Optimization of a Stern-Gerlach Magnet by Magnetic Field-Circuit Coupling and Isogeometric Analysis

Andreas Pels^{1,2}, Sridhar Balasubramanian², Augusto Garcia-Agundez², Zeger Bontinck^{1,2}, Jacopo Corno^{1,2}, Herbert De Gersem², Sebastian Schöps^{1,2}

¹Graduate School of Computational Engineering, Technische Universität Darmstadt, Germany 2 Institut für Theorie Elektromagnetischer Felder, Technische Universität Darmstadt, Germany

Stern-Gerlach magnets are used to magnetically separate a beam of atoms or atom clusters. The design is difficult since both the magnetic field gradient and its homogeneity should be maximized. This paper optimizes the pole-shoe shapes starting from a reference geometry given in literature. The main contributions of the paper focus on reducing computational time and increasing accuracy, which is achieved by replacing large parts of the model by a magnetic equivalent circuit and by introducing Isogeometric Analysis (IGA) in the remaining field model part, respectively. A highly accurate evaluation of local field quantities is possible thanks to the very smooth field representations, even across elements, offered by IGA's spline-based framework.

Index Terms—Finite element analysis, magnetic circuits, magnetostatics, optimization.

I. INTRODUCTION

MAGNETIC separation of a beam of atoms or atom clus-
ters is done with a Stern-Gerlach magnet [\[1\]](#page-1-0). A deflection of the atoms or the cluster is measurable by combining a highest possible magnetic field gradient with a sufficiently large magnetic field aligning the magnetic moments. Besides twowire configurations, Rabi-type and sextupole Stern-Gerlach magnets are common technology. In a Rabi-type magnet, two ferromagnetic pole shoes are shaped such that the two-wire field is reconstructed. A Stern-Gerlach magnet is designed such that a magnetic field with a sufficiently homogeneous gradient is obtained in a particular region in the gap between the poles.

This paper aims at a further optimization of the poleshoe shapes of the Rabi-type magnet described in [\[2\]](#page-1-1) on the basis of finite-element (FE) and Isogeometric Analysis (IGA) models. The optimization procedure requires the solution of numerous FE models. For reasons of computational efficiency, the optimization is carried out using a 2D model. Two further original improvements of the 2D FE model turned out to be necessary to obtain both a sufficiently accurate as well as a sufficiently fast model. The overall 2D FE model is replaced by an IGA model of the pole region, coupled to a magnetic equivalent circuit modelling the remaining parts of the 2D cross-section. This approach promises fast and accurate simulations while representing the Computer Aided Design (CAD) geometry exactly.

II. MAGNET MODEL

The Stern-Gerlach magnet is operated with a DC current. The magnetic field can be calculated sufficiently accurate with the nonlinear magnetostatic formulation of the Maxwell's equation on the domain V , see Fig. [1](#page-0-0)

$$
\vec{\nabla} \times \left(\mu^{-1}(\vec{B}) \ \vec{\nabla} \times \vec{A} \right) = \vec{J} \tag{1}
$$

Fig. 1. 3D model of the Stern-Gerlach magnet (CST EM STUDIO).

with μ the (nonlinear) permeability, $\vec{B} = \vec{\nabla} \times \vec{A}$ the magnetic flux density, \vec{A} the magnetic vector potential and a current density \vec{J} . The magnetic field gradient in x-direction $\tau = \frac{d|\vec{B}|}{dr}$ d_{x} is obtained from the solution for the magnetic vector potential \overline{A} by post-processing. The average magnetic field gradient in the beam area V_{beam} is then calculated by

$$
\tau_{\text{av}} = \frac{1}{|V_{\text{beam}}|} \int_{V_{\text{beam}}} \tau(x, y) \, \text{d}V \tag{2}
$$

using numerical quadrature. The inhomogeneity of the magnetic field gradient is quantified by

$$
\epsilon = \sqrt{\frac{1}{|V_{\text{beam}}|} \int_{V_{\text{beam}}} \left(\frac{\tau(x, y)}{\tau_{\text{av}}} - 1 \right)^2 \, \mathrm{d}V} \,. \tag{3}
$$

