Computing the Scalar Magnetic Potential using Spherical Harmonics

Christian Bauer

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supervised by
Prof. Dr. Benjamin Stamm
Abstract

Today's electronic devices become smaller and smaller, therefore hitting the physical boundary of electrons as the basis for correct computations. Spintronic devices which are based on ferromagnetic materials might be able to further lower this boundary, but their properties have to be studied thoroughly in order to make use of them. Hence, micromagnetic simulations need to be run successively multiple times. Since running such simulations is quite expensive, a lot of research is put into the process' speed-up. Therefore, in this paper a novel approach to the computation of the scalar magnetic potential is presented. This calculation is one of the most expensive ones in micromagnetic simulations thus it could lead to a speed-up in the simulation of spherical magnetic materials. The presented algorithm is restricted to the unit sphere. It is tested with two test cases and as a physical example, the scalar magnetic potential of a homogeneously magnetized unit sphere is computed. The method can also be efficiently extended to multiple spherical geometries by means of the fast multipole method which is a topic for future research.

1 Introduction

Today's electronic devices tend to become smaller and smaller while increasing their performance. However, the physical limits of such silicon-based devices have almost been reached. Hence, in order to further ensure faster data transportation at lower power consumption and lower cost a shift from electronic to spintronic devices might be inevitable. In spintronic devices information is stored by manipulating the electron's spin which can be done very quickly and very cheaply. Additionally, since electron spin doesn't depend on energy, it is non-volatile. Possible applications of those properties include for example magnetic random access memory (Parkin, Hayashi, and Thomas 2008) or spin transistors the latter of which can in turn decrease the size and increase the speed of computer components. Another interesting application is the control of electron spin waves via magnonic crystals. These spin waves carry information with shorter wavelengths than electromagnetic waves of equivalent frequencies. Therefore, a minimization of microwave devices might be possible. Furthermore, magnonic waveguide devices, such as microwave resonators, filters, etc. can be fabricated, because magnonic crystals can produce frequency band gaps which disallow the propagation of spin waves of specific frequencies. (Ma et al. 2011; Wang et al. 2014)

Since an electron’s quantum properties are well studied, the real challenge in advancing the production of spintronic or microwave devices lies in the thorough comparison of theory with experiments. Therefore, a lot of research is put into micromagnetic simulation of such phenomena. An important part of such simulations
is the calculation of the demagnetization energy more precisely the calculation of the scalar magnetic potential. (Hirohata 2015; Bolte et al. 2004)

In this paper a novel approach for the computation of the scalar magnetic potential is developed. This method uses spherical harmonics in order to efficiently solve Poisson-type interface problems using a spherical geometry. Hence, the application could be simulations of magnonic crystals which consist of spherical iron inclusions. In the following sections the physical model is introduced first. Afterwards, the mathematical solution of Poisson’s problem is derived and discretized. Finally, the simulation results are presented and a look into possible future research topics is given.

2 Physical Model

Magnonic crystals are magnetic metamaterials created by geometrical structuring (cf. fig. 1). These structures are built out of small inclusions of ferromagnetic materials in a matrix of non-ferromagnetic material or the other way around. Through a periodic distribution of such inclusions the magnetic properties of magnonic crystals are altered, consequentially controlling the spin wave (cf. fig. 2) excitation as well as its propagation. In order to simulate this behavior, a modified version of the Landau-Lifshitz-Gilbert (LLG) equation is often used (Abert 2013). However, in the following sections only the standard LLG equation is explained. Starting with a short introduction to the quantized view of magnetism we will zoom out to describe magnetism continuously.

The fundamental nature of magnetism lies in the material’s quantum mechanical properties. An electron’s position is described in term of its wave function. Observing the position over a period of time yields different orbitals which then can be described by three integer quantum numbers, essentially describing an energetic property. Since the electron also rotates around itself, there is a fourth integer quantum number describing the spin. This number is proportional to the magnetic moment of a magnetic dipole (Bolte et al. 2004). These dipoles or elementary magnets are the building blocks of magnetic matter. They interact with each other thereby generating the material’s magnetic properties. This interaction in ferromagnets yields an energetically favored parallel spin alignment. The alignment of elementary magnets \( m_i \) and \( m_j \) is assumed to be parallel if they are less than the exchange interaction length \( \lambda \) apart from each other, i.e.

