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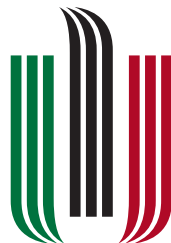
Macrospin models:
scalable simulations of multilayer spintronic devices

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ROZPRAWA DOKTORSKA

Modele makrospinowe:
skalowalne symulacje wielowarstwowych układów
spintronicznych

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Abstract

The advances in spintronics enabled technologies such as low-energy non-volatile magnetic memory, sensitive magnetic field detectors, and microwave nano-oscillators. Progress in those areas relied not only on experimental breakthroughs but also on a variety of modelling frameworks that guide material optimisation or clarify mechanisms underlying physical behaviour.

The thesis builds on that tradition by contributing modelling tools tailored to contemporary challenges in the field such as multivariable optimisation of device performance. The first contribution is technical and involves the development of the open source macrospin simulation package called *cmtj* that is used to fit experimental data or prototype new architectures. The package is grounded in modelling frameworks provided by the stochastic Landau–Lifshitz–Gilbert–Slonczewski equation and Smit–Beljers formalism.

As the second contribution, the *cmtj* software is employed in three experimental contexts: (i) numerical modelling of harmonic Hall voltage detection in the Ta/CoFeB sample, (ii) explanation of the multilevel switching phenomenon in a trilayer spin-orbit torque Co/Pt/Co system with strong interlayer exchange coupling and Dzyaloshinskii–Moriya interaction, and (iii) the study of desynchronisation fields in electrically coupled in-series CoFeB/MgO/CoFeB magnetic tunnel junctions. For each, extensive simulations highlight the flexibility of the macrospin model and provide detailed insight into the experimental observations.

Finally, *cmtj* is applied to extrapolate to novel device architectures. Using reinforcement learning, it is demonstrated how a controller can steer an oscillator to synchronise with a desired frequency in a few tuning steps or learn a current impulse shape that leads to magnetisation switching in a simple memory cell model.

Streszczenie

W ostatnich latach postępy w spintronice doprowadziły do powstania niskoenergetycznych pamięci nieulotnych MRAM, czułych detektorów pola magnetycznego oraz nanooscylatorów działających w zakresie mikrofalowym. Rozwój tych urządzeń opierał się w dużej mierze na różnorodnych technikach modelowania, które wyjaśniły mechanizmy leżące u podstaw ich działania lub umożliwiły optymalizację materiałów.

Niniejsza rozprawa wpisuje się w tę tradycję, prezentując narzędzia modelowania dostosowane do współczesnych wyzwań tej dziedziny takich jak optymalizacja układów w przestrzeni wielu parametrów. Pierwszym wkładem rozprawy jest otwarty pakiet symulacyjny *cmtj*, który może być użyty do dopasowywania wyników eksperymentalnych lub prototypowania nowych urządzeń spintronicznych. W ramach pakietu zostały zaimplementowane różne metody numeryczne oparte m.in. na równaniu Landaua–Lifshitz–Gilberta–Slonczewskiego oraz modelach Smita–Beljersa.

Druga część pracy opisuje użycie programu symulacyjnego *cmtj* do zamodelowania trzech zjawisk eksperymentalnych: (i) numerycznego opisu harmonicznego detekcji napięcia Halla w próbce Ta/CoFeB, (ii) wyjaśnienia wielostopniowego przełączania w strukturze Co/Pt/Co z torkiem spin–orbita, silnym sprzężeniem międzywarstwowym oraz interakcją Dzyaloshinskii–Moriya, (iii) opisu mechanizmu pól desynchronizacji w sprzężonych elektrycznie i szeregowo połączonych magnetycznych złączach tunelowych na stacku CoFeB/MgO/CoFeB. W każdym z powyższych przypadków obszerne symulacje makromagnetyczne dostarczają wielu cennych wskazówek ułatwiających interpretację pomiarów eksperymentalnych.