The optimal situation is obtained when τ_{av} is maximal and ϵ is minimal. The reference geometry of [\[2\]](#page-1-1) is shown in Fig. [1.](#page-0-0) The corresponding magnet is already in operation. The coils and the outer yoke parts will not be replaced and, hence, remain unaffected by the optimization. Moreover, changes to the pole geometry may change the magnitude of the magnetic flux but only marginally change the magnetic flux distribution in the outer parts. This motivates considering only the pole region of the Rabi-type magnet in the following. The partial computational domain including the pole tips is denoted by V_p .

We propose to represent the outer part by a generalized magnetic field-circuit coupling based on [\[3\]](#page-1-2). The partial model V_p is embedded as a reluctance \mathcal{R}_p together with a magnetomotive force \mathcal{F}_{mmf} representing the coil and a reluctance \mathcal{R}_{y} representing the outer yoke parts in a magnetic circuit. The flux through the circuit is denoted by Φ . The total reluctance is $\mathcal{R}_{\text{tot}} = \mathcal{R}_{\text{p}} + \mathcal{R}_{\text{y}}$. Hopkinson's law reads $\mathcal{F} = \mathcal{R}_{\text{tot}} \Phi$.

III. DISCRETIZATION AND FIELD-CIRCUIT COUPLING

Let the FE shape functions $\vec{\omega}_i$ of the reduced model be numbered so that $j \in \{1, \ldots, M\}$ are associated with edges inside V_p and $j \in \{M+1, N\}$ associated with edges at $S_p :=$ ∂V_p . The magnetic vector potential is discretized by

$$
\vec{A}_p(\vec{x}) = \sum_{j=1}^M a_j \vec{\omega}_j + \Phi \vec{\chi}, \qquad (4)
$$

where $\vec{\chi}|_{S_p} := \frac{\vec{A}_\star}{\Phi_\star}|_{S_p}$ with \vec{A}_\star , Φ_\star taken from solving [\(1\)](#page-0-1) on the original domain V and continued into the interior of V_p . The weighted residual approach leads to $\mathbf{K}_{aa} \mathbf{a} + \mathbf{K}_{ab} \Phi = \dots$ where $\mathbf{K}_{aa} \in \mathbb{R}^{M \times M}$ is the usual stiffness matrix and

$$
\left(\mathbf{K}_{\mathrm{ab}}\right)_{i1} = \int_{V_{\mathrm{p}}} \mu^{-1} \vec{\nabla} \times \vec{\omega}_i \cdot \vec{\nabla} \times \vec{\chi} \mathrm{d}V,\tag{5}
$$

where $i = 1, 2, ..., M$. An additional equation feedbacks the magnetomotive force of the partial model to the external circuit. The magnetomotive force of V_p is calculated by

$$
\mathcal{F}_{\mathbf{p}} = \int_{\tilde{S}_{\mathbf{p}}} \vec{H} \cdot d\vec{s} = \int_{\tilde{S}_{\mathbf{p}}} \left(\mu^{-1} \vec{\nabla} \times \vec{A} \right) \cdot d\vec{s},\tag{6}
$$

where $\tilde{S}_{\rm p}$ is an adequate part of $S_{\rm p}$. Introducing [\(4\)](#page-1-3) into [\(6\)](#page-1-4) and integrating by part leads to $\mathcal{F}_p = \mathbf{K}_{ba} \mathbf{a} + \mathcal{R}_p \Phi$ where $\mathbf{K}_{\text{ba}} \in \mathbb{R}^{1 \times M}$ can be interpreted as a weighting in a Petrov-Galerkin framework by a new test function $\vec{\chi}'$. Finally, the field-circuit coupled system of equations is

$$
\begin{bmatrix} \mathbf{K}_{aa} & \mathbf{K}_{ab} \\ \mathbf{K}_{ba} & \mathcal{R}_{p} + \mathcal{R}_{y} \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \Phi \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{F}_{mmf} \end{bmatrix} . \tag{7}
$$

