both films are compared to experimental data. While in Pt/CoFeB a strong symmetric and asymmetric exchange energy leads to an observable dispersion, the dispersion in W/CoFeB is found to be rather flat in the experiment. The simulation series tries to evaluate if this is mediated by much weaker interactions in the W/CoFeB layer stack or by the presence of a strong perpendicular magnetic anisotropy. In fact, the W/CoFeB films are out-of-plane magnetized in remanence due to a strong perpendicular magnetic anisotropy. The magnetization is pulled in-plane by an external in-plane field in the simulation as well as the experiment.

In the second part, waveguides of CoFeB with varying widths, antenna and external fields are examined in order to design dispersion curves which are close to one another. This allows to design simple magnonic filter devices, like spectrum analyzer, delay lines, etc.

4.1. Ultrathin film simulations

In this example the dispersion relation of spin waves in ultrathin films with a thickness of $\approx 0.6\text{nm}$ are examined. Based on experimental data obtained by Brillouin Light Scattering measurements of spin waves, simulations are performed.

As the dispersion relation gives insight into various physical properties of the studied system, such as the interfacial Dzyaloshinskii-Moriya interaction (DMI) \[37]\ and the exchange constant, it has come to be a major object of investigation. Recently, a facile extraction method of the exchange constant and interfacial DMI from BLS measurement data was reported \[38]: To obtain the symmetric exchange constant, it is suggested to average over the Stokes and anti-Stokes signal to eliminate the DMI-induced frequency shift. Afterwards, a parabolic fit delivers the constant in question by using an approximation of the dispersion relation $f(k)$ \[32]:

$$f(k)_{\text{sw}} = f_{\text{FMR}} + \beta |k| + Jk^2 + \frac{\gamma}{\pi M_s} Dk$$  \hspace{1cm} (4.1)
where the averaging over Stokes and anti-Stokes $f(k)$ eliminates the DMI term and leaves

$$f(k)_{\text{sym}} = f_{\text{FMR}} + \beta |k| + Jk^2$$

(4.2)

for the symmetric exchange approximation.

On the other hand, the asymmetric contribution can be extracted by

$$f(k)_{\text{asym}} = \frac{|f(k)_{\text{stokes}} - f(-k)_{\text{stokes}}|}{2} = \frac{\gamma}{\pi M_s} Dk$$

(4.3)

Thus, from a simple angle-resolved BLS measurement, it is possible to obtain a series of material constants. Nevertheless, a few assumptions need to be made in order to extract the two exchange constants and it is, thus, of interest to compare the results from this simple estimation to a full micromagnetic simulation. In addition, this problem constitutes an appropriate test case for the framework, since parameter sweeps and and automatized analysis can be used here with a rather simple physical system. Thus, in the following, parameter sweeps will be performed for the two material systems in order to obtain a best fit between the experimental data and the numerical simulations. The best fit is determined by the simulation with the minimal difference to the interpolated experimental data.

![Simulation geometry and field configuration](image)

Figure 4.1: The simulation geometry and field configuration for (a) in-plane geometry and (b) out-of-plane geometry. The perpendicular magnetic anisotropy field is represented by $H_{\text{PMA}}$.

For both material systems, a series of common basic elements of the simulation are fixed. The magnetization component $m_x$, pointing in the direction of the dynamic field, was used for evaluation. For both films, an infinitely extended thin film of a thickness of 0.6 nm is simulated using periodic boundary conditions (PBC). The basic simulated area is 20.48 µm x 1 µm in size and...
4.1 Ultrathin film simulations

is fictively prolongated to infinity to mimic a plain film [16], like shown in Figure 4.1. For both material systems, several parameters like the external field, the perpendicular anisotropy constant, or the symmetric and asymmetric exchange constants are varied in a range centered around the parameters extrapolated from the experiment. In this process, first, the series of the corresponding ground states is being simulated. In all simulations, the in-plane magnetic field is essentially applied along the y-axis, with a small tilting angle of 1° to break the symmetry of the system. Consequently, the dispersion in these magnetization landscapes is determined by the excitation of the system with a short pulse that is localized in a 20 nm wide region in the center of the films extending along the y-direction and, thus, leading to spin wave propagation into the x-direction. A sinc-pulse in the time-domain is used to ensure a broadband spin wave excitation up to a predefined maximum frequency. The consequent data are Fourier transformed from the space-time into the frequency-wave vector domain in order to extract the dispersion relation. As the system in this geometry features one dominant mode that can be excited by the antenna field, the dispersion can then be simply extracted as the frequency position of the maximum Fourier intensity at a given wave vector, as described in subsection 3.3.1. In the following, the simulation series and the analysis and parameter fits in the two material systems will be discussed, starting with Pt/CoFeB.

4.1.1 Pt/CoFeB Sample

For the Pt/CoFeB/MgO series, a clear symmetric and antisymmetric dispersion have been observed in the experiment, which is shown in Figure 4.2. To confirm the parameters obtained from the fitting described in Equation 4.2 and Equation 4.3, the symmetric exchange constant $A_{ex}$ and the asymmetric exchange constant $D$ are varied in the simulation series. Additionally the perpendicular magnetic anisotropy (PMA) strength is being optimized by a comparison to experimental data showing the evolution of the spin wave resonance frequency at an incidence angle of 5° ($k = 11.81$ rad/µm) as a function of field. Other parameters, namely the applied external field and the saturation magnetization are taken from the experiment. The investigated single layer sample consists of Pt(5 nm)/Co$_{20}$Fe$_{60}$B$_{20}$(0.6 nm)/MgO(2 nm)/Ta(5 nm). Table 4.1 shows the resulting parameter space that has been varied. As is highlighted in Figure 4.2 (b), for each parameter set, the Fourier spectrum is obtained in the frequency wave vector domain and the dispersion of the Damon-Eshbach spin wave mode is clearly visible. The maximum intensity at each wave vector is determined and associated with the resonance frequency of the spin wave mode. This way, the white line shown on top of the intensity map is constructed. The figure shows the best fit obtained in the simulated parameter space: $A_{ex} = 20$ pJ/m, $D_{ind} = 1.3$ mJ/m², $K_{u1} = 0.50$ mJ/m². These parameters are the same from the experimental ones: $K_{u1} = 0.50$ mJ/m², $D_{ind} = 1.3$ mJ/m², except for $A_{ex} = 27.5$ pJ/m, which is slightly higher in the experimental approximation. Figure 4.2 (a) shows the best fit (orange)
4.1 Ultrathin film simulations

Table 4.1: List of the parameters used in the Pt/CoFeB sweep.

