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DOCTORAL DISSERTATION SUMMARY

Macrospin models: scalable simulations of multilayer spintronic devices

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AUTOREFERAT ROZPRAWY DOKTORSKIEJ

Modele makrospinowe: skalowalne symulacje wielowarstwowych układów spintronicznych

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Aim and motivation of the thesis

The primary motivation of the thesis was to bring modern modelling and software development techniques to rapid prototyping and fitting to experimental data in spintronics. To this end, the author designed the open-source PYTHON simulation package CMTJ[1], which can serve as the basis for further projects. Its versatility was demonstrated in the thesis by considering different multilayer structures, as well as various modelling approaches such as dynamic models, energy-based models [1], Bayesian modelling [2], and reinforcement learning [3].

Some of the existing approaches to macrospin modelling involve SPICE [4, 5, 6] or Verilog simulation environments [7], but these approaches often suffer from performance issues, making them less suitable for large-scale modelling. The thesis draws on the notion of digital twins, a concept that has gained attention in recent years, particularly in the context of Industry 4.0 [8]. In the digital twin approach, a physical model (in the context of the thesis, a spintronic device inside a measurement station) is accompanied by a virtual model (a set of equations and a controller, provided by the software package); real-world operations can first be simulated in the software before a twin solution is deployed in the laboratory. In particular, the final chapter of the thesis is inspired by the experiment on plasma control in a tokamak fusion reactor, where the algorithm was first trained in the simulated environment before it was deployed in situ [9].

The thesis first presents the technical contribution of the core software package, CMTJ, together with an overview of the numerical techniques used to model multilayer spintronic devices that are indispensable for understanding the research problems addressed in the remainder of the thesis. Those problems are the following:

1. Multilevel switching under field reversal in Co/Pt(wedge)/Co samples [10].
2. Synchronisation and desynchronisation of the magnetic tunnel junctions (MTJs) connected in series [11].
3. Real-time control of spintronic devices for current-induced switching and synchronisation problems [12].

The first two problems arise from the need to explain phenomena observed in experimental data, with the initial challenge being formal analysis and realistic modelling of the experiments. The third research problem is primarily theoretical and has not yet been verified experimentally at the time of writing. In this case, the focus was on realistic assumptions and the prediction of results without access to experimental data.

The following sections provide a brief synopsis of these research problems.

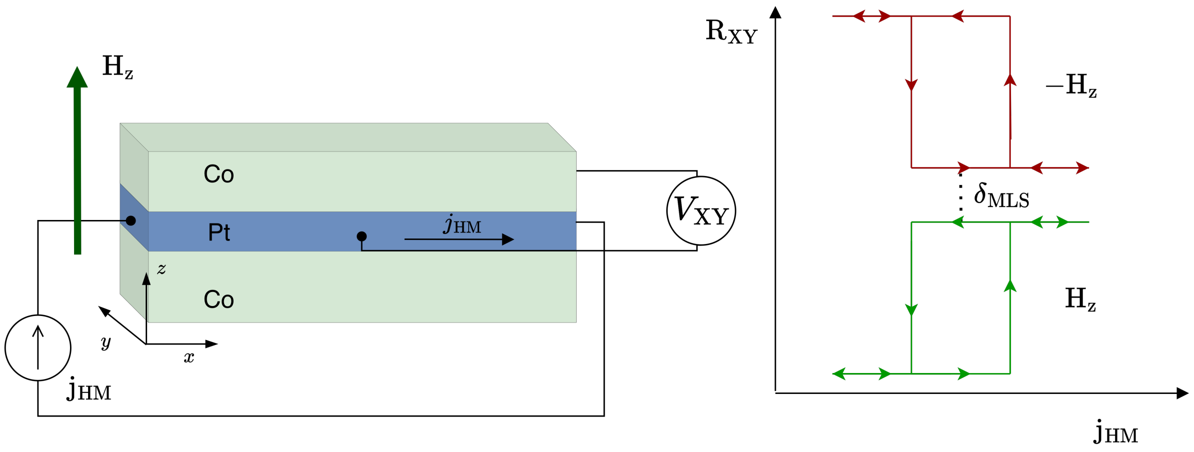

Figure 1: *A schematic representation of the multilevel switching (right), alongside the simulated ferromagnet/heavy metal/ferromagnet (FM/HM/FM, wedge not pictured) stack. The* R_{XY} *measurement serves as a proxy indicator of the magnetisation direction, with the dominant contribution from the AHE resistance.*

