Machine Learning for Skyrmion Dynamics under Multi-physics Coupling: Enhancing Micromagnetic Simulations through Automation

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***Abstract*—Skyrmions, one of the magnetic textures, are often simulated to design and build new electronic devices as a type of beyond-CMOS technologies. Landau-Lifshitz-Gilbert (LLG) equation is the most fundamental formula describing the motion of magnetic moments in the ferromagnetic materials. To enhance micromagnetic simulation workflows based on the non-linear LLG equation for Skyrmion dynamics, machine-learning (ML) methods will be used to accelerate the complex computation while bypassing the conventional and necessary Fast Fourier Transform (FFT) calculations. A micromagnetic toolkit [1] built on COMSOL Multiphysics (developed by Theoretical spintronics group at FUDAN University) will be implemented to model and simulate the transient and dynamic response of the Skyrmions. By adjusting the key parameters within the LLG equation, such as Dzyaloshinskii-Moriya Interactions (DMI) strength, material size, and anisotropy constant, the presence of Skyrmion, dynamic response and its annihilation, switching time can be determined accurately and extracted as the key label features. COMSOL with MATLAB Simulink will be scripted to automate parameters sweep to generate large number of datasets for model training. We will construct a ML model: a convolutional encoder first compresses the magnetisation pattern as it extracts key spatial features by calculating convolutions, fully connected layers will be followed to predict skyrmion dynamics. The resulting model is intended to lower computational complexity for existing micromagnetic computation with satisfied generalization capability.**

***Index Terms*— Skyrmions, Spintronics, Multi-physics Simulation, Machine Learning, AI for Science**

I. Introduction

Since the middle of the 20th century, silicon-based semiconductor is used widely for the information storage and transmission. Though the number of transistors used in CMOS technologies is increasing exponentially every year according to the Moore's law for obtaining higher gain and signal-to-noise ratio (SNR) [2], the power budgets have started to limit its increment. Beyond-CMOS technology has been developed due to its potential of dealing with the scalability problem and achieving lower energy consumption [3].

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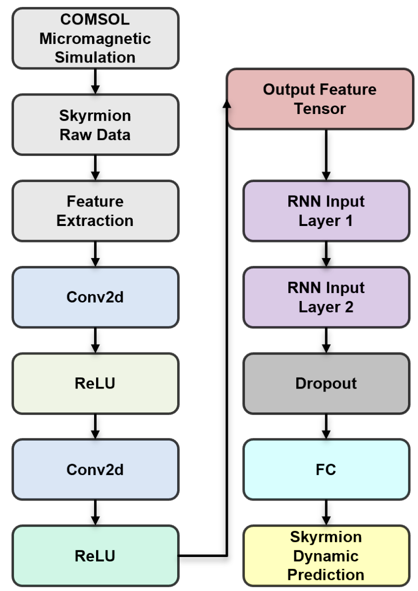

Fig. 1. Workflow

A new class of devices created from the field of condensed matter physics, called spintronics, is one of the beyond-CMOS technology in the post-von Neumann computing architecture. Spintronic device has the advantage of high degree of scalability and low power consumption due to the property of combining both electron spin and its charge to provide more degree of freedom (DOF) compared to CMOS technology [4]–[6]. Magnetic skyrmion is a type of the topology protected magnetic textures, which exhibits high endurance and rapid information carriers.

Skyrmions can be driven by various external field without causing damage to itself. In rotationally symmetric systems, skyrmion crystals can rotate as a whole in a fixed direction under a temperature gradient (clockwise or counter clockwise, depending on its direction) [7]. Skyrmions can also be driven by spin waves, electric currents, and alternating magnetic fields [8]. However, the topological protection of skyrmions is not absolute, when external interference is strong enough, skyrmions can also be annihilated. Moreover, current-driven skyrmions are also annihilated depending on constricted geometries [9].

It is significant to simulate skyrmion dynamics under different setup to understand its behavior and build a wide range of beyond-CMOS electronic devices. Although the LLG dynamics are typically solved using the finite difference method (FDM), this approach introduces computational complexity due to the long-range interactions between cells [10]. Now, researchers have pointed out that the machine leaning methods can be used to accelerate the calculation process. Though the neural network they designed have successfully boosted the rate of simulation ten time faster than traditional FDM methods, it still faces the issue of weak generalization capability and scalability, especially in Multiphysics coupling.

II. Methodology

A. Automated Simulation Pipeline

Due to the highly nonlinear nature of the LLG equation and its strong dependence on specific geometric structures, it is almost impossible to solve the equation using mathematical techniques. However, as the efficiency of solving partial differential equations using computers has significantly improved, and therefore the ordinary computers can be used to solve partial differential equation systems.

Using appropriate micromagnetic simulation software is significant as we are focusing on the skyrmion dynamics when external field is involved. COMSOL Multiphysics can not only be used to implement complex system simulation, but also provide a flexible platform for coupling with other physics module, such as heat transfer and AC/DC. Micromagnetic module is developed using the weak form of the LLG equation by Yuchao Wei [1]. We can easily achieve the micromagnetic simulation by simply adjusting the parameters inside the LLG equation, variables, and the boundary conditions.

Post-proceeding modules are provided as well in COMSOL. Users can easily plot the animation of the transient response, and extract the distribution of high-resolution magnetic moments at one specific frame as a 'csv' file. Parameter sweep will be used to generate sufficient number of datasets for the feature extraction and ML model training procedures.

B. Feature Engineering

To prepare the data for supervised classification or regression, a structured feature extraction process should be designed to process simulation raw data output. Magnetization components can be visualized and quantified over spatial grids within COMSOL. From these raw fields, both global and local features are derived. Global features include mean, total energy, and DMI strength, while local features consists of skyrmion radius, distance between skyrmion and boundary of the rectangular membrane, and motion vectors. Additionally, binary and multiclass behavior labels, such as annihilation, translation, and stationary will be manually assigned. For the image-based pipelines, raw magnetization maps will be flattened into 2-Dimensional (2D) tensor format for convolutional architectures.

C. ML Model Training

As shown in Figure 1, we propose a machine learning architecture that combines convolutional and recurrent layers to classify skyrmion behavior (annihilation, motion, or static) under varied external field conditions. Raw magnetization maps generated from COMSOL micromagnetic simulations are first passed through stacked 2D convolutional layers with ReLU activations to extract spatial features. These encoded feature tensors are then fed into a recurrent neural network (RNN) to capture temporal evolution, followed by dropout regularization and a fully connected layer for final classification.

In addition to our proposed image-based CNN–RNN model, classical machine learning classifiers (e.g., Random Forest, XGBoost) will also be trained for benchmarking purposes. All models will be trained using stratified train-validation-test splits, and evaluated using standard metrics including accuracy, precision, and confusion matrices to interpret error distributions. The best-performing models will be saved and tested on both public and in-house datasets to assess robustness and generalization.

III. conclusion and Impact

This aim of this study is to accelerate the simulation process by classifying the dynamic response of skyrmion bypassing the traditional calculation process. We will use COMSOL Multiphysics software to generate large numbers of datasets to extract features and train the customized CNN-RNN model to predict skyrmion behavior (annihilation, motion, or static) under varied external field conditions, providing valuable insights for guiding the design of skyrmion-based devices in which they are used as information carriers.

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