<table>
<thead>
<tr>
<th>$D_{\text{ind}}$ mJ/m²</th>
<th>$A_{\text{ex}}$ pJ/m</th>
<th>$K_{\text{ul}}$ mJ/m²</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.15</td>
<td>15</td>
<td>0.46</td>
</tr>
<tr>
<td>1.2</td>
<td>20</td>
<td>0.50</td>
</tr>
<tr>
<td>1.25</td>
<td>25</td>
<td>0.54</td>
</tr>
<tr>
<td>1.3</td>
<td>27.5</td>
<td>0.58</td>
</tr>
<tr>
<td>1.35</td>
<td>30</td>
<td>0.63</td>
</tr>
<tr>
<td>1.4</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.83</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.88</td>
</tr>
</tbody>
</table>

Together with the experimental data and the dispersion that results if the experimental parameter are used.

![Figure 4.2](image)

**Figure 4.2:** The dispersion relation of Pt/CoFeB in Damon Eshbach geometry with pronounced interfacial DMI. (a) The dispersion relation obtained from the experimental measurement, the best-fitting simulation and the simulation with the experimentally approximated parameters. (b) The Fourier transformed simulation data of the $y$-component of magnetization in time and space and the detected dispersion relation as the white curve.

As is visible from the figure, the experimental parameters lead to a stronger increase of the frequency than the experiment and the best fit due to the larger assumed symmetric exchange. Nevertheless, the obtained value $A_{\text{ex}} = 20$ pJ/m from the best fit is still quite large for this material system.
4.1 Ultrathin film simulations

4.1.2 W/CoFeB Sample

In the Pt/CoFeB system, a quite strong DMI constant and a quite strong symmetric exchange constant have been observed in the experiment and confirmed in the simulations. A correlation between these two quantities has been reported in literature [39]. This statement constitutes one of the main driving points beyond this analysis. In fact, in W/CoFeB (W(5 nm)/Co\textsubscript{20}Fe\textsubscript{60}B\textsubscript{20}(0.6 nm)/MgO(2 nm)/Ta(5 nm)), overall a very flat dispersion has been observed in the experiment. An asymmetric contribution could nevertheless be extracted and yields a very weak DMI of $D = 0.08$ mJ/m\textsuperscript{2} (see Fig. 4.5 (a)). In turn, a look at the symmetrized dispersion, which is shown in Fig. 4.5 (b), yields a very low slope as well - in fact, it is hardly perceivable within the experimental error. An application of the same analysis as before yields a best fit for a very weak exchange constant of only $A_{\text{ex}} = 3.18$ pJ/m. While this is in line with the picture of a correlation of DMI and symmetric exchange, the value is very low for this material system. In the following, the influence of the perpendicular magnetic anisotropy and perpendicular magnetized ground state of the film on the dispersion will be analyzed and a fitting to the dispersion will be performed in order to give an upper limit for the symmetric exchange constant from the simulations.

To this end, two parameters will be varied. Namely the symmetric exchange constant $A_{\text{ex}}$ and the PMA constant $K_{u1}$:

As the film is naturally out-of-plane magnetized, a typical resonance behavior along a hard axis of anisotropy is observed. As the field is increased, the magnetization starts to reorient along its hard axis, leading to a decrease of the resonance frequency as the internal fields are reducing. At some point, a softening point is reached and for larger fields, the magnetization is aligned along the hard axis. For further increasing fields, the resonance frequency now increases monotonously with
4.1 Ultrathin film simulations

Figure 4.4: The top figure shows the frequency extracted from the dispersion relation of the simulations, the experimental stokes and anti-stokes measurements and the analytically calculated one at a wave vector of \( k = 6.11 \text{ rad/\text{µm}} \) over the externally applied in-plane field. The bottom figure show the angle of average magnetization between the in- and out-of-plane component over the externally applied in-plane field.

Table 4.2: List of the parameters used in the W/CoFeB sweep.

<table>
<thead>
<tr>
<th>( A_{\text{ex}} ) pJ/m</th>
<th>( K_{\text{u1}} ) mJ/m²</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.815</td>
</tr>
<tr>
<td>4</td>
<td>0.825</td>
</tr>
<tr>
<td>6</td>
<td>0.833</td>
</tr>
<tr>
<td>8</td>
<td>0.842</td>
</tr>
<tr>
<td>10</td>
<td>0.847</td>
</tr>
<tr>
<td>...</td>
<td>0.850</td>
</tr>
<tr>
<td>30</td>
<td>0.950</td>
</tr>
<tr>
<td>32</td>
<td>1.000</td>
</tr>
</tbody>
</table>

the ever increasing internal field. From this characteristic behavior, the perpendicular anisotropy constant can be fitted. For this, a two-dimensional space is simulated (see Table 4.2) where the magnetic field and the PMA are varied. The dispersion is again mapped by excitation with a sinc function and the resonance frequency at \( k = 6.11 \text{ rad/µm} \) is extracted and compared to the
4.1 Ultrathin film simulations

Figure 4.5: Asymmetric and symmetric fit of the experimental data.

experiment. The best fit is obtained for $K_s = 0.847 \text{mJ/m}^2$
With the PMA constant being determined, the next quantity of interest is the symmetric exchange.
In a next simulation series, the magnetic field is fixed to the experimental value of 400mT, the
exchange constant is varied from 2pJ/m to 32pJ/m and the dispersion relation is extracted for each
simulation in the wave vector range accessible by BLS.
A best fit, which is shown in Figure 4.6 by the orange curve, is obtained for an exchange constant
of 25 pJ/m. Evidently, this value is much larger than the one from the estimation given in Figure 4.5 (b), for which the corresponding dispersion is shown by the green curve in Figure 4.6 and, in fact, quite comparable to the value in Pt/CoFeB. For completeness, also the dispersion curve for
the parameters extracted from the Pt/CoFeB series is shown by the dark violet curve. The reason
for the large discrepancy between the best fit and the simple estimation from the symmetrized dis-
persion becomes evident from Figure 4.6:
In the case of a dominant PMA, the resulting dispersion relation has a negative slope for small
wave vectors, even in the Damon-Eshbach geometry. In fact, this behavior is well described by the
analytical formula [40].

$$ f = f_0 \pm f_{\text{DMI}} = \frac{\gamma \mu_0}{2\pi} \sqrt{(H + J k_{sw}^2 + P(k_{sw} t) M_s)(H + J k_{sw}^2 - P(k_{sw} t) M_s - H_{K_{eff}})} \pm \frac{\gamma}{\pi M_s} D k_{sw} $$

with $\gamma$ as the absolute value of the gyromagnetic ratio, $H$ representing the in-plane applied field,
$M_s$ the saturation magnetization, $J = \frac{A_{sw}}{\mu_0 M_s^2}$ the spin wave stiffness, $H_k$ the uniaxial anisotropy field,
$H_{K_{eff}} = H_k - M_s$ the effective anisotropy field and $P(k_{sw} t) = 1 - \frac{1 - \exp(-|k_{sw}| t)}{|k_{sw}| t}$. The red curve in
4.2 Waveguide Studies

Figure 4.6 shows this analytical calculation, which is resembling the numerical result, which is given by the orange curve, to a large extent. The origin of the slight shift of about 50 MHz between simulation and theory could not be identified, despite a large error analysis. Despite the small shift, both, numerics and analytical theory highlight that in systems with large PMA, one has to be extremely careful with simplified extractions of the material parameters. The negative slope of the dispersion falsifies the analysis given in Equation 4.4. A proper theory needs to be fitted to the results or, if no proper theory is at hand, a parameter sweep as provided by the framework should be applied to obtain a correct estimate of the material parameters.