\[
m_i \approx m_j, \quad \text{for } |r_i - r_j| < \lambda,
\]

with \( r \) as the location of an elementary magnet. (Abert 2013)

\[\text{There are actually different types of magnetism with ferromagnetism being the strongest}\]
magnetic vortices. Figure 2: Schematics of a Spin Wave Propagation Along $e_k$. Magnetic moments (orange arrows) precess with a periodic spatial phase difference, determining the spin-wave wavelength $\lambda$. (Wintz et al. 2016)
The foundation of micromagnetic simulations is the continuous description of the quantized states that form magnetism. The continuous distribution of magnetic dipoles can thus be written as

$$\int_\omega M(r) \, dr \approx \sum_i \mathbb{1}_\omega(r_i)m_i,$$

with the magnetization $M$ which depends solely on the position $r$ and the magnetic moment $m_i$ of the $i$th dipole. $\mathbb{1}_\omega$ is an index function that denotes the inside of the $i$th magnetic moment’s volume $\omega$ which is located at the position $r_i$. However, this only holds for $\omega \geq \lambda^3$, and therefore, such simulations are valid in length scales greater than 1 nm (cf. Abert 2013). Since the computation of the underlying equations is quite expensive the length scales also have an upper limit of about 1000 nm (Abert 2013).

In order to simulate a ferromagnetic material, the change in time of the material’s magnetization distribution needs to be computed. This can be achieved by solving the LLG equation for the magnetization $\mathbf{M}$

$$\frac{\delta \mathbf{M}}{\delta t} = -\gamma (\mathbf{M} \times \mathbf{H}_{\text{eff}}) - \frac{\alpha \gamma}{M_s} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}}).$$

(1)

Herein, $M_s$ describes the saturation magnetization

$$\mathbf{M}(r) = M_s \cdot \mathbf{m}(r), \quad \text{with} \quad |\mathbf{m}(r)| = 1 \text{ and } M_s \in \mathbb{R}.$$n

There are two dimensionless coefficients $\gamma$ and $\alpha$ in the equation which describe the magnetization vector’s change of orientation with respect to the direction of the effective magnetic field $\mathbf{H}_{\text{eff}}$. The gyromagnetic ratio $\gamma$ is a parameter that describes the magnetization’s rotation around the direction of the effective field (cf. fig. 3) and the damping coefficient $\alpha$ tries to align both fields’ direction. The effective magnetic field $\mathbf{H}_{\text{eff}}$ is a magnetic field which is applied to the setting of interest. (García-Cervera, Gimbutas, and Weinan 2003)

In order to solve the LLG equation an initial condition is necessary. Such an initial condition for the magnetic field $\mathbf{M}$ is usually obtained by minimizing the total energy

$$E_{\text{Total}} = E_{\text{Exchange}} + E_{\text{Anisotropy}} + E_{\text{Zeeman}} + E_{\text{Demagnetization}}.$$n

(2)

In the steady-state of a system the ferromagnet’s magnetization minimizes eq. (2) which is obtained by summing up several distinct energies. Depending on

and the commonly known one. Besides that there are paramagnetism, diamagnetism, and antiferromagnetism, however, these are not covered in this seminar work.
Figure 3: Precession Around the Effective Field with Damping. The magnetization \( \mathbf{M} \) rotates around the effective field \( \mathbf{H}_{\text{eff}} \), as described with the coefficient \( \gamma \) (left), and the damping \( \alpha \) (middle) results in a spiralling motion (right). (Abert 2013)

the type of simulation some of the terms can be neglected, if their impact is small enough. (Huber 2013; García-Cervera, Gimbutas, and Weinan 2003; Abert 2013; Bolte et al. 2004)

The exchange energy

\[
E_{\text{Exchange}} = -\sum_{i \neq j}^{N} J_{ij} (S_i S_j) \tag{3}
\]

is responsible for the spontaneous magnetization of a body. It is based on the Coulomb interaction and the quantum mechanical Pauli exclusion principle and energetically favors a parallel alignment of the spins \( S_i \) and \( S_j \). In eq. (3), \( J_{ij} \) denotes an exchange integral. (Huber 2013) The continuous description of the exchange energy reads

\[
E_{\text{Exchange}} = \frac{A_{\text{ex}}}{V} \int_{\omega} (\nabla \cdot \mathbf{M})^2 d\omega, \tag{4}
\]

with a measure for the exchange stiffness denoted \( A_{\text{ex}} \) and the magnet’s volume \( V \). While the exchange energy has limited range, its magnitude causes spontaneous long-range ordering in ferromagnets.