Research problem 1: Multilevel switching in Co/Pt(wedge)/Co samples

In Co/Pt(wedge)/Co samples with strong Dzyaloshinskii-Moriya interaction (DMI), interlayer exchange coupling, and strong spin-orbit interaction due to the presence of the heavy-metal (Pt), a phenomenon dubbed multilevel switching (MLS) was observed. When sweeping the current magnitude, the anomalous Hall effect resistance (AHE) hysteresis loop measured under positive external magnetic field bias H_z undergoes a vertical shift relative to the loop measured at $-H_z$. Here, the AHE resistance R_{AHE} (and thus R_{XY}, as shown in Fig.1) acts as an internal indicator of the magnetisation direction. Two hypotheses on the origins of the MLS were proposed:

1. The interfacial asymmetry at the two HM interfaces leads to asymmetric AHE resistance contributions under field reversal.
2. A marked difference in the perpendicular magnetic anisotropy energy between the upper and lower cobalt layers, in combination with strong interlayer exchange, causes MLS.

The first proposal was based on the evidence provided by the earlier work on the same sample by Ogrodnik et al. [13] in which the §asymmetry between the upper and lower Co/Pt interfaces was demonstrated by both XRD and Monte Carlo simulations. Similarly, values for magnetic anisotropy energy and interlayer exchange coupling were derived from the same work. After multiple simulations, neither hypothesis could be rejected, and the thesis remarks on the possibility that a combination of the two causes MLS. Regarding the first hypothesis, using the anisotropy and coupling values reported in [13], and introducing an asymmetry correction factor to both torques and R_{AHE} in the resistance equation allowed the shifted AHE hysteresis to be reproduced under field reversal. However, the second hypothesis was also partially supported. If we assume a relatively large anisotropy energy in the lower Co layer and set the anisotropy for the upper Co layer to be even greater by a factor ΔK then, in a strong coupling regime the MLS hysteresis can be reproduced without the need for the additional correction factor in R_{AHE}. However, because the values of the anisotropy energy in the lower Co, though reasonable, fall outside the range reported in [13], this explanation was not pursued by Grochot et al. [10]. The impact of DMI was also tested and rejected as either a cause of the MLS and an amplifying factor.

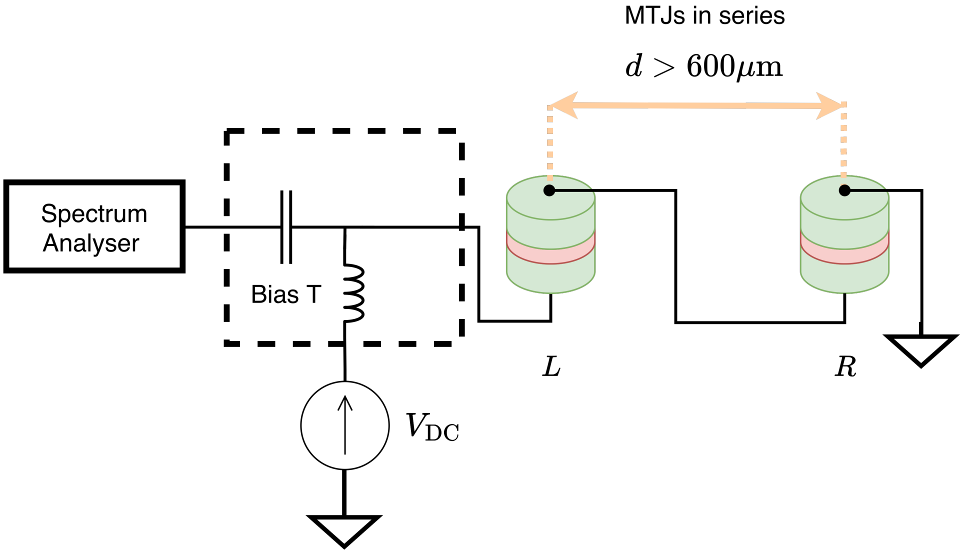

Figure 2: *Schematic for the experimental setup for two MTJs coupled through a series electrical connection.*

Research problem 2: Synchronisation and desynchronisation of MTJs

Synchronisation of two or more MTJs has been a topic of intensive research in recent years. A common method to achieve synchronisation uses long-range dipole interaction [14, 15, 16], but recent research explored a variety of coupling methods through current control [17, 18, 19].