Ostatnia część pracy przedstawia integrację oprogramowania *cmtj* z modelami uczenia ze wzmocnieniem. Zademonstrowano kontroler, który w niewielkiej liczbie kroków automatycznie dostraja oscylator spintroniczny do zadanej częstotliwości oraz kontroler kształtowania impulsu prądu w celu uzyskania przełączenia w układzie ferromagnetyk–metal ciężki lub w złączu tunelowym.

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Index of terms and symbols

Constants

γ_0	gyromagnetic ratio	$2.208 \times 10^5 \text{ m A}^{-1} \text{ s}^{-1}$
$\hbar$	reduced Planck constant	$1.055 \times 10^{-34} \text{ J s}$
μ_0	vacuum magnetic permeability	$1.266 \times 10^{-6} \text{ N A}^{-2}$
e	elementary charge	$1.602 \times 10^{-19} \text{ C}$
h	Planck constant	$6.626 \times 10^{-34} \text{ J Hz}^{-1}$

Experimental

CIMS	Current Induced Magnetisation Switching
FMR	Ferromagnetic resonance
MTJ	Magnetic Tunnel Junction
PIMM	Pulse-induced Magnetometry
SD	Spin Diode
VSD	Voltage Spin Diode

Interactions and effects

AHE	Anomalous Hall effect
AMR	Anisotropic Magnetoresistance
DMI	Dzyaloshinskii–Moriya interaction
IEC	Interlayer Exchange Coupling
IMA	In-plane magnetic anisotropy
ISHE	Inverse Spin Hall effect
PMA	Perpendicular magnetic anisotropy
REE	Rashba-Edelstein effect

RKKY Ruderman–Kittel–Kasuya–Yosida interaction

SHE Spin Hall effect

SMR Spin Hall Magnetoresistance

SOT Spin Orbit Torque

STT Spin Transfer Torque

VCMA Voltage Controlled Magnetic Anisotropy

Layer types and devices

AFM Antiferromagnet

FM Ferromagnetic layer

HM Heavy metal layer

NM Nonmagnetic layer

SAF Synthetic antiferromagnet

SHNO Spin Hall Nano Oscillator

STO Spin Torque Oscillator

Symbols

α_G Gilbert's damping parameter

λ angular parameter (Slonczewski parameter)

$\mathbf{m}$ unit magnetisation vector

$\mathbf{p}$ or $\boldsymbol{\sigma}$ unit spin current polarisation vector

D DMI constant Jm^{-2}

H_{DL} damping-like torque magnitude Am^{-1}

H_{FL} field-like torque magnitude Am^{-1}

K_u magnetic anisotropy constant (1st order) Jm^{-3}

$\mu_0 M_s$ magnetisation saturation T

ϕ azimuth angle from + x-axis rad

θ polar angle from + z-axis rad

θ_{SH} spin Hall angle

J IEC constant Jm^{-2}

j or j_e charge current density Am^{-2}

Introduction

If we classify the development of spin devices with respect to their application, several major directions emerge: storage and memory, oscillators and detectors, and methods for efficient computing. Among those, applications in low-power, non-volatile memory have significantly driven interest in spintronics for many years, and much research has been invested in making the designs not only faster and denser, but also more energy efficient. Alternative methods of spin control, notably through spin-orbit torque, have recently gained traction as suitable replacements to spin torque transfer switching, which suffer from excessive Joule heat limiting widespread industrial adoption.

The discovery of new effects in spintronics applicable to spin devices and a deeper understanding of their potential advantages and limitations resulted in emerging branches of research focused on new logic units based on spintronic gates and alternative methods of computing. A representative example of the former has been demonstrated by Zhang et al.¹ where careful manipulation of the gate geometry and spin textures permits a replication of the basic Boolean AND and OR gates. Alternatively, quantum-gate designs have been attempted employing localised electric control to modify spin transport properties, effectively modulating the probability of electron transposition to the receiving electrode². The term 'alternative methods of computing' represents perhaps a broader and more loosely defined front of research, spanning from ideas such as reservoir-like spin wave encoded neural networks³, through memristors⁴, and computation based on nano oscillators⁵, to probabilistic computing – where a probabilistic bit, often modelled by a nanomagnet with low energy barrier⁶ or a magnetic tunnel junction⁷, becomes the primary unit of computation⁸. Generally, the computational aspects of modern spintronics concentrate around neuromorphic computing concepts⁹. Unlike classical neural network architectures, neuromorphic computation primarily relies on temporal integration of incoming impulses and randomly initialised static network graphs known as reservoirs¹⁰.

