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# Simulations of magnetic particles with arbitrary anisotropies

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**Abstract**

To simulate the behavior of realistic magnetic particles in magnetic particle imaging it is not enough to perform simulations assuming only a uniaxial magnetic anisotropy energy due to the complex coupling between the magnetic and the mechanic degrees of freedom of the particle in multidimensional excitation fields. Most particles can only be approximated of having uniaxial magnetic anisotropy energy. As such, this work will discuss the shortcoming of currently used models focusing on only uniaxial anisotropy and show how a theoretical model must be defined to allow for arbitrary anisotropy energies. First simulation results showing the differences between different anisotropy energies will be presented at the workshop.

## I Introduction

Magnetic particle imaging leverages the nonlinear magnetic response of magnetic materials in an external magnetic field [1]. As such, magnetic nanoparticles are used as tracer material in a spatially encoded external magnetic field which yields a spatially encoded magnetic response from the particles. Due to this encoding MPI can reconstruct the concentration distribution of the particles within the encoding area (field of view) and has shown great potential for different applications such as vascular imaging or cell tracking.

Since the quality of reconstructions highly depends on the differentiability of the particle's response in two adjacent points in space and this response is dependent on the physical properties of the particle and the encoding field sequence, having a simulation to correctly model and predict the response of the particles is desirable to eliminate experimental uncertainty. Furthermore, simulations give full access to modify and change all physical parameters which might not yet be accessible in an experimental context.

One of the parameters which strongly influences the particle response is the magnetic anisotropy energy (MAE) of the particle. The magnetic anisotropy energy can be modeled in different ways and one of the most common used anisotropy models is that of uniaxial anisotropy which only depends on the angle between the particles magnetization and one energetically preferred body fixed axis also called easy axis. The model of uniaxial anisotropy is the simplest and allows modeling real particles to a certain degree if the particles exhibit a strong uniaxial behavior [2]. Unfortunately, this only covers a small amount of particle classes since particles exhibit different effects on the nanoscale (e.g. different surface anisotropies due to geometry) which makes the total magnetic anisotropy energy a sum of different magnetic anisotropy energies. Experimental measurements of single particles also reveal more complex magnetic anisotropy energies [3] such as biaxial anisotropy.

To remove the limitation of a uniaxial magnetic anisotropy energy a theoretical model must be used which allows the usage of arbitrary magnetic anisotropy energies within the corresponding Langevin equations of coupled particle rotation and magnetization dynamics. Simulation models previously published [4-6], which solely rely on modeling the particles orientation using the body fixed easy axis, are not suited for arbitrary anisotropy energies. Thus, this work will discuss and show, how such a simulation model with arbitrary MAE must be set up.

# II Theoretical model

The model used to describe the particle rotation and the magnetization dynamics are all based on the Yolk-Egg model [7, 8] and consists of coupled Langevin equations for the magnetization movement (a modified Landau-Lifschitz-Gilbert equation) and the mechanical rotation (a modified Euler equation) of the particle. The corresponding angular velocities for the mechanical rotation $\vec{\omega}_n$ (ignoring the inertia of the particle and any vorticity of the surrounding medium) and the rotation of the magnetization vector $\vec{\omega}_m$ are given as [9]:

$$\begin{aligned}\vec{\omega}_n =&\frac{1}{6\eta V_H}(M_S V_M \vec{m}\times\vec{B}_{eff}+\vec{\tau}_{eff}) \quad \text{and}\\ \vec{\omega}_m =&-\frac{\gamma}{1+\alpha^2}\vec{B}_{eff}+\frac{|\gamma|\alpha}{(1+\alpha^2)}(\vec{m}\times\vec{B}_{eff})+\\ &\frac{1}{6\eta V_H}(M_S V_M(\vec{m}\times\vec{B}_{eff})+\vec{\tau}_{eff})\end{aligned}$$

$\eta$ is the viscosity of the surrounding medium, $V_H$ ($V_M$) is the hydrodynamic (magnetic) volume, $\vec{m}$ is the unit magnetisation vector, $M_S$ is the saturation magnetization, $\gamma$ is the (electron) gyromagnetic ratio, $\alpha$ is the damping constant, $\vec{B}_{eff}$ is the effective magnetic field given as $\vec{B}_{eff}=\frac{1}{M_S V_M}\frac{\partial U}{\partial \vec{m}}+\vec{B}_{noise}$ and $\vec{\tau}_{eff}$ is the effective torque given as $\vec{\tau}_{eff}=-\frac{\delta U}{\delta\phi}+\vec{\tau}_{noise}$. $B_{noise}$ and $\vec{\tau}_{noise}$ are Gaussian white noise terms describing the thermal influence on the motion. $U$ is the total energy/potential of the particle consisting of the Zeeman energy $M_S V_M \vec{m}\cdot\vec{B}_{ext}$ and the MAE, e.g. for uniaxial anisotropy it is given as $K_u V_M(\vec{m}\cdot\vec{n}_3)^2$ where $K_u$ is the anisotropy constant and $\vec{n}_3$ is the energetically preferred body axis (which is most commonly the z-axis). $\delta\phi$ is the infinitesimal rotation operator as derived in [10].