The anisotropy energy results from spin-orbit interactions. It describes the alignment of a magnetization parallel to certain axes depending on the material’s lattice structure. These axes are called easy axes. For a magnet with only one easy axis, the anisotropy energy is denoted by

\[
E_{\text{Anisotropy}} = K_{u1} \int_{\omega} \sin^2 (\varphi) \, d\omega + K_{u2} \int_{\omega} \sin^4 (\varphi) \, d\omega. \tag{5}
\]
Figure 4: Time Spent for Different Computations in a Micromagnetic Simulation over Number of Cells. From bottom to top: Demagnetization energy, Exchange energy, Anisotropy energy, Zeeman energy, numerical integration, and numerical derivation. (Bolte et al. 2004)

Hereby, $K_{u1}$ and $K_{u2}$ are the uni-axial anisotropy constants and $\varphi$ is the angle between the magnetization and the easy axis. (Bolte et al. 2004; Abert 2013)

Interactions with an external magnetic field are described in the Zeeman energy

$$E_{\text{Zeeman}} = -\mu_0 \int_\omega \vec{M} \cdot \vec{H}_{\text{external}} d\omega$$

which is minimized, if the magnetization is parallel to the external field. (Huber 2013; Abert 2013; Bolte et al. 2004)

The demagnetization energy is based on Maxwell’s equations and accounts for the electrons’ dipole-dipole interactions. In its continuous description the demagnetization energy reads

$$E_{\text{Demagnetization}} = -\frac{\mu_0}{2V} \int_\omega \vec{M} \cdot \vec{H}_{\text{demag}} d\omega.$$  (7)

Herein, the demagnetization field $\vec{H}_{\text{demag}}$, also referred to as stray field, is introduced. The stray field energy describes a long-ranged interaction in which the demagnetization, that is induced by the magnetization itself, counteracts the magnetization. Calculating the stray field is one of the most important steps in evaluating the effective field, because the demagnetization field often dominates the other terms. (Huber 2013; Kaliche 2016; Abert 2013)
Since it is of such importance and its computation is quite expensive (cf. fig. 1), a lot of effort is put into finding an efficient method to compute the demagnetization field and therefore the demagnetization energy (Kaliche 2016; Fredkin and Koehler 1990; Abert et al. 2013, cf.). The stray field depends on the magnetostatic potential \(u\), which is essentially the equivalent to the well-known electrostatic potential, as follows

\[ \vec{H}_{\text{demag}} = -\nabla u. \]  

(8)

The magnetostatic potential in turn depends on the magnetization

\[ \Delta u = \text{div}(\vec{M} \chi_\omega) \]

\[ \chi_\omega = \begin{cases} 0, & \text{inside } \omega \\ 1, & \text{outside } \omega \end{cases} \]  

(9)

with the index function \(\chi_\omega\) denoting the inside of the magnetic material’s volume \(\omega\). Therefore, eq. (9) can also be written as

\[ \Delta u = \text{div}(\vec{M}) \quad \text{in } \omega \]

\[ [\partial_n u] = -\vec{M} \cdot n \quad \text{on } \Gamma \]

\[ \Delta u = 0 \quad \text{in } \mathbb{R}^3 \setminus \omega \]

\[ [u] = 0 \quad \text{on } \Gamma, \]  

(10)

where eq. (9) has been split in an interior and an exterior part. Additionally, \(n\) and \(\partial_n\) were introduced to denote the outward pointing surface normal and the derivative in the direction of \(n\), respectively. Furthermore, the notation \([\cdot]\) was introduced to identify a jump condition, i.e. \([u] = u_n^i + u_n^e = 0\) with \(n_i\) and \(n_e\) unit normals pointing outwards and inwards the domain \(\omega\), respectively.

Since eq. (8) is easily solvable and cheap to compute, in the following sections the solution method to eq. (9) or rather eq. (10) will be looked into in more detail.