In 2018, Taniguchi et al. [20] proposed a theoretical method of electrical coupling in which two MTJs are coupled through an electrical connection. In that model, for a series connection of two MTJs, the synchronisation depends on the relative alignment of the pinned layer of the first MTJ and free layer of the second MTJ. The thesis analyses and simulates this experimental setup for a series connection of two MTJs, separated by more than 600 µm to exclude dipole interaction from the picture (see Fig.2 for a schematic setup). For this configuration, a field scan was performed; for each value of the external field magnitude, a spectrum was collected first for the coupled pair and then separately for each MTJ. The analysis of the experimental results showed that in the coupled pair, the two MTJs oscillated with a common mode, up to a threshold field, beyond which the oscillation splits into two modes. Therefore, in the thesis, the simulations were devised to explore this behaviour of "desynchronisation". The explanation that ultimately proved satisfactory was due to the observation that the model by Taniguchi et al. [20] required a modification that accounts for the parametric dispersion of two coupled MTJs. Previous works on the topic, for example, Arun et al. [21], focused on the ideal case, assuming two junctions with identical magnetic and electric parameters. However, in our simulations, we allowed the magnetic parameters, namely the saturation magnetisation $\mathrm{M_s}$ and the magnetic anisotropy constant $\mathrm{K_u}$ to vary up to $\pm 10\%$ from the values determined by fitting experimental ferromagnetic resonance curves to a single decoupled MTJ. This approach allowed for a reproduction of desynchronisation fields in the simulations which closely matches the experimental picture. A sample desynchronisation is shown in Fig.3. Furthermore, one can balance the magnetic anisotropy or $\mathrm{M_s}$ disparity between two MTJs to lower or raise that desynchronisation threshold. This behaviour enables tunable devices that use voltage-controlled magnetic anisotropy (VCMA) to control the disparity of magnetic anisotropy and thus the moment when two devices synchronise or desynchronise under a constant external field; this use case has been demonstrated

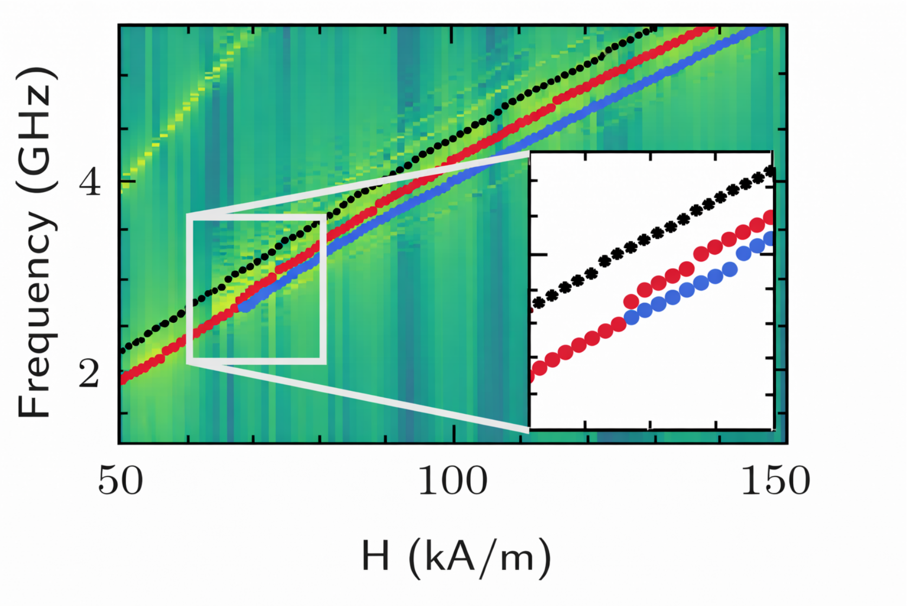

Figure 3: *A simulation reproducing desynchronisation field observed in the experimental data. The background is a frequency spectrum of the magnetoresistance of two MTJs measured in series, the black line is the reference signal of the first MTJ when disconnected from the in-series configuration. The red and the blue lines come from the first and the second MTJ in the series connection respectively. The zoom inset presents the exact moment when at some threshold external magnetic field two MTJs begin to oscillate with different dominant frequencies.*

both in the thesis and in the paper [11], an example is also shown in Fig.4. In the thesis, the author also remarks on the two possible simulation setups: one in which Kirchhoff's current law is strictly preserved, i.e. the total current in the circuit is constant at all times, and another in which small current changes due to synchronising current fluctuations are allowed (in this configuration, the voltage is assumed to be kept constant). Both configurations yield the same results, up to a small correction factor in the current density, and therefore this modelling assumption affects only the interpretation of the result.