Figure 4.6: The dispersion relation of W/CoFeB in Damon Eshbach geometry with strong PMA. (a) The dispersion relation obtained from the experimental measurement, the simulation with the best fitting parameters (orange), the experimental parameters extracted from the symmetrized dispersion relation (green), the best fit parameters found for Pt/CoFeB (purple) and from the analytical calculation (red). (b) The Fourier transformed simulation data of the y-component of magnetization in time and space and the detected dispersion relation as the white curve. Also here, the red curve represents the analytically calculated dispersion relation.

4.2. Waveguide Studies

As the excitation spectrum of waveguides is dependent on a multitude of parameters, such as the thickness, width, external field, and the excitation field of the antenna, the engineering of arbitrary spin wave dispersion relations appears to be possible within certain boundaries. Especially, as modern fabrication processes of waveguides allow for precision down to the nanometer scale, the

1In fact, it was investigated whether the difference is a consequence of the time step, the cell size, the size of the simulated area, the damping as well as the excitation amplitude. None of these parameters had any visible effect on the shift.
The geometry of the waveguide can be used as a real-world tuning parameter for the dispersion relation. Hence, applications with tailored waveguide excitation spectra, of which many are conceivable, are within the realms of possibility.

![Schematic of a potential spectrum analyzer based on spin wave waveguides.](image)

Figure 4.7: Schematic of a potential spectrum analyzer based on spin wave waveguides.

The description of spin wave eigenmodes in waveguides is a nontrivial task. In the backward volume geometry, i.e., in longitudinally magnetized waveguides, semi-analytical formalisms can be used to obtain a proper description in thin films as long as the magnetization is uniform across the film thickness. In contrast, the description of higher order thickness modes is already a very complex task. In the Damon Eshbach geometry, i.e., in a transversely magnetized waveguide, this task becomes just impossible by means of analytic or semi-analytic theories. As the magnetization distribution as well as the internal field landscape in this geometry can only be approximated, it is clear that the spin wave dispersion and mode profiles can only be obtained under crude approximations. Micromagnetic simulations, on the other hand, can give the full picture including a correct description of the static and dynamic demagnetization (section 2.5) as well as of the mode profiles of edge modes as well as waveguide modes, thickness modes and hybridization between the various modes.

In the following, it will be demonstrated that for a proper device design, the analytical approximations of the effective field, which is a decisive factor for the possible spin wave eigenmodes, cannot deliver satisfactory accuracy. The device in question is a magnonic on-chip spectrum analyzer which is based on the width dependence of the internal field in transversely magnetized waveguides. First, an analytical description of the key parameter in the device design, the effective field within the waveguide, is given and the concept of operation is explained. Afterwards, full nu-
4.2 Waveguide Studies

Numerical simulations are used in order to confirm the device performance. The objective is to find a reliable way of designing bandwidths with peaks at desired frequencies for a fixed wave vector. In addition to the effects arising from the magnetization configuration and the internal field landscape on the fundamental waveguide mode, the contribution of higher order waveguide modes and edge modes to the excitation spectrum is studied in the micromagnetic simulations. To structure the device, two magnetic materials will be chosen. Yttrium Iron Garnet, a ferrimagnetic insulator with a low saturation magnetization \( M_{\text{sat}} = 147 \text{kA/m} \) and the aforementioned metallic ferromagnet CoFeB with a high saturation magnetization \( M_{\text{sat}} = 1560 \text{kA/m} \). For the device, which heavily relies on demagnetization effects, these two materials should result in very different frequency regions for the operating device and in the following, their performance will be benchmarked.

Figure 4.5 shows a schematic of the device. An array of finely tuned waveguides will be excited by the same co-planar waveguide (CPW) and the resulting signal will be detected by spin pumping and the inverse spin hall effect (iSHE).

As the excited wave vector range has to be as narrow as possible in order for the concept to work, a CPW-antenna was chosen as initial excitation source, like shown in Figure 4.8. The field distribution of such an antenna has an out-of-plane (\( \perp \)) and in-plane (\( \parallel \)) component. It can be calculated by summing up the Oersted fields of the respective antenna-stripes (see Appendix) \[43\]. The calculated field distribution along the \( y \)-axis, using the configuration shown in Figure 4.8, is displayed in Figure 4.9(a). The corresponding Fourier transformation, shown in (b), confirms that only a narrow range of wave vectors is excited efficiently by the antenna. The minima of excitation in the reciprocal space are positioned at \( n2\pi/d \), where \( d \) is the spacing between the strip lines.

Figure 4.8: Geometry of the CPW.
4.2 Waveguide Studies

Figure 4.9: (a) The in-plane and out-of-plane field distribution of a CPW in the middle of a spin wave waveguide along the width axis. (b) The FFT of the field distributions shown in (a).

4.2.1 Simulation Setup

In Figure 4.10, a section of a waveguide is shown along with the acting magnetic fields. In contrast to section 4.1, the out-of-plane component $m_z$ of the magnetization is extracted for evaluation since the system is in-plane magnetized. The waveguides used in the simulations, have a significantly larger length than width and a fixed height of $t = 50$ nm. Due to this aspect ratio, the remanence magnetization aligns along the length of the waveguide (long axis, $x$). The external field $H_{\text{ext}}$ is applied along the short axis ($y$) and, thus, counteracts the remanence magnetization and pulls the effective field into the $y$ direction. The angle between the long axis and the effective field is represented as $\theta$ in Figure 4.10. The dynamic fields created by the CPW point out-of-the waveguide plane ($z$ axis) and along the waveguide long axis ($x$ axis). For external fields which are too low to compensate the shape anisotropy field $H_s$, the excitation effectively occurs in BV geometry. The thus excited spin waves propagate along the long axis. By increasing the biasing field, a softening point, resembling the one in the ultrathin film simulations, is reached. In this case, the effective field $H_{\text{eff}}$ vanishes and the system will transition into Damon Eshbach geometry when the external field is further increased. Firstly, it is crucial to determine the required conditions for our system to be in Damon Eshbach geometry, as only in this geometry, the basic working principle of the spectrum analyzer can operate and the dependency of the frequency on the waveguide width will be monotonous.