However, each application needs, at some level, simulation support to iterate on the designs or simply to understand various interactions either present within the device itself or with the external factors. To this extent, both research and the industry employ the help of a multitude of simulation

¹ X. Zhang, Ezawa, and Y. Zhou, "Magnetic skyrmion logic gates".

² W. Zhang, "Voltage-driven spintronic logic gates in graphene nanoribbons".

³ Papp, Kiechle, et al., "Experimental demonstration of a concave grating for spin waves in the Rowland arrangement".

⁴ Huang, Xia, et al., "Memristive Artificial Synapses for Neuromorphic Computing"; Chanthbouala, Garcia, et al., "A ferroelectric memristor".

⁵ Houshang, Zahedinejad, et al., "Phase-Binarized Spin Hall Nano-Oscillator Arrays"; Torrejon, Riou, et al., "Neuromorphic computing with nanoscale spintronic oscillators".

⁶ Nomura, Furuta, Tsujimoto, Kuwabiraki, Peper, et al., "Reservoir computing with dipole-coupled nanomagnets"; Taniguchi, Utsumi, and Imamura, "Thermally activated switching rate of a nanomagnet in the presence of spin torque".

⁷ K. Hayakawa, Kanai, et al., "Nanosecond Random Telegraph Noise in In-Plane Magnetic Tunnel Junctions".

⁸ J. Kaiser and Datta, "Probabilistic computing with p-bits"; Camsari, B. M. Sutton, and Datta, "p-Bits for Probabilistic Spin Logic".

⁹ Torrejon, Riou, et al., "Neuromorphic computing with nanoscale spintronic oscillators"; Kurenkov, Fukami, and Ohno, "Neuromorphic computing with antiferromagnetic spintronics".

¹⁰ Taniguchi, Ogiwara, et al., "Spintronic reservoir computing without driving current or magnetic field".

packages that vary in complexity, speed, or degree of fidelity. The situation is not different in spintronics, where there is a selection of methods ranging from ab initio¹¹, atomistic¹², and micromagnetic¹³ to macromagnetic^{14,15}. The latter technique is usually not used in the form of an established, usable, and complete simulation package.

Therefore, this thesis demonstrates the relevance of macromagnetic models, emphasising their clarity and effectiveness in solving simplified problems, thus providing valuable insights into real systems. The reduction in complexity and accuracy is offset by the gains in computational speed, ease of prototyping, and iterative simulation improvements. The software flexibility allows the use of a wide selection of tools to analyse the output of those simple models, and when we combine all of that with the experimental data, it turns out that we develop a fairly sound intuition of the investigated phenomenon. Given this versatility of the macrospin modelling, the thesis presents a broad overview of multiple modelling methods. Throughout its course, we discuss various applications such as current-induced magnetisation switching (CIMS), voltage-spin diode (VSD), harmonic Hall voltage detection, coupled oscillators, or noise modelling.