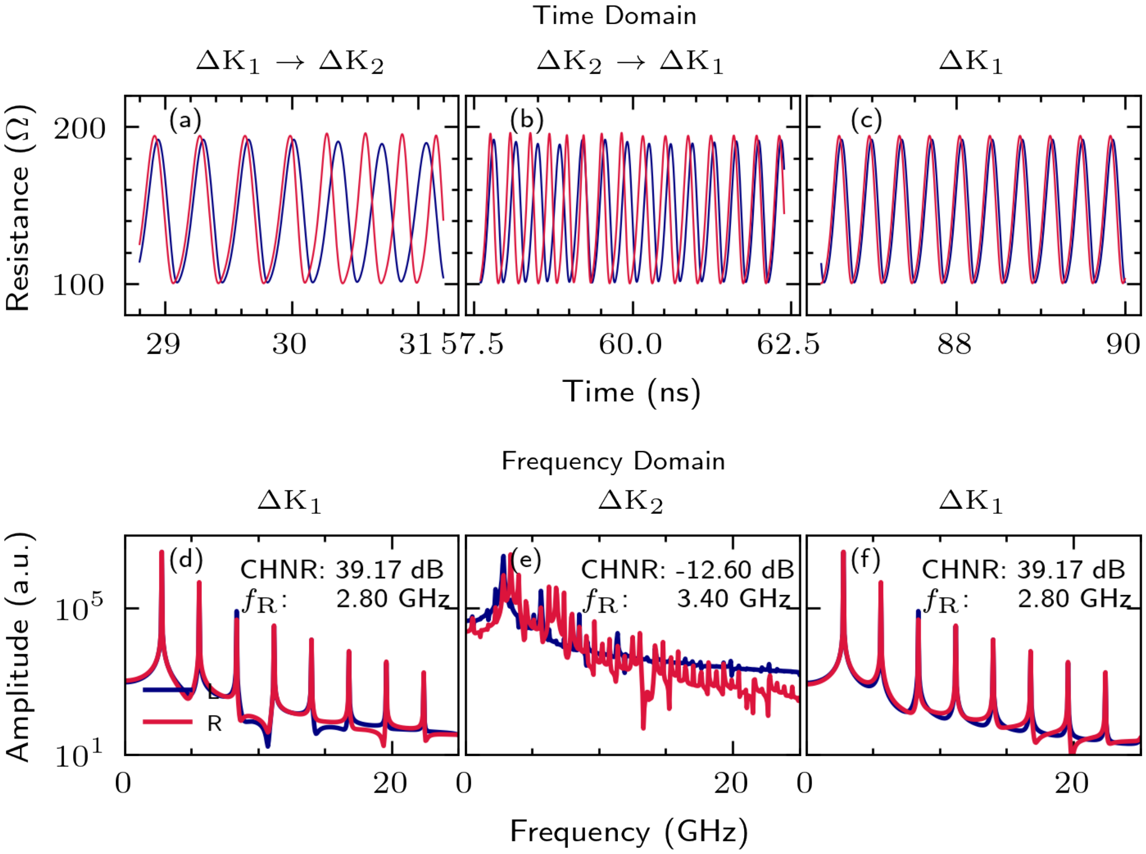

Figure 4: *An example of the VCMA control of synchronisation for the in-series configuration of two MTJs. Each column depicts a transition, obtained by changing the anisotropy of the first MTJ in series. The top row shows the magnetoresistance over time for the first MTJ in series (red) and the second (blue). Going from left to right: we first change the anisotropy of the first MTJ (a, d) causing a desynchronisation, then after some time we change it back to the original value (b, e), an action which after some time leads to a renewed synchronised state (c, f). Depicted in the bottom row are the frequency spectra of steady states observed after each transition. The overlap of the blue and red spectra confirms the synchronised state. CHNR (cross-harmonic noise ratio) is used in the thesis as one of the synchronisation measures, the larger it is, the stronger the synchronisation.*

Research problem 3: Real-time control of spintronic devices

The final part of the thesis demonstrates various approaches to employing CMTJ for reinforcement learning (RL) tasks. The two cases described in the thesis are real-time control of the spin-torque oscillator (STO) and current-induced magnetisation switching (CIMS). The schematic configurations for these tasks are shown in Fig.5 and Fig.6.