3 Mathematical Model

From the previous section it is clear that the magnetostatic potential can be expressed with eq. (10) which in an abstract form reads

\[ \Delta u = f \quad \text{in } \omega \]

\[ [\partial_n u] = g \quad \text{on } \Gamma \]

\[ \Delta u = 0 \quad \text{in } \mathbb{R}^3 \setminus \omega \]

\[ [u] = 0 \quad \text{on } \Gamma. \]  

(11)
By restricting $\omega$ to a unit sphere, eq. (11) can be solved using spherical harmonics and utilizing potential theory. This is shown in the next paragraphs.

The eq. (11) can be represented as two problems, s. t. the solution is $u = u_f + u_g$. Starting with the first problem, i. e.

\[
\Delta u_f = f \quad \text{in } \omega \\
u_f = 0 \quad \text{on } \Gamma, 
\]

and following the method of Quan (2016), a solution of the form

\[
u_f(\theta, \phi, r) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} v(r) Y_{\ell m}(\theta, \phi)
\]

is obtained. Note that in order to combine the solution to both problems, $u_f$ needs to be extended by 0 in $\mathbb{R}^3 \setminus \omega$. Herein, $Y_{\ell m}$ are the spherical harmonics (cf. Appendix A for further details). Since the implementation of this method is part of this seminar work, it is explained in Section 4.

Now, the second problem needs to be solved as well. After stating the first problem as in eq. (12) the second one reads

\[
\Delta u_g = 0 \quad \text{in } \mathbb{R}^3 \setminus \Gamma \\
[u_g] = 0 \quad \text{on } \Gamma \\
[\partial_n u_g] = g - \partial_n u_f|_{\omega} \quad \text{on } \Gamma.
\]

This problem is a classical example of potential theory and the solution is a single layer potential of the form

\[
u_g = \int_{\Gamma} \frac{\sigma(s)}{|x - s|} ds
\]

with

\[
\sigma(s) = \frac{1}{4\pi} [\partial_n u_g] = \frac{1}{4\pi} \left(g - \partial_n u_f|_{\omega}\right).
\]

Since the single layer potential and potential theory in general are well-understood topics in mathematics and physics respectively, the reader is hereby kindly referred to the literature, e. g. Folland (1995).

### 4 Numerical Method

As previously stated, the numerical implementation is based on the work of Quan (2016). In order to solve eq. (12) on a unit ball, it is multiplied by $-1$ to obtain

\[
-\Delta u_f = -f \quad \text{in } B_1(0) \\
u_f = 0 \quad \text{on } \partial B_1(0).
\]
Here, \( B_1(0) \) describes a unit ball centered at 0. Using the ansatz

\[
\begin{align*}
  u(\theta, \phi, r) &= \sum_{\ell'=-\infty}^{\infty} \sum_{m'=0}^{\ell'} \ u_{\ell',m'}(r) Y_{\ell',m'}(\theta, \phi)
\end{align*}
\]

eq (17) is written as

\[

- \Delta \left( \sum_{\ell',m'} u_{\ell',m'}(r) Y_{\ell',m'}(\theta, \phi) \right) = -f
\]

Herein, the notation \( \sum_{\ell',m'}(\cdot) \) actually means \( \sum_{\ell'=-\infty}^{\infty} \sum_{m'=-\ell'}^{\ell'} (\cdot) \). Now remembering the Laplacian operator in spherical coordinates

\[
\Delta u = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial u}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 u}{\partial \phi^2}
\]

and using the fact that the ansatz is made out of two independent functions, which are dependent on the radius \((r)\) and the angles \((\theta, \phi)\), respectively, eq. (18) is simplified to

\[

- \sum_{\ell,m} \Delta (u_{\ell',m'} Y_{\ell',m'}) + 2 (\nabla u_{\ell',m'} \cdot \nabla Y_{\ell',m'}) + u_{\ell',m'} \Delta (Y_{\ell',m'}) = -f. \tag{19}
\]

Notice that the dependencies of the functions \( u_{\ell',m'} \) and \( Y_{\ell',m'} \) are dropped from now on. Because the gradients of \( u_{\ell',m'} \) and \( Y_{\ell',m'} \) are orthogonal, \( 2 (\nabla u_{\ell',m'} \cdot \nabla Y_{\ell',m'}) = 0 \) holds and therefore

\[

- \sum_{\ell,m} \Delta (u_{\ell',m'} Y_{\ell',m'}) + u_{\ell',m'} \Delta (Y_{\ell',m'}) = -f. \tag{20}
\]