IV. SIMULATION AND OPTIMIZATION

IGA is a rather new technique for the discretization of partial differential equations. It can be understood as a generalization of the standard FEM method, however with more regular basis functions employed for the approximation process [\[4\]](#page-1-5). The geometry mapping and the basis functions are described in terms of traditional or non-uniform rational B-splines (NURBS) [\[4\]](#page-1-5), [\[5\]](#page-1-6), [\[6\]](#page-1-7). Consequently the geometry is represented in the language of CAD and this allows natural communication with possible manufacturers of the pole tips. Secondly, highly smooth solutions can be obtained while in classical FEM the basis functions are typically limited to $C⁰$ across the element boundaries. We use the software package GeoPDEs since curlconforming B-splines are provided and it supports a multipatch framework; 3D generalization is also possible [\[4\]](#page-1-5). For use of

Fig. 2. Optimized and original geometry of the pole of the magnet.

the partial model in GeoPDEs, the geometry is split in multiple patches, each one discretized in the reference geometry [\[4\]](#page-1-5). To further speed up the simulations, the nonlinear saturation is frozen, i.e., a constant but inhomogeneous reluctivity $\nu = \nu(\vec{B}_{\star}(\vec{x}))$ is used where \vec{B}_{\star} is taken from the nonlinear computation of the full model.

The cost function for the optimization should combine the requirements for a high average magnetic field gradient τ_{av} and a low inhomogeneity factor ϵ . The function is defined as

$$
f(x, y, w) = \frac{\tau_{\rm w}}{|\tau_{\rm av}|} + \epsilon - \frac{\tau_{\rm w}}{|\tau_{\rm av}|} \epsilon,
$$
 (8)

where x, y, w are the vectors of geometrical DOFs $(x - y)$ coordinates, y-coordinates, weights) of the control points. The weighting by $\tau_w = 8$ T/m ensures that all quantities are approximately equally treated with a slight tendency to prefer the minimization of the inhomogeneity factor. The goal of the optimization is then to minimize [\(8\)](#page-1-8). The pole geometry was optimized using Matlab's Optimization Toolbox. The optimization procedure in GeoPDEs lasts about 6 hours. Building and solving the equation system with field-circuit coupling in GeoPDEs takes approximately half a minute. The optimized and the reference geometry are compared in Fig. [2.](#page-1-9)

ACKNOWLEDGMENT

This work was supported by the 'Excellence Initiative' of German Federal and State Governments and the Graduate School CE at TU Darmstadt.

REFERENCES

- [1] W. Gerlach and O. Stern, "Das magnetische Moment des Silberatoms," *Z. Phys. A-Hadron. Nucl.*, vol. 9, pp. 353–355, 1922.
- [2] B. Masschaele, T. Roggen, H. De Gersem, E. Janssens, and T. T. Nguyen, "Design of a strong gradient magnet for the deflection of nanoclusters," *IEEE Trans. Appl. Supercon.*, vol. 22, no. 3, pp. 3 700 604–3 700 604, 2012.
- [3] D. A. Philips, "Coupling finite elements and magnetic networks in magnetostatics," *Int. J. Numer. Meth. Eng.*, vol. 35, no. 10, pp. 1991– 2002, 1992.
- [4] C. de Falco, A. Reali, and R. Vázquez, "GeoPDEs: A research tool for Isogeometric Analysis of PDEs," *Adv. Eng. Softw.*, vol. 42, no. 12, pp. 1020–1034, Dec. 2011.
- [5] A. Buffa, G. Sangalli, and R. Vázquez, "Isogeometric analysis in electromagnetics: B-splines approximation," *Comput. Method. Appl. M.*, vol. 199, no. 17-20, pp. 1143–1152, Mar. 2010.
- [6] T. Hughes, J. Cottrell, and Y. Bazilevs, "Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement," *Comput. Method. Appl. M.*, vol. 194, pp. 4135–4195, Oct. 2005.