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Transformer Neural Networks for Predicting Magnetization Dynamics

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Publication date:
2022

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Pollok, S., Kotewitz, S. T., Lassen, N. M., & Bjørk, R. (2022). *Transformer Neural Networks for Predicting Magnetization Dynamics*. 256-257. Abstract from 67nd Annual Conference on Magnetism and Magnetic Materials, Minneapolis, United States.

Session HOC

NEW APPROACHES IN COMPUTATIONAL MAGNETISM

Michael Joseph Donahue, Chair

National Institute of Standards and Technology, Gaithersburg, MD, United States

INVITED PAPER

HOC-01. Generative deep learning for permanent magnet microstructures. A. Kovacs[1,2], A. Kornell[1,2], Q. Ali[1,2], J. Fischbacher[1,2], M. Gusenbauer[1,2], H. Oezelt[1,2], M. Yano[3], N. Sakuma[3], A. Kinoshita[3], T. Shoji[3], A. Kato[3] and *T. Schrefl*[1,2] *1. Christian Doppler Laboratory for Magnet design through physics informed machine learning, Wiener Neustadt, Austria; 2. Department for Integrated Sensor Systems, University for Continuing Education Krems, Wiener Neustadt, Austria; 3. Advanced Materials Engineering Div., Toyota Motor Corporation, Mishuku Susono, Japan*

Traditionally, imaging, magnetic measurements, and micromagnetic simulations have been applied to understand the impact of microstructure on the magnetic properties. Here, we apply a data-driven approach to map the microstructure of a nano-crystalline permanent magnet to its demagnetization curve. We represent the demagnetization curve by a few discrete anchor points and train a neural network regressor to predict these points from the granular structure. Once the model is trained, hysteresis properties can be estimated without the need of time-consuming simulation. To reduce the required number of micromagnetic simulations, we combine unsupervised and supervised learning. In a first step, we learn low-dimensional representations of the grain structures. This can be done in an unsupervised fashion. In a second step, we learn the mapping from a low-dimensional latent code that represents a grain structure to anchor points of the demagnetization curve. Through the dimensionality reduction step, we can reduce the number of trainable parameters in the neural network for prediction of the hysteresis properties. Therefore, less training data is needed. Fig. 1 compares the predictions the demagnetization curve for previously unseen granular structures with the ground truth. The mean absolute errors are $0.015M_s$ (magnetization) and $0.02H_A$ (anisotropy field) for the remanence and coercivitiy. For dimensionality reduction, we apply a variational autoencoder. It maps a 2D image of the grain structure to a latent code. Hereby we achieve a compression rate of 98 percent. Variational autoencoders are generative models which can generate new samples within the input space which differ from the original training set. Like face morphing, we generate new magnets by linear interpolation between two points in the latent space. Fig. 2 shows the generation of new magnet microstructures through morphing. The financial support by the Austrian Federal Ministry for Digital and Economic Affairs, and the Christian Doppler Research Association is gratefully acknowledged.

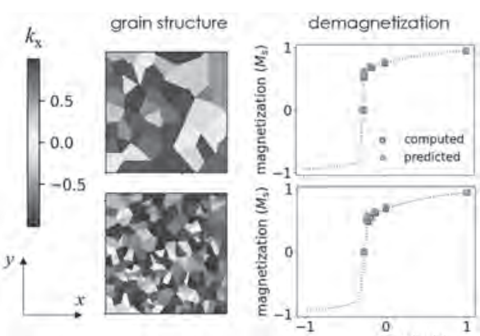

Fig. 1. Predictions of demagnetization properties from the granular structure.

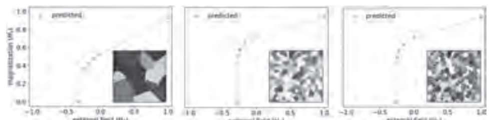

Fig. 2. The structure in the center was generated by morphing from the two other structures shown.