As the external field strength and the waveguide width $w$ are easily altered parameters in real-world setups, it is apparent to use them as sweeping parameters.
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In addition, to avoid the formation of domain walls in the groundstate relaxation the applied field is rotated one degree from the short to the long axis. Also the damping at the edges was increased to avoid reflections. In a real setup, the waveguide could be chosen of sufficient length to make sure that all the spin wave energy is damped out and the length over which magnetization dynamics are detected is maximized.

So far, sinc-function fields have been used to obtain a broadband excitation. In the previous studies of the ultrathin films, the dispersion was very flat and, consequently, the analysis was not conducted until the limits of the maximum frequency resolved in the simulation. Moreover, the analysis was more concerned with the frequency-wave vector dependence in the analyzed films. In the waveguide studies, the entire analyzed frequency span will be important, as, at least for CoFeB, the resonance frequency can easily approach a few tens of GHz. The thus excited intensity pattern is decisive for the device operation. In this context, it should be noted that a sinc function in numerical simulations is always truncated, as it has a finite amplitude even at very large times. This can lead to artifacts around the position of the maximum frequency, as is depicted in Figure 4.11. Here, it also can be seen that the amplitude after the cutoff frequency is still substantial and as such, all frequencies are excited. In turn, it is possible to use a very short Gaussian pulse to obtain a broad band excitation. Such a pulse does not feature a homogeneous excitation efficiency up
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(a) Dispersion relation and excitation spectrum for a waveguide excited with a sinc signal with a nominal cut-off frequency at 16 GHz.

(b) Dispersion relation and excitation spectrum for the same waveguide excited with a gauss pulse

Figure 4.11: Comparison of the dispersion relation and resulting frequency spectrum of a waveguide excited with a) a sinc signal and b) a gauss pulse. The externally applied field is $\mu_0 H_{ext} = 0.15T$, the waveguide is in Damon Eshbach mode. The width is $\approx 3\mu m$.

to a cut-off value, as is expected from an ideal sinc. However, it becomes evident in Figure 4.12 that the sinc in the numerical simulation also does not truly fulfill this condition. In contrast, if the Gaussian pulse is chosen sufficiently short, it is approximately homogeneous in the interesting frequency range. This has to be taken into account whenever intensity information from broadband excitation is the goal of a numerical investigation and, for this purpose, it is beneficial to use a short Gaussian pulse. Therefore, such an excitation will be used for the remaining simulations.

To determine whether the system is in Damon Eshbach or Backward Volume geometry, the angle $\theta$ of the average effective field $\mu_0 H_{eff}$ of the ground state between the long and short axis is calculated and compared to the corresponding dispersion relation. Using this method, an angle of
4.2 Waveguide Studies

(a) The sinc and gauss signal applied to the CPW in the simulations. The cut-off frequency of the sinc is 16 GHz.

(b) The fast Fourier transform of the sinc and gauss signal in (a).

Figure 4.12: Comparison of the sinc and gauss signal and the discrete Fourier transform thereof. The parameters used are the ones applied in the simulations.

$\theta \geq 75$ is deemed as Damon Eshbach geometry.

For both material systems, at first a broad parameter scan across the external field and width is conducted. The respective material parameters can be found in Table 4.3. The width is altered by changing the cell size and the amount of cells such that is constituted by $N_y = 2^n$ cells. The field is varied in different boundaries for the two materials, as is shown in Table 4.3. The reason for this is the different saturation magnetization, as will be discussed below.

This scan roughly shows how the parameters influence the different states of the system and allows to determine sensible windows for the externally applied field and width for the device operation. Typically, higher external fields push the dispersion relation to higher frequencies, if the magnetization aligns with this field [41]. However, as mentioned above, if the waveguide is still magne-
4.2 Waveguide Studies

(a) Frequency-wave vector space and excitation spectrum for a waveguide in backward volume mode

(b) Frequency-wave vector space and excitation spectrum for a waveguide with a vanishing effective field.

Figure 4.13: Comparison of the dispersion relation and resulting frequency spectrum of waveguides in a) BWVM state and b) with a vanishing effective field $\mu_0 H_{\text{eff}}$.

Table 4.3: Material parameters used in the YIG and CoFeB waveguide simulations [38].

<table>
<thead>
<tr>
<th>Material</th>
<th>$M_{\text{sat}}$ (kA/m)</th>
<th>$A_{\text{ex}}$ (pJ/m)</th>
<th>$\alpha$</th>
<th>$f_{\text{max}}$ (GHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>YIG</td>
<td>147</td>
<td>3.5</td>
<td>$4 \cdot 10^{-4}$</td>
<td>32</td>
</tr>
<tr>
<td>CoFeB</td>
<td>1560</td>
<td>17.6</td>
<td>$4.3 \cdot 10^{-3}$</td>
<td>32</td>
</tr>
</tbody>
</table>

tized longitudinally, this relation is not true. In this case, the effective internal field decreases and, consequently, the dispersion relation drops with increasing field (see also subsection 4.2.3).

This happens when the chosen field is too low and, hence, cannot compensate the shape anisotropy field. Hence, the system is either in a highly volatile state as the effective field vanishes when the external field is equal to the anisotropy field or it is still in the Backward Volume geometry, as can
Table 4.4: Simulation parameters used in the waveguide sweeps for YIG and CoFeB.

<table>
<thead>
<tr>
<th>YIG</th>
<th>$\mu_0H_{ext}[T]$</th>
<th>$N_y$</th>
<th>$C_y[nm]$</th>
<th>CoFeB</th>
<th>$\mu_0H_{ext}[T]$</th>
<th>$N_y$</th>
<th>$C_y[nm]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>16</td>
<td>4</td>
<td></td>
<td>0.15</td>
<td>16</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>32</td>
<td>5</td>
<td></td>
<td>0.17</td>
<td>32</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>0.15</td>
<td>64</td>
<td>6</td>
<td></td>
<td>0.19</td>
<td>64</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>128</td>
<td></td>
<td></td>
<td>0.21</td>
<td>128</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>256</td>
<td></td>
<td></td>
<td>0.23</td>
<td>256</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>512</td>
<td></td>
<td></td>
<td>0.25</td>
<td>512</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.19</td>
<td></td>
<td></td>
<td>0.27</td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>0.65</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

be seen in the exemplary dispersion relations shown in Figure 4.13 (b). The required field strength to reach the desired Damon Eshbach mode decreases with a larger width, as the relative strength of the demagnetization fields at the edges weakens [41]. After the softening point is overcome, the frequency rises relatively quickly and, thus, is potentially pushed out of the resolvable frequency window. In particular, the impact of secondary peaks, originating from higher modes, is of interest for practical applications, as their presence might be detrimental to the device performance. Thus, extensive care has to be taken when choosing the parameter space. In summary, a reasonable parameter space has to be found, where the magnetization is in Damon Eshbach geometry and the frequencies of first and higher order modes are resolvable in a feasible simulation time frame. Once this step is completed, the behavior of the excitation spectra of the waveguides under varying widths and external fields can be analyzed.