In the STO synchronisation task, the controller (RL agent) can change the external field magnitude and direction as well as the input bias current. The aim is to force a given STO to match its oscillating frequency to the frequency specified by the task. The agent is rewarded for taking fewer steps and using less energy (which is proportional to the magnitude of the field and the current density). For the CIMS task, two configurations were considered: SOT and STT. Each had a different geometry, but in the simulation the agent was given control only of the input current density and was tasked to switch the magnetisation from the starting position to the opposite position using as little energy as possible.

Several assumptions, common to both simulation configurations, were made to make the simulations more realistic, and thus challenging. First, selected device parameters are always sampled at random from the uniform distributions designed to satisfy two key properties:

1. The maximum and minimum parameter values represent a realistic dispersion encountered in spintronic device fabrication scenarios.
2. The parameter ranges are chosen so that every sampled instance remains solvable and the controller may complete the task successfully.

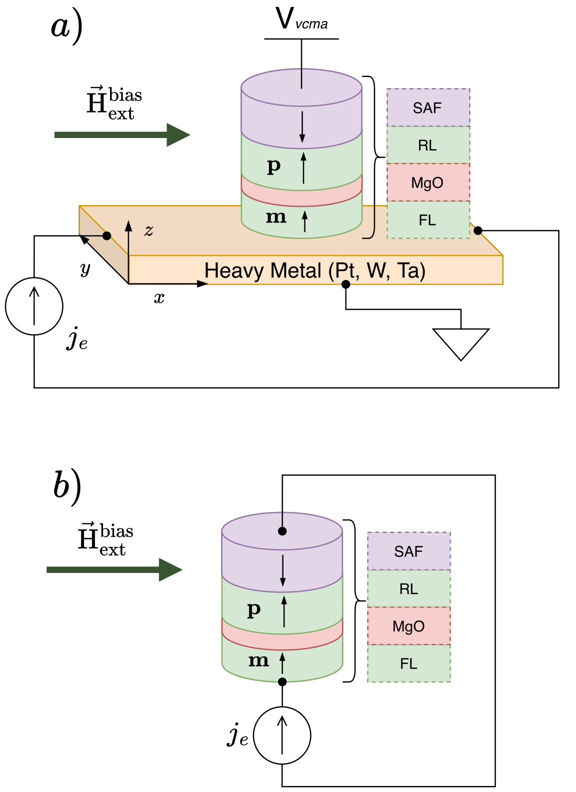

Figure 5: *Schematic configurations for CIMS task: (a), spin-orbit torque (SOT) switching; (b), spin-transfer torque (STT) switching.*

Furthermore, the initial conditions, as well as the success criteria for a given task, are sampled at random at the beginning of each simulation episode. At no point during the training or the evaluation does the controller have access to the sampled magnetic parameters of the models; in other words, the device is treated as a black box by the RL agent. Secondly, the measurement inputs, called observations in the RL terminology, are provided to the controller at a lower sampling rate than the solver time step, which introduces a delay in control and creates a coarser timescale. The simulation and the measurement are not asynchronous; that is, they share the same clock. We note that this assumption should be revisited in future research.