Utilizing that the spherical harmonics obey \( r^2 \Delta Y_{\ell m} = -l(l + 1) Y_{\ell m} \) yields another simplification:

\[

- \sum_{\ell,m} \Delta (u_{\ell',m'} Y_{\ell',m'}) = -l(l + 1) u_{\ell',m'} \frac{Y_{\ell',m'}}{r^2} \tag{21}
\]

\[

\Leftrightarrow - \sum_{\ell,m} \frac{1}{r^2} \left( 2 \frac{\partial u_{\ell',m'}}{\partial r} + r \frac{\partial^2 u_{\ell',m'}}{\partial r^2} \right) Y_{\ell',m'} - u_{\ell',m'} \frac{l(l + 1)}{r^2} Y_{\ell',m'} = -f
\]

\[

\Leftrightarrow \sum_{\ell',m'} - \frac{1}{r^2} \left( 2 \frac{\partial u_{\ell',m'}}{\partial r} + r \frac{\partial^2 u_{\ell',m'}}{\partial r^2} \right) Y_{\ell',m'} + \frac{\ell' (\ell' + 1)}{r^2} u_{\ell',m'} Y_{\ell',m'} = -f.
\]
Multiplying by $r$ and denoting $w_{\ell',m'} = ru_{\ell',m'}$ further simplifies eq. (21). Now the variational formulation is derived: first w.r.t. $\theta$ and $\phi$, then w.r.t. $r$. Therefore, eq. (21) is multiplied by $\mathcal{Y}_{\ell m}$, which is used as a test function here, and integrated over the unit sphere’s surface $S^2$.

$$
\int_{S^2} \sum_{\ell',m'} \left( -\frac{1}{r} \frac{d^2}{dr^2} (w_{\ell',m'}) \mathcal{Y}_{\ell'm'} + \frac{\ell(\ell + 1)}{r^2} u_{\ell',m'} \mathcal{Y}_{\ell'm'} \right) \mathcal{Y}_{\ell m} dS = - \int_{S^2} f \mathcal{Y}_{\ell m} dS.
$$

(22)

Using the orthonormality property of the spherical harmonics, i. e.

$$
\int_{S^2} \mathcal{Y}_{\ell'm'} \mathcal{Y}_{\ell m} dS = \delta_{\ell\ell'} \delta_{m'm},
$$

with the Kronecker delta $\delta_{ij}$, this simplifies to

$$
- \frac{d^2}{dr^2} w_{\ell',m'} + \frac{\ell(\ell + 1)}{r^2} u_{\ell,m} = - \int_{S^2} f \mathcal{Y}_{\ell m} dS.
$$

(23)

It remains to formulate the weak solution with respect to the radius for each $\ell$ and $m$. Hence, a multiplication with a test function $z(r) \in H^1_0((0,1))$ and an integration over the domain $(0,1)$ is done

$$
\left( \frac{d}{dr} w_{\ell m}, \frac{d}{dr} z \right)_{(0,1)} + \ell(\ell + 1) \left( \frac{w_{\ell m}}{r^2}, z \right)_{(0,1)} = (f_{\ell m}, z)_{(0,1)}, \quad \forall z(r) \in H^1_0((0,1)).
$$

(24)

Note that $w_{\ell m} \in H^1_0((0,1))$ and $f_{\ell m} = (rf, \mathcal{Y}_{\ell m})_{S^2}$ where $(\cdot, \cdot)_\Omega$ denotes the scalar $L^2$-product integrated over the domain $\Omega$.

In the following paragraphs, the discretization is performed. First, a truncation in $\ell$ and therefore in $m$ is introduced, s. t. $\ell = 0, \ldots, \ell_{\text{max}}$. For $H^1_0((0,1])$ the subspace $\mathcal{V}_N = \text{span} \{ r(1-r)L_i'(2r-1) | i = 1, \ldots, N \}$ is chosen, hence, each $w_{\ell m}$ is represented as $w_{\ell m}^N(r) = \sum_{i=1}^N [w_{\ell m}^N]_i r(1-r)L_i'(2r-1)$ and $z(r)$ are the basis functions $z(r) = r(1-r)L_j'(2r-1)$, $j = 1, \ldots, N$. Here, the $L_i$’s denote the Legendre polynomials of degree $i$, thus the inputs are shifted by $2r - 1$, because the Legendre polynomials are only defined in $[-1,1]$. Furthermore, $L_i'$ denote the derivatives of $L_i$. Plugging the representations for $w_{\ell m}(r)$ and $z(r)$ into eq. (24) yields