CONTRIBUTED PAPERS

HOC-02. Transformer Neural Networks for Predicting Magnetization Dynamics. *S. Pollok*[1], S.T. Kotewitz[1], N.M. Lassen[1] and R. Bjørk[1] *1. Department of Energy Conversion and Storage, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark*

For modern applications, e.g., magnetic storage devices [1], we need to describe magnetic effects inside material on a nanometer length scale. Using a continuum approach, the micromagnetic formalism [2] allows exactly for this. Within this formalism, a material is modeled with local magnetization vectors *m*, resolving magnetic structures, e.g., domain walls. Existing simulation frameworks, e.g., MagTense [3], are validated by solving standardized benchmarks, e.g., μMAG Standard Problem #4 [4]. In this work, we present a data-driven approach for predicting magnetization dynamics, and validate it on exactly this standard problem. We create a large dataset of magnetization dynamics using MagTense [3], and by optimizing the parameters of a neural network, we are able to generalize dynamics across the physical setup, and subsequently, to ask for solutions of the whole parameter space. We use convolutional neural networks to embed *m* into a low-dimensional latent space. Here, time evolution is then performed with the recent Transformer [5] architecture, which allows for overcoming memory constraints and computational limitations of numerical approaches. As shown in Fig. 1, we embed the external magnetic field H_{ext}, the exchange interaction constant A_{exch}, and the anisotropy constant K along with the local magnetization vectors (m_x, m_y, m_z) into latent space. From the obtained 128-dimensional vector, we can then reconstruct the global sample magnetization M with a mean error of 5 mT per time step, as depicted in Fig. 2. Previously, Kovacs et al. [6] have similarly modeled magnetization dynamics in latent space. In contrast to that approach, we are able to represent a spatially varying external magnetic field of increased range, and to include crystal anisotropy and exchange interaction into our model.

[1] S. Tehrani *et al.*, Proceedings of the IEEE, Vol. 91, no. 5, pp. 703–714 (2003). [2] W. F. Brown Jr., Journal of Applied Physics, Vol. 30, no. 4, pp. S62–S69 (1959). [3] R. Bjørk *et al.*, Journal of Magnetism and Magnetic Materials, Vol. 535, p. 168057 (2021). [4] B. McMichael *et al.*, μMAG Standard Problem #4. URL: https://www.ctcms.nist.gov/~rdm/mumag.org.html (2000). [5] A. Vaswani *et al.*, Advances in Neural Information Processing Systems, Vol. 30 (2017). [6] A. Kovacs *et al.*, Journal of Magnetism and Magnetic Materials, Vol. 491, p. 165548 (2019).

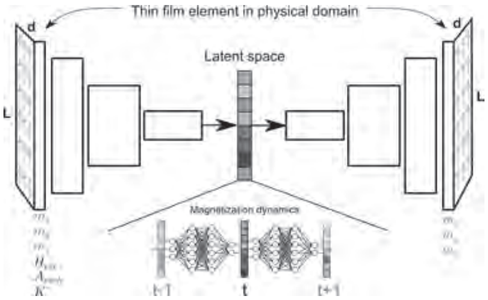

Fig. 1: Deep learning architecture for modeling magnetization dynamics. Using a Transformer [5], the low-dimensional embedding of all contributions is integrated in time before it is mapped back to the original physical domain.

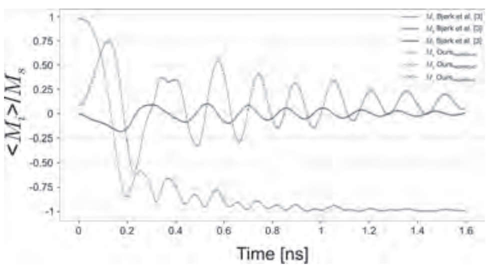

Fig. 2: Reconstruction of the normalized global sample magnetization *M* from latent space. The reconstructed spatial components M_x, M_y, and M_z are compared to the published solution of Bjørk et al. [3].

HOC-03. Artificial Neural Networks for the Analysis of Ferromagnetic Resonance Spectra. D.W. Slay[1] and *M. Charilaou*[1] *1. Physics, University of Louisiana at Lafayette, Lafayette, LA, United States*