With the angular velocities the coupled Langevin equations describing the motion are derived. Depending on how the state of the particles is represented different equations are obtained. The most common one found in literature is using Cartesian coordinates and the vectors $\vec{m}$ and $\vec{n}_3$ [4-6] which yields the equations:

$$\frac{\partial\vec{n}_3}{\partial t}=\vec{\omega}_n\times\vec{n}_3 \quad \text{and} \quad \frac{\partial\vec{m}}{\partial t}=\vec{\omega}_m\times\vec{m}$$

with the implicit condition of $|\vec{m}|=1$ and $|\vec{n}_3|=1$. These equations can only be used, if the potential shows axial symmetry since the rotation of the particle is not fully described. Thus, this is only fullfilled for the case of uniaxial anisotropy (which allows the reduction of the rotational gradient of the potential to $\delta U/\delta\phi=\vec{n}_3\times\partial U/\partial\vec{n}_3$. A second drawback of the method is that it requires an extra normalization step in any explicit step-wise solver since the system is overdetermined (6 equations but only 4 free variables) making the numerical method non-linear and mathematical questionable [11, 12]. This drawback could be solved by using implicit solvers, like the implicit midpoint method [12], which has yet to be done in an MPI related context.

The best way to describe the state of the particle is to use Euler angles $\vec{\Phi}_n=(\varphi_n,\theta_n,\psi_n)$ and spherical coordinates $\vec{\Phi}_m=(\theta_m,\varphi_m)$ representing the orientation of the particle and the magnetization direction, respectively. This yields the coupled Langevin equations:

$$\frac{\partial\vec{\Phi}_n}{\partial t}=\mathbf{E}_{313}(\vec{\Phi}_n)\vec{\omega}_n \quad \text{and} \quad \frac{\partial\vec{\Phi}_m}{\partial t}=\mathbf{E}_{Sphere}(\vec{\Phi}_m)\vec{\omega}_m$$

with $\mathbf{E}_{313}$ and $\mathbf{E}_{Sphere}$ being projection matrices to map the angular velocities onto the change of state [13]. The general rotational gradient of the potential is then given by

$$\begin{aligned}\partial U/\partial\phi &= \vec{n}_3\times\partial U/\partial\vec{n}_3+(\vec{\theta}_n\cot\theta_n+\vec{n}_3)\frac{\partial U}{\partial\varphi_n}\\ &=\vec{\varphi}_n\frac{\partial U}{\partial\theta_n}-\frac{1}{\sin\theta_n}\vec{\theta}_n\frac{\partial U}{\partial\psi_n}+(\vec{\theta}_n\cot\theta_n+\vec{n}_3)\frac{\partial U}{\partial\varphi_n}\end{aligned}$$

with

$$\begin{aligned}\vec{\varphi}_n =&(\cos\psi_n,\sin\psi_n,0),\\ \vec{\theta}_n =&(\sin\psi_n\cos\theta_n,\cos\psi_n\cos\theta_n,-\sin\theta_n) \quad \text{and}\\ \vec{n}_3 =&(\sin\psi_n\sin\theta_n,-\cos\psi_n\sin\theta_n,\cos\theta_n).\end{aligned}$$

The additional term in the rotational gradient in comparison to the uniaxial case is creating a torque which creates a spinning motion around the axis $\vec{n}_3$.

Since common particles have an ellipsoidal shape and a cubic crystalline structure, they exhibit uniaxial anisotropy due shape and cubic anisotropy due to their crystalline structure. The total anisotropy can be written as a sum of both. Cubic anisotropy, only considering first order terms, is defined as:

$$E_{cubic}=K_{c,1}V_M(\alpha_1^2\alpha_2^2+\alpha_1^2\alpha_3^2+\alpha_2^2\alpha_3^2)$$

with $\alpha_i=(\mathbf{R_0}\vec{n}_i(\varphi_n,\theta_n,\psi_n))\cdot\vec{m}$. $\mathbf{R_0}$ is a constant rotation matrix which describes the fact that the anisotropy axes do not need to be aligned with the body fixed coordinate system.

Another more phenomologic approach to describe the anisotropy energy is used in [14] where an anisotropy tensor $\mathbf{K}$ is introduced. The introduced additional energy term reads:

$$E_{tensor}=\vec{m}^T\mathbf{R}_{313}^{-1}(\varphi_n,\theta_n,\psi_n)\mathbf{K}\vec{m}$$

with the inverse of the rotation matrix $\mathbf{R}_{313}^{-1}=\mathbf{R}_{313}^{\mathbf{T}}$. In our case it is defined as the following clockwise rotations:

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around z-axis by $\phi_n$, around new x-axis by $\theta_n$ and last around new z-axis by $\varphi_n$. The rotation matrix is necessary since the anisotropy tensor is only well defined (constant) in the body fixed coordinate system of the particle and thus must be transformed back to the space fixed coordinate system. It should be noted that the anisotropy tensor already includes the uniaxial case and as such it is enough to write the total anisotropy as a sum of $E_{cubic}$ and $E_{tensor}$.

# III Conclusions

This work introduces a theoretical model to describe the coupled magnetic and mechanical motion of magnetic particles. It is discussed that the common approach of using Cartesian coordinates with only $\vec{n}_3$ and $\vec{m}$ cannot fully describe the motion of the particle and is not suited for arbitrary anisotropy energies. Thus, a theoretical model is introduced representing the magnetic (mechanical) state of the particle in spherical coordinates (Euler angles). With this representation, coupled Langevin equations are derived which can accommodate arbitrary anisotropy energies. At the workshop, first results comparing the different anisotropies will be presented and discussed.

# Author's Statement

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