Contents and contributions of this thesis

This thesis makes several distinct contributions to the field. The first contribution is the development of the standardised numerical library CMTJ, which serves as the simulation backbone for the following work. The principal methods implemented in this library are detailed in the first chapter, [Numerical methods](#), including key equations, numerical techniques employed, points of optimisation, and the associated numerical effects. The chapter also provides the theoretical foundation for this thesis. In the second chapter, [Modelling spin Hall devices](#), we use the CMTJ library to explore models that reflect the effects of interfacial asymmetry on spin Hall bars, using experimental data from Co/Pt/Co systems as validation ground. Additionally, we focus on electrical detection techniques, in particular harmonic Hall voltage detection on CoFeB/Ta devices. The following two chapters, [Modelling magnetic tunnel junctions](#) and [Dynamic control of devices](#), focus on the role of magnetic tunnel junctions (MTJs) as oscillators and detectors. In [Modelling magnetic tunnel junctions](#), we examine electric coupling and its effect on the synchronisation of the two devices. The simulation results are compared with the available experimental data. Subsequently, we investigate the stochastic behaviour of the MTJs by modelling $1/f^\alpha$ noise. The final chapter, [Dynamic control of devices](#), further develops the idea of real-time tuning of the MTJ-based detector to a desired frequency using the reinforcement learning approach. The concluding chapter discusses the potential implications of the proposed solutions and identifies new avenues for future research.

All figures, diagrams, and simulations used in this thesis, unless explicitly

¹¹ Hafner and Kresse, “The Vienna AB-Initio Simulation Program VASP”; Giannozzi, Andreussi, et al., “Advanced capabilities for materials modelling with Quantum ESPRESSO”.

¹² Müller, Hoffmann, et al., “*Spirit*”.

¹³ M. J. Donahue and D. G. Porter, *OOMMF User's Guide, Version 1.0*; Vansteenkiste, Leliaert, et al., “The design and verification of MuMax3”.

¹⁴ Xiao, Zangwill, and M. D. Stiles, “Macrospin models of spin transfer dynamics”.

¹⁵ Mojsiejuk, Ziętek, Grochot, et al., “cmtj”.

stated otherwise, were created by the author of this thesis, even if they are inserted by citing another publication. For clarity, we map the chapters to relevant publications together with specific contributions from the author of this thesis, indicating that the results presented in this thesis are complementary to the author's published works:

- **Chapter Numerical methods**

The author created, programmed, packaged, and documented the CMTJ library. The fitting of the experimental data with the simulations was also carried out by the author.¹⁶

¹⁶ Mojsiejuk, Ziętek, Grochot, et al., “cmtj”.

- **Chapter Modelling spin Hall devices**

The author proposed the model and performed the numerical simulations for asymmetric switching in the Co/wedge Pt/Co sample.¹⁷

The author created the model and simulated all the fits to the experimental data for the Ta/CoFeB sample.¹⁸

¹⁷ Grochot, Ogrodnik, et al., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”.

¹⁸ Ziętek, Mojsiejuk, et al., “Numerical model of harmonic Hall voltage detection for spintronic devices”.

- **Chapter Modelling magnetic tunnel junctions**

The author conducted simulations of the spin-torque oscillators connected in-series. The author also proposed the observation of the desynchronisation based on the analysis of the experimental data.¹⁹

¹⁹ Rzeszut, Mojsiejuk, et al., “Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions”.

- **Chapter Dynamic control of devices**

The author designed the environments and conducted the training of the reinforcement learning algorithms.²⁰

²⁰ Mojsiejuk, Ziętek, and Skowroński, “Reinforcement learning for spin torque oscillator tasks”.

The table below summarises the samples, models, and experiments with chapter references for the ease of the reader:

Investigated phenomena	Sample	Type of modelling used	Chapter
<i>Harmonic Hall voltage detection</i>	Ta/CoFeB	SOT-LLGS	Modelling spin Hall devices
<i>FMR</i>	CoFeB/W(wedge)/CoFeB	Smit-Beljers, Bayesian modelling	Modelling spin Hall devices
<i>Multilevel CIMS</i>	Co/Pt(wedge)/Co	SOT-LLGS, Domain Wall motion models	Modelling spin Hall devices
<i>Electric synchronisation of MTJs</i>	CoFeB/MgO/CoFeB	Electric coupling, LLGS	Modelling magnetic tunnel junctions
<i>Noise modelling and reconstruction</i>	Theoretical	STT-sLLGS, $1/f^\alpha$ noise modelling, Kasdin noise model, multi-domain noise models	Modelling magnetic tunnel junctions
<i>Real-time control of spintronic oscillators</i>	Theoretical	STT-LLGS, reinforcement learning models	Dynamic control of devices