4.2.2 YIG waveguides

In the following, Yttrium Iron Garnet, a ferrimagnetic insulator with a low saturation magnetization (see Table 4.3), is studied as a potential material for the waveguides in the above introduced spectral analyzer design. Firstly, a simulation of a relatively wide ($w = 640$ nm) and one of a narrow waveguide ($w = 160$ nm) are calculated for a field of 250 mT. Then, the angle of the average effective field between the long and short axis of the waveguides is extracted. The resulting angles of 88.92° for the 640 nm wide waveguide and 88.75° for the 160 nm wide one confirm that the magnetization is in DE geometry and, thus, these simulations are of further interest for a preliminary study.

As the effective field distribution can already yield hints about possible mode profiles, a cutline of the $y$ component of the effective field strength across the width is plotted in Figure 4.14. Additionally, the analytically calculated effective field is included, which, however, assumes an uniformly...
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Figure 4.14: Comparison of the effective field and magnetization of a wide and narrow waveguide.

(a) Left: The effective field and its analytical calculation along the short axis of a waveguide with a width of 160nm and an external field of 250mT. Right: The magnetization along the short axis.

(b) Left: The effective field and its analytical calculation along the short axis of a waveguide with a width of 640nm and an external field of 250mT. Right: The magnetization along the short axis.

The formula is derived from [41]:

$$
\mu_0 H_{\text{eff}}(y) = \mu_0 H_{\text{ext}} - \mu_0 M_s N_{yy}(y)
$$

$$
= \mu_0 H_{\text{ext}} - \frac{\mu_0 M_s}{\pi} \left[ \arctan \left( \frac{d}{2(y-y_0)+w} \right) - \arctan \left( \frac{d}{2(y-y_0)-w} \right) \right],
$$

(4.5)

where $N_{yy}$ is the demagnetization tensor element along the short axis of the homogeneously magnetized waveguide and $y_0$ being the center of the waveguide in this direction.

As can be seen from Figure 4.14, since $\mu_0 H_{\text{ext}} > \mu_0 M_{\text{sat}}$, the magnetization is mainly homogeneous along the short axis, even for very narrow waveguides. This means that this assumption is well enough fulfilled. One can see, however, that there is still a clear derivation to the numerically
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Figure 4.15: Intensity plots for the peak frequencies in the middle and at the edge of a waveguide with $\mu_0H_{\text{ext}} = 250$ mT.

calculated field.
This will become even more crucial in the case of CoFeB waveguides, as $\mu_0M_{\text{sat}} \approx 1.96$ T in CoFeB is significantly larger than in YIG. It can also be seen that the field distribution varies significantly between the different widths. The narrow waveguide shows a lower effective field and, thus, has a stronger demagnetization field than the wide one. As will be demonstrated below, this will have a large influence on the observed mode profiles.

Exemplary, the two dimensional intensity map of a waveguide mode ($f = 8.77$GHz) and an edge mode ($f = 7.14$GHz) excited by the CPW are shown in Figure 4.15. It can immediately be seen that
the antenna has a very strong non-reciprocal excitation, since almost all of the intensity is located at the left side of the antenna. This phenomenon is known for the Damon-Eshbach geometry and mediated by the interplay of the in-plane and the out-of-plane excitation field components [41]. Thus, since the half with the main part of the signal should be chosen as position for the detector, further evaluations will be limited to this region. The displayed mode pattern and the prevalent edge modes already show that complex dispersion relations and internal field landscapes are to be expected.

With this preliminary knowledge, a broad parameter sweep across the waveguide width from $\approx 0.06 \, \mu m$ to $\approx 3.07 \, \mu m$ and the external field from 50mT to 250mT, as listed in Table 4.4, is conducted. It is to be noted, that the simulation time is reduced to one eighth of the one used in the preliminary simulations, since the parameter space swept includes 90 individual simulations with partly large world sizes and, thus, requires a lot of data and computation resources as it is. This shorter time frame leads to a significantly limited spin wave propagation range due to the finite group velocity. Therefore, the region, in which following evaluations are conducted, is confined further. In order to obtain a rough estimate of a fitting frame, the $x$ position, where the intensity of the mode in the simulation with the shorter time window is significant, is used, as it is shown in Figure 4.16. Also the space directly under the antenna is excluded, since the forced oscillations excited therein could create a discrepancy in the excitation spectra evaluated to the one seen by a detector farther away from the antenna. In conclusion, the evaluation is performed from $x_0 = -2.5\, \mu m$ until $x_0 = -0.8\, \mu m$.  

\footnote{The average deviation of the frequency intensities between the shorter and longer simulation time frames results in 13MHz, which was deemed low enough to perform this approximation.}
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(a) The angle of the effective field $\mu_0H_{\text{eff}}$ for different widths and applied fields. An angle of zero corresponds to a complete alignment to the waveguide length.

(b) The average effective field strength along the short axis of various waveguides, differentiated by the applied external field and the width of the waveguide.

(c) The peak frequency of the excitation spectrum of various waveguides, differentiated by the applied external field and the width of the waveguide.

Figure 4.17: Phase diagrams of the sweep of the external field and waveguide width.
In order to gain an overview over the simulation results, phase maps, representing different characteristics of the systems, are calculated. Namely, the angle of the average effective field $\theta$ between the long and short axis of the waveguides, the strength of the $y$-component of the average effective field and the peak frequency of the excitation spectrum, as shown in Figure 4.17. This data will help along the classification process of the different possible states, like discussed in subsection 4.2.1. In Figure 4.17 (a) the angle of the effective field indicates, that almost all parameter combinations of field and width, excluding low-field, low-width simulations, are magnetized in the Damon Eshbach geometry. Also, as can be seen in (c), the peak frequencies rise, as expected, with an increasing effective field, which is shown in (b). The hatched purple area for low-width low-field combinations is excluded from further evaluation, since the angle $\theta$ is under the threshold value of 75°. Moreover, the peak frequencies stay in the maximum resolvable frequency range of under 32GHz. Thus, for fields above 100mT, all widths can be further investigated.