$$
\sum_{i=1}^N [w_{\ell m}^N]_i \left[ \left( \frac{d}{dr} r(1-r)L_i'(2r-1), \frac{d}{dr} r(1-r)L_j'(2r-1) \right)_{(0,1)} + \frac{\ell(\ell + 1)}{r^2} \left( r(1-r)L_i'(2r-1), r(1-r)L_j'(2r-1) \right)_{(0,1)} \right] = f_{\ell m}^j,
$$

(25)
with \( f^i_{\ell m} = (f_{\ell m}, r(1 - r)L'_i(2r - 1))_{(0,1)} \). Herein, the first scalar product can be simplified a lot. First, substituting \( \zeta = 2r - 1 \) gives
\[
\left( \frac{d}{dr} r(1 - r)L'_i(2r - 1), \frac{d}{dr} r(1 - r)L'_j(2r - 1) \right)_{(0,1)}
= \left( \frac{d}{d\zeta} (\zeta + 1) \left( 1 - \frac{\zeta + 1}{2} \right) L'_i(\zeta), \frac{d}{d\zeta} (\zeta + 1) \left( 1 - \frac{\zeta + 1}{2} \right) L'_j(\zeta) \right)_{(-1,1)}
= \frac{1}{4} \left( \frac{d}{d\zeta} (1 - \zeta^2)L'_i(\zeta), \frac{d}{d\zeta} (1 - \zeta^2)L'_j(\zeta) \right)_{(-1,1)}.
\]
Then, with the equality
\[
\frac{d}{d\zeta} \left( (1 - \zeta^2)L'_i(\zeta) \right) + i(i + 1)L_i(\zeta) = 0, \quad \forall i \geq 1, \forall \zeta \in (-1,1)
\]
the scalar product further simplifies to
\[
\frac{1}{4} \left( -i(i + 1)L_i(\zeta), -j(j + 1)L_j(\zeta) \right)_{(-1,1)}.
\]
Now, applying
\[
\int_{-1}^{1} L_i(\zeta)L_j(\zeta)d\zeta = \frac{2\delta_{ij}}{2j + 1}, \quad \forall i, j \geq 1
\]
finally results in
\[
\frac{1}{8} \left( -i(i + 1) \right) \left( -j(j + 1) \right) \frac{2\delta_{ij}}{2j + 1} = \frac{j^2(j + 1)^2}{4(2j + 1)} \delta_{ij}.
\]
With these simplifications and \( \forall 0 \leq \ell \leq \ell_{\text{max}}, -\ell \leq m \leq \ell, j = 1, \ldots, N, \) eq. (24) reads
\[
[A_{\ell m}]_{i,j} [W_{\ell m}]_j = [f_{\ell m}]_j,
\]
where
\[
[A_{\ell m}]_{i,j} = \frac{j^2(j + 1)^2}{4(2j + 1)} \delta_{ij} + \ell(\ell + 1) \left( (1 - r)^2L'_i(2r - 1), L'_j(2r - 1) \right)_{(0,1)}
\]
\[
[W_{\ell m}]_j = [w^N_{\ell m}]_j,
\]
\[
[f_{\ell m}]_j = f^j_{\ell m}.
\]
Herein, the dimensions are
\[
A_{\ell m} \in \mathbb{R}^{N \times N}, \ x_{\ell m} \in \mathbb{R}^N, \ f_{\ell m} \in \mathbb{R}^N, \ \forall \ell, m.
\]
If, for each $\ell$ and $m$, the solution to this linear system is obtained,

$$w_{\ell m}^N(r) = \sum_{i=1}^N [w_{\ell m}^N]_i r(1 - r) L'_i(2r - 1)$$

can be calculated and

$$w(\theta, \phi, r) = \sum_{\ell=0}^{\ell_{\text{max}}} \sum_{m=-\ell}^{\ell} w_{\ell m}^N(r) Y_{\ell m}(\theta, \phi)$$

is the approximate solution to eq. (12). (Quan 2016)