Magnetic nanoparticles and nanostructures are important elements in a wide range of applications, and the key properties that determine their performance is the saturation magnetization and the magnetic anisotropy, which in turn determine the internal anisotropy fields. Quantifying these internal anisotropy fields is key for understanding nanomagnetic phenomena and for developing novel materials for applications. Ferromagnetic Resonance spectroscopy (FMR) is a powerful technique for quantifying internal anisotropy fields. The interpretation of FMR spectra, however, requires the use of an appropriate model and forward calculations; no inverse methods are available to extract internal fields from FMR spectra. We will present the use of artificial neural networks for spectral recognition, i.e., to identify the internal magnetic anisotropy fields from the FMR spectrum, as illustrated in the figure. We have trained two different types of networks, a convolutional neural network and a multi-layer perceptron, by feeding the networks with FMR spectra that were pre-computed based on a Stoner-Wohlfarth-type model [1] and labeled with the corresponding anisotropy fields. We tested the trained networks with unseen FMR spectra and found that they successfully predict the correct anisotropy fields with a precision of a few militesla. Surprisingly, the neural networks performed well for data that was beyond their training range [2]. These results demonstrate the potential benefit of using artificial neural networks for accelerated high-throughput analysis of magnetic materials and nanostructures.

[1] M. Charilaou: Ferromagnetic resonance of biogenic nanoparticle chains. J. Appl. Phys. 122, 063903 (2017) [2] D. Slay and M. Charilaou: Spectral Recognition of Magnetic Nanoparticles with Artificial Neural Networks. arXiv 2022 (DOI: 10.48550/arXiv.2206.00166)

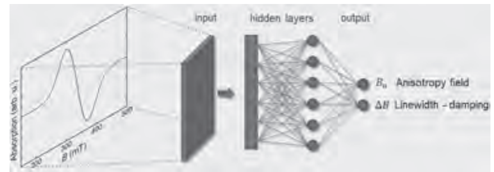

Figure 1

HOC-04. Finite Element Solver for Harmonic Linearized Landau-Lifshitz-Gilbert Equation. *Z. Lin*[1] and V. Lomakin[1] *1. University of California, San Diego, San Diego, CA, United States*

We present a numerical formulation for a linearized Landau-Lifshitz-Gilbert equation (LLGE) based on the finite element method (FEM) for the study of the magnetization dynamics in nanomagnetic structures under weak time-harmonic (given frequency) excitations. The linearized LLGE is obtained by assuming small magnetization deviations around the equilibrium state. Assuming an excitation by an AC field or current at a given frequency, the linearized LLGE is manipulated into a harmonic linearized LLGE for complex magnetization deviation amplitude, which is transverse to the equilibrium state. The resulting linear system of equations is solved by an iterative linear solver. A preconditioner is constructed based on the exchange stiffness matrix and incomplete LU decomposition, which significantly improved the convergence of the linear iterations. The formulation was implemented as a module of the FastMag micromagnetic simulator where all the fields and operators are computed as outlined in [1]. The validity, effectiveness, speed, and scalability of the linear solver are demonstrated by numerical simulations in Figs. 1 and 2. Figure 1 shows the magnetization states obtained by using the introduced harmonic LLGE solver and the full time-domain LLGE solver. The figure shows the magnetization state snapshots at different times. The results show good agreement, but the harmonic LLGE solver is much faster and allows handling complex frequencies, which may be important for understanding the solution behavior. Figure 2 shows the number of linear iterations as a function of the structure size for using different types of the ILU preconditioners. Using the preconditioners significantly reduces the number of iterations and the computational time.

[1] R. Chang, S. Li, M. Lubarda *et al*. Journal of Applied Physics, 109(7): 07D358 (2011).

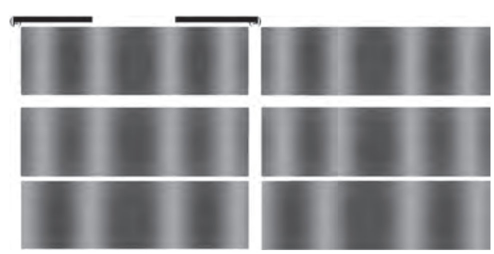

Fig. 1 Magnetization snapshot at t=17.4, 42.8, and 58.9 ns from top to bottom obtained via (a) harmonic linearized LLG solver and (b) non-linear time domain LLGE for a 5×30×100 nm stripe with an excitation field in the middle at 20 GHz frequency and 50 Oe magnitude in the y-direction. The mesh edge length is 2 nm. The material parameters are M_s = 800 emu/cm^3, A_{ex} = 10^{-6} erg/cm, α = 0.01.