Publication list

The list below compiles the entire list of articles by the author relevant to the field of spintronics, to date:

1. Skowroński, W., Łazarski, S., **Mojsiejuk, J.**, Chęciński, J., Frankowski, M., Nozaki, T., Yakushiji, K., Yuasa, S., (Aug. 2019). “High frequency voltage-induced ferromagnetic resonance in magnetic tunnel junctions”. *Applied Physics Letters* 115.7, p. 072401
Contribution: Conducted voltage-induced ferromagnetic resonance simulations of MTJs with strong perpendicular magnetic anisotropy.
2. **Mojsiejuk, J.**, Kulig, P., Chęciński, J., Frankowski, M., (Feb. 2020). “Visualization for Micromagnetics With Synchronized Plotting”. *IEEE Transactions on Magnetics* 56.2, pp. 1–6
Contribution: Developed the software and wrote the article.
3. Ziętek, S., **Mojsiejuk, J.**, Grochot, K., Łazarski, S., Skowroński, W., Stobiecki, T., (July 2022). “Numerical model of harmonic Hall voltage detection for spintronic devices”. *Physical Review B* 106.2, p. 024403
Contribution: Conducted the simulations, wrote the article, and performed a formal analysis.
4. **Mojsiejuk, J.**, Ziętek, S., Grochot, K., Skowroński, W., Stobiecki, T., (Apr. 2023). “cmtj: Simulation package for analysis of multilayer spintronic devices”. *npj Computational Materials* 9.1, p. 54
Contribution: Wrote the article and software, and conducted the simulations.
5. Rzeszut, P., **Mojsiejuk, J.**, Skowroński, W., Tsunegi, S., Kubota, H., Yuasa, S., (June 2023). “Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions”. arXiv:2306.11608 [physics]
Contribution: Conducted the simulations, performed formal analysis of the experimental results, and co-wrote the article.
6. Grochot, K., Ogródnik, P., **Mojsiejuk, J.**, Mazalski, P., Guzowska, U., Skowroński, W., Stobiecki, T., (Apr. 2024). “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, p. 9938
Contribution: Conducted the simulations, excluding the spin-wave simulations, and co-wrote the article.
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., (Aug. 2024). “Magnetization dynamics driven by displacement currents across a magnetic tunnel junction”. *Physical Review Applied* 22.2, p. 024019

Contribution: Conducted micromagnetic simulations. Details in [Magnetization dynamics driven by displacement currents across an MTJ](#)

8. **Mojsiejuk, J.**, Ziętek, S., Skowroński, W., (Sept. 2025). “Reinforcement learning for spin torque oscillator tasks”. arXiv:2509.10057 [physics] (accepted to *IOP Journal of Physics: Conference Series*)

Contribution: Conducted the simulations, performed the formal analysis, and wrote the article.

9. Cierpień, M., Maślanka, D., Gubała, K., **Mojsiejuk, J.**, Grochot, K., Wrona, J., Langer, J., Nan, T., Skowroński, W., (Oct. 2025) “Magnetic tunnel junction made of abundant materials for memory and dynamic applications”, *Scientific Reports* (accepted)

Contribution: Conducted the simulation parameter fitting.

Numerical methods

This chapter gives a gentle introduction to key numerical techniques that are used implicitly or explicitly throughout the remainder of the work. It presents the base versions of the models later used in experimental reproductions, dynamic control, and parameter fitting.

