Fakultät f. Mathematik, **Universität Wien**
Forschungsplattform MMM „Mathematics-Magnetism-Materials“

public PhD defense of Sebastian SCHAFFER, MSc

Physics Informed Machine Learning in the Field of Micromagnetism

Time: Friday, 17. Jan 2025, 15:00 – 17:00

Place: MMM-WPI-SemRoom, 8th floor, Oskar-Morgenstern-Platz 1, 1090 Wien

Zoom: https://univienna.zoom.us/j/65405445489?pwd=VNlu8ESBS1IGOCifbS2YnbhiLVxkIw.1
Meeting ID: 654 0544 5489
Kenncode: 105431

1a) 15h00 – 15h45 – 16h00 c.t. : **Presentation by S. Schaffer + Questions of jury and public**

1b) 16h00 – 16h10 : **closed session of jury**

2) 16h15 : « **deliberation** » + « **celebration** » (drinks & snacks)

PhD jury :

Andreas **Cap** (U.Wien) - president
Massimiliano **D’Aquino** (Univ. Napoli Federico II) - referee
Bruno **Després** (Lab. Jacques-Louis Lions, Paris Sorbonne) – referee
Norbert J. **Mauser** (U. Wien) – PhD director / member

Dirk **Praetorius** (TU Wien) – member
Thomas **Schrefl** (U. Krems) – member

Everyone present with a PhD in computational sciences / mathematics / physics allowed to ask a public question.

Lukas Exl
(Co-director of thesis)

Norbert J Mauser
(head MMM and co-director of thesis)

Abstract:

This thesis investigates advanced neural network methodologies, with a primary focus on Physics-Informed Neural Networks (PINNs), Extreme Learning Machines (ELMs), and hard constrained PINNs and the application to computational micromagnetism. These methods are developed to solve complex physical problems, such as the stray field problem, by embedding physical laws directly into the neural network training process, thereby achieving efficient and accurate solutions without extensive supervised data. The development of highly scalable models could pave the way for large scale micromagnetic simulations and its applications to sustainable technologies such as wind turbines and electric motors.

The initial chapters provide a comprehensive exploration of neural networks, detailing how PINNs and ELMs can be tailored for time-independent partial differential equations (PDEs) such as the Poisson equation. Emphasis is placed on hard constrained PINNs, which enhance optimization by removing constraints, thus achieving higher accuracies comparable to traditional numerical solvers like the Finite Element Method (FEM) and Finite Difference Method (FDM). This approach offers mesh-free optimization without the need for complex discretization schemes, allowing for flexible, reduced-order modeling that mitigates the curse of dimensionality.

Subsequent chapters introduce Constructive Solid Geometry (CSG) using R-functions to enforce hard constraints within the PINN framework. This robust modeling technique ensures the exact satisfaction of essential boundary conditions on intricate geometries, arising in the course of the stray field computation. Further, the challenges of magnetostatics are addressed. Particularly the computation of magnetostatic self-energy. By employing the splitting ansatz proposed by Garcia-Cervera and Roma, the research derives energy bounds on finite domains and develops an alternating scheme for the efficient computation of scalar or vector potentials. This scheme facilitates the minimization of magnetostatic self-energy, essential for precise micromagnetic simulations.

The culmination of this work is the application of hard constrained PINNs to the full 3D minimization of Gibbs free energy. By incorporating the Cayley transform, the neural network outputs are constrained to the Lie group of rotation matrices SO(3), ensuring the physical integrity of the magnetization configuration. This innovative approach accurately models continuous magnetization distributions while minimizing total Gibbs free energy, including exchange energy, anisotropy energy, and magnetostatic self-energy. The thesis demonstrates the efficacy of this method through the solution of the NIST µMAG Standard Problem #3 and the simulation of demagnetization processes in hard magnetic materials.

Overall, this thesis makes its contribution to computational micromagnetism by integrating hard constraint physics informed neural network techniques into energy minimization frameworks. However, the developed methods have further applicability beyond magnetostatics to other areas of physics and engineering.

Short Biography: ***Sebastian Alexander Schaffer*** (born 1992) is an Austrian computational scientist. After completing high school in Zeltweg, he earned a bachelor's degree in Process Engineering from the TU Wien. His growing interest in computer science and numerical mathematics led him to pursue a master's degree in Computational Science at Univ. Wien. In his master's thesis, supervised by L. Exl and N. J. Mauser he explored machine learning methods for predicting magnetization dynamics, yielding 2 publications. He continued as PhD student in the field of computational sciences with focus on machine learning in micromagnetism, as full time employee half at the WPI and half at the research platform MMM of Univ. Wien, where he is teaching in Mathematical Modelling and Applied Machine learning.

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