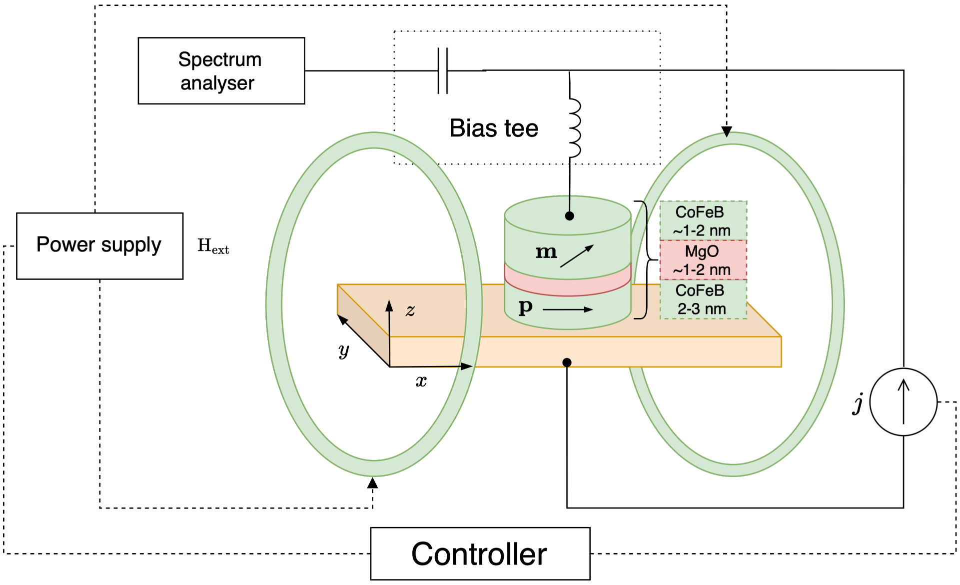

Figure 6: *A configuration for the controller-driven simulation of the spin torque oscillator synchronising to the desired target frequency.*

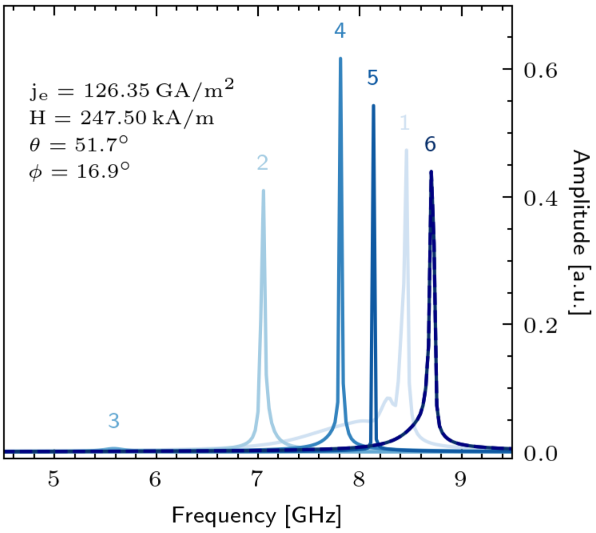

Figure 7: *Sample RL synchronisation task. Final controller values are shown in the box. The peaks, numbered from 1 to 6, represent the STO spectrum at each tuning step of the controller.*

Third, the controller, or RL agent, is allowed to make continuous actions, meaning that the output value can be any real number in the specified parameter range. For both tasks, Soft Actor Critic (SAC) [22], Twin Delayed Deep Deterministic (TD3) [23] and Proximal Policy Optimisation (PPO) [24] algorithms were the best performing, although the optimal choice of the algorithm depended on the particular task.

Some modifications of the task, particularly in SOT switching, turned out to be difficult for all the models, for example, the trade-off between the low-current usage and a fast switching. Across the distribution of the magnetic parameters, the RL agent favoured a conservative strategy by choosing to complete the task successfully, rather than using input currents close to the theoretical minimum which ensure quick switching. Such problems can be alleviated by fine-tuning specific parameter ranges of the sampling distributions to a particular experimental setup. STO synchronisation was the simpler task of the two: the controller learnt to achieve a target frequency within a very small number of steps, often only five control steps were needed to reach the synchronisation. In Fig.7 we show a sample run of the RL controller in the STO task, where in six controller steps, the RL agent synchronises to the target frequency ≈ 8.7 GHz.

Outlook

The results presented in this thesis indicate that CMTJ can serve not only as a simulation package for prototyping spintronic models but also as a foundation for a broader computational framework that connects modelling, parameter identification, and control. The natural continuation of this work is therefore twofold: to increase the physical realism of the models and to shorten the distance between simulation and experiment. In that sense, the long-term perspective of the project is the development of a practical digital-twin workflow for spintronic devices, in which model parameters are updated from measurements, candidate control strategies are first tested in silico, and then transferred to the laboratory setup.