Landau-Lifshitz-Gilbert-Slonczewski equation

The key equation in spintronics is the Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation²¹ and its variations. The minimal form of the LLGS equation can be derived through standard spin algebra calculations. We begin with a microscopic Zeeman Hamiltonian²²:

$$\mathcal{H} = -\frac{g\mu_0\mu_B}{\hbar}\hat{\mathbf{S}} \cdot \mathbf{H} = \gamma_e\mu_0\hat{\mathbf{S}} \cdot \mathbf{H} \quad (1)$$

where $\gamma_e = -g\mu_B/\hbar$, and $\hat{\mathbf{S}} = \{\hat{S}_x, \hat{S}_y, \hat{S}_z\}$ is the spin angular momentum operator with 3 components defined in terms of the Pauli matrices $\frac{\hbar}{2}\boldsymbol{\sigma}_i$ with $i = \{x, y, z\}$. However, instead of considering a single spin operator, the introduction of a density operator $\rho = \sum_n p_n |\Psi_n\rangle\langle\Psi_n|$, $p_n \geq 0$, $\sum_n p_n = 1$ allows us to write $\langle\hat{S}\rangle$ as a statistical ensemble over local spins:

$$\langle\hat{S}\rangle = \text{Tr}(\rho\hat{S}) \quad (2)$$

Adopting a Heisenberg picture, the time evolution of that ensemble is given by:

$$\frac{d}{dt}\langle\hat{S}\rangle = \frac{i}{\hbar}\langle[\mathcal{H}, \hat{S}]\rangle = \frac{i}{\hbar}\langle[\gamma_e\mu_0\hat{\mathbf{S}} \cdot \mathbf{H}, \hat{S}_j]\rangle = \frac{i}{\hbar}\gamma_e\mu_0\mathbf{H}_i\langle[\hat{S}_i, \hat{S}_j]\rangle = \frac{i}{\hbar}i\hbar\gamma_e\mu_0\epsilon_{ijk}\mathbf{H}_i\langle\hat{S}_k\rangle \quad (3)$$

where we used the fact that ρ is time-independent. ϵ_{ijk} is the Levi-Civita symbol. The components $\langle\hat{S}_k\rangle, \mathbf{H}_i$ behave as the components of a cross product: $(a \times b)_j = \epsilon_{jkl}a_kb_l$, hence:

$$\frac{d}{dt}\langle\hat{\mathbf{S}}\rangle = \gamma_e\mu_0\langle\hat{\mathbf{S}}\rangle \times \mathbf{H} \quad (4)$$

If we define magnetisation per unit volume as:

$$\mathbf{M} = \frac{\gamma_e N}{V}\langle\hat{\mathbf{S}}\rangle \quad (5)$$

²¹ Landau and Lifshitz, “On the Theory of the Dispersion of Magnetic Permeability in Ferromagnetic Bodies”.

²² Lakshmanan, “The fascinating world of the Landau-Lifshitz-Gilbert equation”.

using $\gamma_0 = \mu_0|\gamma_e|$, then the familiar precessional term of the LLG equation emerges:

$$\frac{d}{dt}\mathbf{M} = -\gamma_0\mathbf{M} \times \mathbf{H} \quad (6)$$

To this fundamental equation, Gilbert added a damping term derived from the Lagrangian framework²³. Finally, Slonczewski and Berger independently calculated the form of the damping and field-like torques²⁴ that arise from the spin transfer torque (STT) effect. A Landau-Lifshitz (LL) form of the LLGS equation that combines these results is given by²⁵:

$$\frac{1 + \alpha_G^2}{\gamma_0} \frac{d\mathbf{m}}{dt} = -\mathbf{m} \times \mathbf{H}_{\text{eff}} - \alpha_G \mathbf{m} \times (\mathbf{m} \times \mathbf{H}_{\text{eff}}) + a_j \varepsilon \beta \mathbf{m} \times \mathbf{p} - a_j \varepsilon (\mathbf{m} \times (\mathbf{m} \times \mathbf{p})) \quad (7)$$

where we use magnetisation vector normalised by magnetisation saturation, $\mathbf{m} = \mathbf{M}/M_s$, $\mathbf{H}_{\text{eff}}$ is the effective field term, β determines the field-like to damping-like torque ratio. β is phenomenological and stack-dependent; many simulations set it to 0 or equal to the damping parameter α_G , although sometimes a larger scaling factor is used for the field-like torque²⁶. The variable a_j is defined in terms of current density j :