Exemplary, the excitation spectrum for a fixed external field of 250mT is analyzed for the different waveguide widths. The spectra are calculated by integrating the intensity over all wave vectors for each frequency in the FFT of the space and time domain up to a maximum wave vector of $6\pi/d$, where $d = 500$ nm (see subsection 3.3.1 for details about the FFT process). This wave vector corresponds to the third minima of the CPW excitation in the reciprocal space and was chosen because, up to this wave vector, the amplitude of excitation has already decayed significantly, as can be seen in Figure 4.9. The resulting spectra are presented in Figure 4.18. In all cases, a monotonous rise of the peak frequencies with the width of the waveguides can be seen. Moreover, the form of the peak frequencies stays very consistent, with a standard deviation of the full-width-half-maximum of only 30MHz. However, they show a very distinct frequency gap between roughly 7.5GHz and 8.5GHz. As the intensity maps of the preliminary simulations in Figure 4.15 already suggest, this could be attributed to the presence of edge modes, which typically have a lower frequency than the fundamental or higher order modes in DE geometry.

In these maps, the intensity distribution for the frequencies with the highest intensity along the mid and along the edge are compared for a width of 160nm in (a) and 640nm in (b). This map is derived by a Fourier transformation in time of the signal over the waveguide, i.e., into the space-frequency domain. Consequently, only the intensity at the given peak frequency is shown as a function of space.

This suspicion becomes even more substantiated when looking at the mode profiles along the short axis of these waveguides, displayed in Figure 4.20. First of all, it should be noted that the obtained mode profiles look already quite complex and do not necessarily resemble simple cosine shaped waveguide modes or clearly confined edge modes. Nevertheless, the profiles confirm that there are indeed edge modes, as their main part of intensity is mainly distributed at the edges, whereas
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Figure 4.18: The excitation spectra for the Damon Eshbach magnetized simulations of the initial broad scan. The peak frequency is marked by a vertical line and the full-width-half-maximum area is shaded in the respective color. The standard deviation of all different full-width-half-maximum is shown as $\sigma_{\text{fwhm}}$.

Figure 4.19: The peak frequency and the corresponding effective field along the different wave guide widths.

the higher frequency mode is distributed along the center. This picture also shows, that these edge modes are more prevalent in the narrow waveguide, shown in (a). As can be seen in Figure 4.14 (a), in narrow waveguides there is hardly a region of homogeneous internal field, whereas there is a large drop of the fields at the edges of the waveguide resulting in strong potential wells for edge modes [?]. Apparently, this results in the fact that in the narrow waveguides, more intensity can be transferred into an edge mode excitation than into the waveguide mode excitation. This can be
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(a) Narrow waveguide: Mode profile for a waveguide of 160nm and an external field of 250 mT.

(b) Wide waveguide: Mode profile for a waveguide of 640nm and an external field of 250 mT.

Figure 4.20: Comparisons of the mode profiles along the short axis for the peak frequencies in the middle and at the edge between a narrow and wide waveguide with an external field of 250 mT.

seen in Figure 4.22 where the Fourier spectra of the respective excitation in the two waveguides are shown in the frequency-wave vector domain. In both, the spectra of the waveguide and edge modes are close to each other and they share a similar shape and slope of their dispersion. However, in the narrow waveguide, the relative intensity in the excited edge mode is much higher than the one in the waveguide mode, while this is opposite in the wider waveguide. This behavior is also apparent in Figure 4.21 where the intensities integrated along the short axis of the waveguide are shown as a function of the x-coordinate. In the narrow waveguide, the intensity of the edge mode is higher than the one in the waveguide mode, and both modes decay with a similar decay length. In such a waveguide, the dominant spin wave that would be detected by the iSHE would, thus, be the edge mode. This could potentially be mitigated by confining the iSHE detector to the central area. However, it should be noted that the excitation strength of the waveguide mode is significantly
lower and, thus, only a comparatively small voltage could be detected. In contrast, in the wider waveguide, the energy inserted into the waveguide mode is larger than in the one inserted into the edge mode, resulting in the jump in frequency visible in Figure 4.18 and Figure 4.19.

In summary, the results of the parameter sweep show that, as the spectral peaks rise monotonously with the waveguide width, a basic requirement for the proposed spectrum analyzer is fulfilled. Also, the consistent form of the peaks could make further processing of the spin wave signal more approachable. However, two distinct modes are excited, one propagating along the middle of the waveguide and one along the edges. In narrow waveguides with widths of under $\approx 300$ nm, mainly edge modes are excited, whereas for wider waveguides, the waveguide modes are carrying a larger intensity. This results in a gap of roughly 1 GHz between the respective spectra. It can be argued that, nonetheless, independent of the frequency range, YIG waveguides could still be used for the proposed device, as the key requirements are fulfilled. Still, since the peak frequency range is not extensive, the use of materials with a higher Ms, such as CoFeB, are an interesting alternative,
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(a) Narrow waveguide: Frequency-wave vector space and frequency spectrum for a waveguide of 160nm and an external field of 250 mT.

(b) Wide waveguide: Frequency-wave vector space and frequency spectrum for a waveguide of 640nm and an external field of 250 mT.

Figure 4.22: Comparison of the Frequency-wave vector space and resulting frequency spectrum of a narrow and wide waveguides with $\mu_0 H_{\text{ext}} = 250$ mT

since they promise a larger frequency span. In the following, the application of CoFeB in such a spectrum analysis device will thus be investigated.

4.2.3 CoFeB waveguides

In this section, the results of a width sweep from $\approx 0.06 \mu$m to $\approx 3.07 \mu$m and of a simultaneous field sweep from 150mT to 650mT are presented. The data set consists of 450 individual simulations and a raw size of roughly 400 GB. The material parameters used in the simulations can be found in Table 4.1.

Analogous to [subsection 4.2.2] firstly the $y$-component of the effective field and the magnetization
4.2 Waveguide Studies

along the short axis is extracted for a narrow waveguide of 160nm with a field of 650mT, shown in Figure 4.23. This time, the waveguide shows a significantly larger demagnetization field and a very inhomogenous magnetization, especially at the edges. This causes substantial derivations of roughly 400mT to the analytically calculated effective field at the edges. Hence, it is evident that, in this material, numerical approaches to this problem are crucial.

![Figure 4.23](image)

Figure 4.23: The effective field component in $y$ direction and the magnetization along the width for a narrow waveguide with a width of 160nm and a field of 650mT.

Similar to the discussion in the previous subsection 4.2.2 for YIG, we will first address the angle $\theta$ of the average effective field between the short and long axis, which is plotted for each width and field combination as shown in Figure 4.24 (a). The data clearly shows that the required field strength to pull the magnetization into DE geometry is much higher now, due to the larger Ms. The latter also results in a much larger difference between narrow and wide waveguide than this was the case in YIG.