Finally, eq. (14) is solved. Remember that the exact solution to this problem can be derived through a single layer potential. With $\partial_n w_{\ell m}^N(r) = \partial_r w_{\ell m}^N(r)$, which is

$$\partial_r w_{\ell m}^N(r) = \sum_{i=1}^N [w_{\ell m}^N]_i ((1 - r)L'_i(2r - 1) - r L'_i(2r - 1) + r(1 - r)2L''_i(2r - 1)), $$

the coefficients

$$\sigma_{\ell m} = \frac{1}{4\pi} [\partial_n u_g] = \frac{1}{4\pi} \left(g_{\ell m} - \partial_n w_{\ell m}^N(r) \right)$$

are obtained at the Lebedev integration points on the unit sphere’s surface. These coefficients are then used to calculate a density

$$[\sigma]_{\ell m} = \sum_{\ell, m} \sigma_{\ell m} Y_{\ell m}. $$

With this density the single layer potential $\mathcal{S}$, and therefore the solution to eq. (14), reads

$$\mathcal{S}(\theta, \phi, r; [\sigma]_{\ell m}) = \sum_{\ell, m} \frac{4\pi}{2\ell + 1} [\sigma]_{\ell m} Y_{\ell m}(\theta, \phi) \left\{ \begin{array}{ll} r^\ell, & \text{inside } B_1(0) \\ \left(\frac{1}{r}\right)^{\ell+1}, & \text{outside } B_1(0) \end{array} \right\}. $$

Note that in order to obtain the overall solution to eq. (14) both solutions must be added

$$u(\theta, \phi, r) = u_f(\theta, \phi, r) + u_g(\theta, \phi, r) = \sum_{\ell m} w_{\ell m}^N(r) Y_{\ell m}(\theta, \phi) + \mathcal{S}(\theta, \phi, r). $$

5 Numerical Results

In order to test the implementation, two test cases are created. The test cases validate the implemented methods which solve eqs. (12) and (14).
For the first test case we set $f = 1$ in eq. (12) which therefore yields the exact solution

$$u_f(\theta, \phi, r) = u_f(r) = \frac{r^2 - 1}{6}.$$  

As depicted in fig. 5a the numerical solution matches the exact one. However, there is an error which originates in the discretization of the sphere’s radial component. If the amount of integration points in $r$ the error will decrease (cf. fig. 5b).

For the second problem, eq. (14), for the case $g = 1$ and $\partial_n u_f = 0$ the exact solution is known and reads

$$u_g(\theta, \phi, r) = u_g(r) = \begin{cases} -1, & \text{in } \omega \\ -\frac{1}{r}, & \text{in } \mathbb{R}^3 \setminus \omega. \end{cases}$$

In the fig. 6a it is obvious that the numerical solution indeed matches the exact one and the error is $||u_g - u_g, \text{approx}||^2 = 3.3049 \cdot 10^{-30}$. Since $\sigma$ could be computed exactly in this test case, the error is negligible as expected. Note that at $r = 1$ a kink in the derivative of $u$ w.r.t. $r$ can be observed. This is the jump which was demanded from the underlying partial differential equation (PDE).

Last but not least a physical example is provided. Hereby, a constant magnetization $\mathbf{M} = M_0 = (0, 0, 1)^T$ is assumed. Therefore, the boundary conditions become $f = \text{div} \mathbf{M} = 0$, and $g = -\mathbf{M} \cdot \mathbf{n}$ and the exact solution

$$u(x, y, z) = \begin{cases} \frac{z}{3}, & \text{in } \omega \\ \frac{z}{3r}, & \text{in } \mathbb{R}^3 \setminus \omega. \end{cases}$$

can be calculated. Since $f = 0$, the first problem doesn’t play a role at all. Instead, the solution to the second problem is also the solution to the homogeneously
magnetized unit sphere. Again, $\sigma$ could be computed exactly and therefore, the obtained results are exact (cf. fig. 6b) with a negligible error of $||u - u_{\text{approx}}||^2 = 2.9158 \cdot 10^{-31}$.