$$a_j = \frac{\hbar j}{e\mu_0 M_s t_{\text{FM}}} \quad (8)$$

e is the electron charge and ε depends on λ , the parameter of the spacer layer derived by Slonczewski, and P , the efficiency of the spin current polarisation ($0 \leq P \leq 1$):

$$\varepsilon = \frac{P\lambda^2}{\lambda^2 + 1 + (\lambda^2 - 1)\mathbf{m} \cdot \mathbf{p}} \quad (9)$$

The polarisation vector $\mathbf{p}$ is normalised to have unit length, $|\mathbf{p}| = 1$.

In spin orbit torque (SOT) dominant systems such as heavy-metal/ferromagnet (HM/FM) stacks, the LLGS equation is more naturally expressed by grouping the torque terms under more generic field-like ($\mathbf{H}_{\text{FL}}$) and damping-like ($\mathbf{H}_{\text{DL}}$) torque magnitudes (here, expressed as effective fields in A/m)²⁷:

$$\frac{d\mathbf{m}}{dt} = \frac{-\gamma_0}{1 + \alpha_G^2} [\mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha_G \mathbf{m} \times \mathbf{m} \times \mathbf{H}_{\text{eff}}] + \frac{-\gamma_0}{1 + \alpha_G^2} [(\mathbf{H}_{\text{FL}} - \alpha_G \mathbf{H}_{\text{DL}})\mathbf{m} \times \mathbf{p} + (\mathbf{H}_{\text{DL}} + \alpha_G \mathbf{H}_{\text{FL}})\mathbf{m} \times (\mathbf{m} \times \mathbf{p})] \quad (10)$$

if α_G is sufficiently small, the torque mixing terms can be neglected in favour of the dominant term. See the appendix of [Pub. 1: Numerical model for the harmonic Hall voltage detection](#) for derivation of the LL form of the equation for SOT.

Fig.1 shows the idea behind the damping and field-like torques along with the standard effective field precession and damping terms. The contributions from the latter tend to cause the magnetisation alignment along a particular axis, whereas the former produces a precession about the said axis.

²³ Gilbert, “Classics in Magnetism A Phenomenological Theory of Damping in Ferromagnetic Materials”.

²⁴ Slonczewski, “Current-driven excitation of magnetic multilayers”; Berger, “Emission of spin waves by a magnetic multilayer traversed by a current”.

²⁵ We refer to a form of an LLGS equation which does not contain implicit dependency on the $\frac{d\mathbf{m}}{dt}$ as the LL-form (Landau-Lifshitz) of the LLGS equation.

²⁶ Arun, Gopal, et al., “Influence of Field-Like Torque in Synchronization of Spin Torque Oscillators”.

²⁷ Nguyen and Pai, “Spin-orbit torque characterization in a nutshell”.

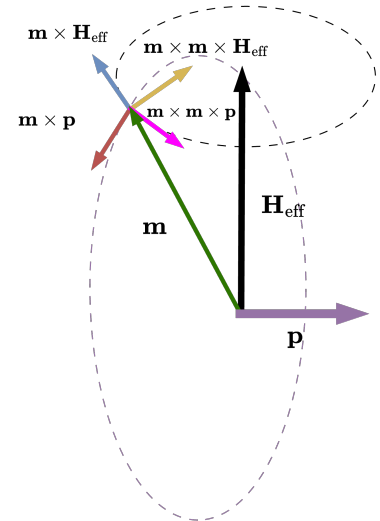


Figure 1: The main idea behind the damping-like and field-like contributions. Here, $\mathbf{m}$ is marked with a green vector, $\mathbf{H}_{\text{eff}}$ is the effective field vector coloured black, and in purple we mark the $\mathbf{p}$ which is the polarisation vector of a reference layer. The dashed lines represent the precession cones about a specific axis designated by $\mathbf{H}_{\text{eff}}$ (dashed black) or $\mathbf{p}$ (dashed purple). In both cases, the precession is produced by the field-like terms (the orange and blue vectors), whereas the damping-like contributions pull the magnetisation vector $\mathbf{m}$, aligning it with the specific axis – again, either $\mathbf{H}_{\text{eff}}$ or $\mathbf{p}$. Those vectors are coloured yellow or pink, respectively.