The resulting demagnetization field also results in larger changes of the effective field for the different widths, which is shown in Figure 4.24 (b).

The resulting peak frequency of the excitation spectra, shown in (c), rises with increasing effective field in the $y$ direction accordingly, once the magnetization has rotated. For an effective field angle below 45 degrees, the peak frequency also rises with decreasing applied field, due to the stronger effective field along the long axis. As mentioned above, in this scenario, the frequency is not monotonously increasing with the waveguide width and, thus, the spectral analysis will be flawed. Hence, these field-width combinations will be excluded from the analysis. Also, for high widths and high fields, the peak frequency reaches the maximum resolvable frequency of 32 GHz. Afterwards, the primary peaks are pushed out of the resolvable range and cannot be correctly represented anymore. The parameter range where this effect happens will be excluded from further
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(a) The angle of the averaged effective field $\mu_0 H_{\text{eff}}$ for different widths and applied fields. An angle of zero corresponds to a complete alignment to the waveguide length.

(b) The average field strength of the effective in width direction for different combinations of the applied external field $\mu_0 H_{\text{ext}}$ and waveguide width.

(c) The peak frequency of the excitation spectrum of various waveguides, differentiated by the applied external field and the width of the waveguide. The purple shaded area has an angle $\theta < 75$ of the effective field and the green shaded area has a peak frequency $f_{\text{peak}} \geq 31$.

Figure 4.24: Phase diagrams of the initial broad sweep of the external field and waveguide width.
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Figure 4.25: The excitation spectra for the Damon Eshbach magnetized simulations with an angle $\theta \geq 82^\circ$ and $\mu_0 H_{\text{ext}} = 250 \text{ mT}$ of the initial broad scan. The peak frequency is marked by a vertical line and the full-width-half-maximum area is shaded in the respective color. The standard deviation of all different full-width-half-maximum is shown as $\sigma_{\text{fwhm}}$.

analysis, by using the corresponding effective field and maximum frequency as a threshold value. The resulting parameter space is marked in Figure 4.24 (c), where the hatched green and purple areas are excluded from the analysis. Thus, as the parameter boundaries are found for this material system, the behavior and characteristics of the excitation spectra can now be examined.

Figure 4.26: Frequency-wave vector space and frequency spectrum for a waveguide of 160nm and an external field of 650 mT.
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For a fixed external field, the excitation spectrum for different widths is analyzed. As in the case of YIG, the spectra are calculated by integrating the intensity over all wave vectors for each frequency in the FFT of the space and time domain up to the third minimum of the CPW excitation for all widths that have not been excluded by the criteria mentioned above. The phase diagram of the effective field in the width direction in Figure 4.24(b) suggest that low external fields show only a narrow effective field range within the operation regime and, thus, only a small frequency shift along the different waveguide widths. This is confirmed by the spectra shown in Figure 4.25. The overlap of the spectra of the different waveguides is large and the shift of the peak frequencies in the range of only a few hundreds of MHz. As these spectra would create unfavorable characteristics for a spectrum analyzer, where the intensity in an individual waveguide should correspond to the presence of a given frequency component, a field value where the phase diagrams in Figure 4.24 indicate a larger frequency shift is chosen for investigation.

With an external field of 0.65T, the peak frequencies for different widths show a significant variation from about 15 GHz to 30 GHz, as shown in Figure 4.27(a). As in the other cases, the shape of the peaks stays relatively consistent with a standard deviation of the full-width-half-maximum of 180 MHz. However, very narrow peaks with comparable amplitude have emerged between 10GHz and 15GHz. Similar to the case of YIG, these peaks at lower frequencies are due to the formation of edge modes which can be excited in the potential wells at the waveguide edges. The fact that the modes are very narrow in frequency already hints, however, that they feature a very flat dispersion.

In order to gain further insights about their nature, the Fourier intensity in the frequency-wave vector space is shown in Figure 4.26 with a logarithmic scale for the intensity. The lower frequency modes can clearly be distinguished and their very flat dispersion in comparison to the waveguide mode is visible. Thus, unlike in YIG, in CoFeB, the group velocity, and, hence, the energy transport, will also be noticeable reduced for the edge mode. As the proposed detectors do not have to be positioned directly under the CPW-antenna, the excitation spectra at a certain distance from the antenna are of additional interest and could concurrently exhibit the absence of these edge modes. In Figure 4.27(b), the spectra, integrated over the width ranging from $x = -2.5$ to $x = -10 \, \mu m$ away from the antenna are shown for an externally applied field of 650mT. Here, the lower-frequency peaks have vanished completely. In order to get a more quantitative result, the mode intensity map and the decay of these modes is displayed in Figure 4.21 for an exemplary waveguide with the same field of 650mT and a width of 160nm. This confirms that the intensity of the edge modes has decayed significantly faster than for the waveguide mode, although their intensity near the antenna is slightly larger in this example. Hence, the detector can easily be positioned sufficiently far away.

3Contrary to the YIG simulations, the spin waves propagate until the end of the waveguide in the chosen time frame, as their group velocity is significantly larger in CoFeB.
4.2 Waveguide Studies

(a) The evaluation region was chosen from -10µm to -0.8µm.

(b) The excitation spectra for the same simulations as in (a). However, the evaluation region was changed to reach from -10µm to -2.5µm.

Figure 4.27: Comparison of the excitation spectra an external field of 650mT but different evaluation regions. The peak frequency is marked by a vertical line and the full-width-half-maximum area is shaded in the respective color. The standard deviation of all different full-width-half-maximum is shown as $\sigma_{\text{fwhm}}$.

from the antenna such that the edge modes have decayed sufficiently.

In conclusion, the resulting phase diagrams from the parameter sweeps crystallized as useful classification tool for the various states of the waveguide system and allowed to make first guesses, not only concerning the boundaries of the applicable parameter space (DE geometry and resolvable frequencies) but also about the range of applied external fields where a strong dependence of the effective field on the width is maintained. These preliminary results favored high fields of 0.5T and larger, and widths in between 100 nm and 300 nm. Further investigations indicated a strong presence of edge modes also in these systems. However, their group velocity turned out to be very low in comparison to the waveguide mode and, thus, their contribution to the spectra at distances in the range of a few µm away from the antenna could be shown to be negligible. Hence, it can
4.2 Waveguide Studies

(a) The intensity map for the peak frequencies in the middle and at the edge waveguide with an external field of 650mT and a width of 160nm.

(b) Decay of the intensities of edge and waveguide mode along the long axis for a waveguide with an external field of 650mT and a width of 160nm.