A particularly promising direction is further investigation of the $1/f^{\alpha}$ noise, also described in the thesis and available in the CMTJ package. The critical challenge in modelling this type of noise process is an adequate parametrisation of the noise parameters in the simulation. At the moment, there does not exist a good method to extract those parameters from the experiment or compute them theoretically, and, as a result, the simulation focuses mainly on qualitative rather than quantitative reproduction of the noise effects.

In the case of electrically coupled MTJs, the thesis shows that parameter dispersion is not a secondary perturbation but a central ingredient of the observed synchronisation–desynchronisation transition. This immediately opens several directions for future study. First, the analysis should be extended from pairs of oscillators to larger coupled networks, where dispersion may play a constructive and destructive role depending on the desired collective state. Secondly, the control of synchronisation through voltage-controlled anisotropy deserves further attention, as it offers an interesting path toward tunable oscillator networks without changing the geometry of the device.

List of publications

The results of the publication marked with (*) were included the doctoral thesis.

1. Skowroński, W., Łazarski, S., **Mojsiejuk, J.**, Chęciński, J., Frankowski, M., Nozaki, T., Yakushiji, K., Yuasa, S., “High frequency voltage-induced ferromagnetic resonance in magnetic tunnel junctions”. *Applied Physics Letters* 115.7 (Aug. 2019), p. 072401. DOI: `10.1063/1.5113681`

2. **Mojsiejuk, J.**, Kulig, P., Chęciński, J., Frankowski, M., “Visualization for Micromagnetics With Synchronized Plotting”. *IEEE Transactions on Magnetics* 56.2 (Feb. 2020), pp. 1–6. DOI: `10.1109/TMAG.2019.2949515`

3. (*) Ziętek, S., **Mojsiejuk, J.**, Grochot, K., Łazarski, S., Skowroński, W., Stobiecki, T., “Numerical model of harmonic Hall voltage detection for spintronic devices”. *Physical Review B* 106.2 (July 2022), p. 024403. DOI: `10.1103/PhysRevB.106.024403`

4. (*) **Mojsiejuk, J.**, Ziętek, S., Grochot, K., Skowroński, W., Stobiecki, T., “cmtj: Simulation package for analysis of multilayer spintronic devices”. *npj Computational Materials* 9.1 (Apr. 2023), p. 54. DOI: `10.1038/s41524-023-01002-x`

5. (*) Rzeszut, P., **Mojsiejuk, J.**, Skowroński, W., Tsunegi, S., Kubota, H., Yuasa, S., *Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions*. arXiv:2306.11608 [physics]. June 2023

6. (*) Grochot, K., Ogrodnik, P., **Mojsiejuk, J.**, Mazalski, P., Guzowska, U., Skowroński, W., Stobiecki, T., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”. *Scientific Reports* 14.1 (Apr. 2024), p. 9938. DOI: `10.1038/s41598-024-60492-x`

7. (*) Safeer, C., Keatley, P. S., Skowroński, W., **Mojsiejuk, J.**, Yakushiji, K., Fukushima, A., Yuasa, S., Bedau, D., Casanova, F., Hueso, L. E., Hicken, R. J., Pinna, D., Van Der Laan, G., Hesjedal, T., “Magnetization dynamics driven by displacement currents across a magnetic tunnel junction”. *Physical Review Applied* 22.2 (Aug. 2024), p. 024019. DOI: `10.1103/PhysRevApplied.22.024019`

8. (*) **Mojsiejuk, J.**, Ziętek, S., Skowroński, W., “Reinforcement learning for spin torque oscillator tasks”. *Journal of Physics: Conference Series* 3161.1 (Jan. 2026), p. 012025. DOI: `10.1088/1742-6596/3161/1/012025`

9. Cierpiał, M., Maślanka, D., Gubała, K., **Mojsiejuk, J.**, Grochot, K., Wrona, J., Langer, J., Nan, T., Skowroński, W., “Magnetic tunnel junction made of abundant materials for memory and dynamic applications”. *Scientific Reports* 15.1 (Oct. 2025), p. 35227. DOI: `10.1038/s41598-025-20842-9`

10. (*) Cierpiał, M., Grochot, K., **Mojsiejuk, J.**, Pawlak, J., Kanak, J., Wrona, J., Nan, T., Skowronski, W., “Spin-orbit-torque-induced magnetization switching in alpha-W-based magnetic tunnel junction”. *Journal of Physics D: Applied Physics* (Dec. 2025). DOI: `10.1088/1361-6463/ae2edc`

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