6 Conclusion

In this seminar report, an introduction to the physics of magnetism has been first given and the importance of the scalar magnetic potential’s computation has been highlighted. Afterwards, a novel method for the computation of the scalar magnetic potential on a unit sphere has been derived and implemented. This method follows the work of Quan (2016) and uses potential theory; more precisely a single layer potential was used. Additionally, two test cases have been implemented in order to verify the code. Last but not least a physical example from Kaliche (2016) has been implemented as well. The derived method is able to solve for the scalar magnetic potential with just a discretization in the radial component of the unit sphere.

Since the presented method is restricted on the unit sphere, it should be extended to spherical geometries in future research. Furthermore, multiple spheres (say hundreds or thousands of spheres) have to be considered, too. This can be done by application of the fast-multipole method. Finally, the algorithm can be included into a micromagnetic simulation in order to simulate a magnonic crystal and analyze its properties.
References


### A Spherical Harmonics

We denote by \( \{Y_{\ell m}\}_{\ell \in \mathbb{N}, -\ell \leq m \leq \ell} \) the set of real spherical harmonics (for the unit sphere \( S^2 \) in \( \mathbb{R}^3 \)), normalized in such a way that

\[
\langle Y_{\ell m}, Y_{\ell' m'} \rangle_{S^2} = \int_{S^2} Y_{\ell m}(s) Y_{\ell' m'}(s) \, ds = \int_0^\pi \int_{-\pi}^\pi Y_{\ell m}(\theta, \phi) Y_{\ell' m'}(\theta, \phi) \sin \theta \, d\theta \, d\phi = \delta_{\ell \ell'} \delta_{mm'},
\]

where \( \delta_{nm} \) denote the Kronecker delta-function. The spherical harmonics can be extended to the surface \( \partial B_r(x_0) \) of a sphere with center \( x_0 \) and radius \( r \) by considering the functions

\[
Y_{\ell m}\left(\frac{x - x_0}{r}\right)
\]
and the scaled inner product
\[ \langle u, v \rangle_{\partial B_r(x_0)} = \frac{1}{r^2} \int_{\partial B_r(x_0)} u(s) v(s) ds = \int_{S^2} u(x_0 + rs') v(x_0 + rs') ds'. \]

Then, the set of spherical harmonics on \( \partial B_r(x_0) \) are also orthonormal with respect to this scaled inner product, i.e.
\[ \langle Y_{\ell m} \left( \cdot - x_0 \right), Y'_{\ell' m'} \left( \cdot - x_0 \right) \rangle_{\partial B_r(x_0)} = \langle Y_{\ell m}, Y'_{\ell' m'} \rangle_{S^2} = \delta_{\ell \ell'} \delta_{mm'}. \]

Note that the purpose of the scaled inner product is to avoid to scale the basis functions by the factor \( 1/r \) in order to have the same set of basis functions on all spheres. Further, the system of spherical harmonics is complete in \( L^2(\partial B_r(x_0)) \) and the Sobolev norms are given by the simple formula: let
\[ u(x) = \sum_{\ell=0}^{+\infty} \sum_{m=-\ell}^{\ell} [u]_{\ell}^m Y_{\ell m} \left( \frac{x - x_0}{r} \right), \]
with
\[ [u]_{\ell}^m = \left\langle u, Y_{\ell m} \left( \frac{x - x_0}{r} \right) \right\rangle_{\partial B_r(x_0)} = \int_{S^2} u(x_0 + rs) Y_{\ell m}(s) ds \]
then
\[ (u, v)_{L^2(\partial B_r(x_0))} = r^2 \left\langle u, v \right\rangle_{\partial B_r(x_0)} = r^2 \sum_{\ell=0}^{+\infty} \sum_{m=-\ell}^{\ell} [u]_{\ell}^m [v]_{\ell}^m, \]
\[ \|u\|^2_{H^s(\partial B_r(x_0))} = r^2 \sum_{\ell=0}^{+\infty} \sum_{m=-\ell}^{\ell} ([u]_{\ell}^m)^2 (1 + \ell^2)^s, \]
for some function \( v \) having a similar structure than \( u \) in (31). We can now extend this formalism to functions whose support is on all spheres \( \Gamma_1, \ldots, \Gamma_M, \Gamma_\infty \) by setting
\[ u|_{\Gamma_i}(x) = \sum_{\ell=0}^{+\infty} \sum_{m=-\ell}^{\ell} [u_i]_{\ell}^m Y_{\ell m} \left( \frac{x - x_0}{r} \right). \]