Figure 4.28: Intensity map of middle and edge mode and its integration over the y axis for a waveguide with a width of 160nm and an external field of 650mT.

It be stated that these derived results clearly indicate the applicability of CoFeB waveguides in the proposed spectrum analyzer.
4.2 Waveguide Studies

4.2.4 Discussion

In this Chapter, the application of the framework for the design of a magnonic spectrum analyzer based on the width dependence of the effective field in transversely magnetized waveguides was discussed. This problem is very hard to tackle analytically and the framework has proven useful to identify suitable working regions. From the perspective of the framework, this constituted a nice example to show how parameter sweeps and a specialized automatized analysis can go hand in hand to predict the device performance in a large parameter span by the creation of phase maps, the automatized analysis of spectra or plotting of mode profiles. From the point of view of the materials under investigation, some clear pros and cons could be identified for either material system, that will be discussed in the following.

**YIG**

- Low saturation magnetization:
  + Does not need high external fields for DE magnetization.
  - Narrow peak frequency range as the effective field quickly reaches the external one.

- Strong edge modes:
  - Two distinct peak frequency ranges with a large gap of 1 GHz in-between.
  - Fundamental and edge mode have similar propagation characteristics → can’t be filtered out easily.

- Narrow peaks:
  + Very consistent peak shape → easier processing of the detected signal.

**CoFeB**

- Larger saturation magnetization:
  - Requires high fields to pull narrow waveguides into DE magnetization.
  + Extensive peak frequency range.

- Less prevalent edge modes:
  + Edge modes can be filtered out by detecting farther away from the antenna.
  + Continuous rise of peak frequency without mode switching.

In conclusion, YIG is likely more suited to perform a spectral analysis with high resolution in a small frequency window which can be easily shifted by a moderate field, whereas CoFeB is very
suitable for the analysis of rather large frequency bands. In contrast, the requirements of large fields might strongly hamper the use of CoFeB, although it should be noted that even higher fields would be needed to push a YIG spectrum analyzer into the same frequency range that is covered in CoFeB.
CHAPTER 5

Conclusion and Outlook

In this Thesis, using Python, a software framework was developed to schedule, perform and analyze series of micromagnetic simulations. Two case studies have been performed to show the usefulness of this software package: Ultrathin films from Pt/CoFeB/MgO and W/CoFeB/MgO were simulated to perform a best fit to experimental data in order to extract material parameters without the use for analytic approximations. In particular, in W/CoFeB/MgO, it could be shown that a simple model can lead to large errors in the estimated values, whereas the framework provides a more appropriate solution with minimum requirements in input and output from the user. In fact, she or he only has to specify the parameter space and provide the experimental data and the framework simulates the entire series, performs an automatized analysis and provides the best fit. The second case study dealt with a problem with increased complexity. The possibility to build a magnonic on-chip spectrum analyzer from a set of transversely magnetized waveguides has been studied. While the thin-film study still dealt with a problem which can be solved with (semi-)analytical theories, the internal field landscape and the corresponding spin-wave spectra in the simulated waveguides can only be described accurately by full micromagnetic simulations. Once again, the framework allows the user to do a full study of the device characteristics with an adapted output function providing the resonance spectra with only minimum requirements to the user. By comparing two quite different materials, YIG and CoFeB, which are both of high relevance to magnonics, the different resulting device characteristics could be identified and guidelines for the device design have been given. While these two examples already demonstrate the large power of the framework, they merely scratch the surface of its potential. The developed parser allows to perform sweeps of more sophisticated manner by the full capability to rescript the MuMax3 files in the Go language by using Python templates. Furthermore, the use of error functions that are already implemented in the fitting can be used to perform more advanced parameter sweeps. In fact, instead of using simple linearly spaced parameter ranges, it is possible to use machine learning algorithms in order to further optimize the parameter sweeps with an adaptive resolution. In addition, as any parameter from the micromagnetic simulation can be used as output quantity, also complex magnonic devices based on spin-wave interference can be simulated and optimized. For instance, the phase can be used as output parameter and nonlinear spin-wave phenomena to
shift the phase can be easily studied in the simulation in order to design nonlinear devices, such as the ones used in directional-coupler based magnonic AND gates. The framework allows to process immense amounts of data and the real-time analysis performed in parallel to the simulations allows to evaluate simulation series of arbitrary complexity by the reduction of the stored data to the minimum resolution needed for a quantitative evaluation. This way, it brings micromagnetic simulations in magnonics to the next level and, as such, it will provide a valuable asset to further studies in the AG Magnetismus.
The Oersted field of the CPW is calculated by the addition of the three Oersted fields created by the individual wires constituting the CPW. It is assumed that the ground lines are out-of-phase with the central wire and carry one half of the current in the central wire respectively. Hereby, the y-direction is chosen to be along the symmetry axis of the antenna. The formula for the in-plane field component created by a current through an individual wire is as follows [43]:

\[
\mu_0 h_{ip}(z, x) = -\frac{I\mu_0}{8\pi ab} \left[ (a-z) \left( \frac{1}{2} \ln \left( \frac{(b-x)^2+(a-z)^2}{(-b-x)^2+(a-z)^2} \right) + \frac{b-x}{a-z} \arctan \left( \frac{a-z}{b-x} \right) \right) - \frac{b-x}{a-z} \arctan \left( \frac{a-z}{b-x} \right) \right] 
+ \frac{b-x}{a-z} \arctan \left( \frac{a-z}{b-x} \right) - \frac{b-x}{a-z} \arctan \left( \frac{a-z}{b-x} \right) \right] 
\]

(5.1)

and has an out-of-plane field component of:

\[
\mu_0 h_{oop}(z, x) = -\frac{I\mu_0}{8\pi ab} \left[ (b-x) \left( \frac{1}{2} \ln \left( \frac{(b-x)^2+(a-z)^2}{(-a-z)^2+(b-x)^2} \right) + \frac{a-z}{b-x} \arctan \left( \frac{b-x}{a-z} \right) \right) - \frac{a-z}{b-x} \arctan \left( \frac{b-x}{a-z} \right) \right] 
+ \frac{a-z}{b-x} \arctan \left( \frac{b-x}{a-z} \right) - \frac{a-z}{b-x} \arctan \left( \frac{b-x}{a-z} \right) \right] 
\]

(5.2)

where \(a\) represents the half-height and \(b\) represents the half-width of the wire. The superposition of the three antenna fields to the field of the CPW is depicted in Figure 4.9 as a function of the y axis, i.e., along short axis of the waveguide. The fields were evaluated at \(z=-101\) nm, corresponding to the top of the waveguide.
Bibliography


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__________________________
Unterschrift