Energy density contributions

The general effective field term in (7, 10) contains contributions from several physical effects. Some of those, along with their principal forms as fields, are given in the *Methods* section of [Pub. 2: Open-source macromagnetic package](#). Here, we briefly review selected contributions in energy form, suitable for algorithms that directly operate on energy expressions rather than fields. For models that operate on the effective field, the macromagnetic scaling of the effective field is taken to be a functional derivative of the energy density $\mathcal{F}$ with respect to the magnetisation vector:

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0 M_s} \frac{\delta \mathcal{F}[\mathbf{m}]}{\delta \mathbf{m}} \quad (11)$$

If we deal with total energy, we also include the volume of the cell, V , in the denominator. For the interaction expressions in J/m^2 , we need to rescale $\mathcal{F}$ by the corresponding layer thickness.

Magnetocrystalline anisotropy, henceforth simply referred to as anisotropy, arises because of the preferred alignment of the magnetic moments with the lattice symmetry axes. A single dominant symmetry axis is typically assumed; thus, the anisotropy energy density term is written with respect to some uniaxial anisotropy axis vector $\mathbf{a}$ as:

$$\mathcal{F}_K = -K_1 (\mathbf{m} \cdot \mathbf{a})^2 - K_2 (\mathbf{m} \cdot \mathbf{a})^4 \quad (12)$$

where K_1 is the first order uniaxial anisotropy constant expressed in J/m^3 , K_2 is the second order anisotropy constant, in the same units. Typically, $K_2 < 0$ ²⁸. In certain models, it is convenient to explicitly distinguish the in-plane and out-of-plane (perpendicular) anisotropy axes, as is done, for example, in (34). Notably, distinguishing these axes simplifies interpreting another term, the demagnetisation energy, which has a form that counteracts the perpendicular anisotropy. Shape anisotropy, as is sometimes called, is primarily influenced by the geometry of the sample, specifically the discontinuity at the edges. Macromagnetically, the energy density of the dipole interaction may look like this:

$$\mathcal{F}_{\text{demag/dipole}} = \frac{\mu_0 M_{s,i} M_{s,j}}{2} \mathbf{m}_i^T \hat{\mathbf{N}}_{ij} \mathbf{m}_j \quad (13)$$

where the tensor $\hat{\mathbf{N}}$ can be a dipole tensor arising from the interaction with another uniformly magnetised body, or it can also encompass the self-demagnetising field, in which case, for the macrospin, we have $i = j$. Often, for most basic strip geometry, the demagnetising field is approximated using the trivial tensor with 1 in the last place of the diagonal of $\hat{\mathbf{N}}$, which reduces to the z axis component of the magnetisation inducing an internal demagnetising energy. In practice we usually use diagonalised version with off-diagonal elements being zero, allowing the simplified demagnetisation

²⁸ Strelkov, A. Timopheev, et al., “Stability phase diagram of a perpendicular magnetic tunnel junction in noncollinear geometry”.

term to be written as:

$$\mathcal{F}_{\text{demag}} = \frac{\mu_0 M_s^2}{2} (\mathbf{m} \odot \mathbf{m}) \hat{\mathbf{N}} \quad (14)$$

with $\odot$ as the Hadamard (element-wise) product. We discuss the dipole interaction, that is, the case when $i \neq j$, in the subsequent paragraph.

Another significant term, not explicitly taken into account in the macrospin simulations, is the exchange interaction energy density that is typically given by²⁹:

$$\mathcal{F}_{\text{ex}} = A_{\text{ex}} (\nabla \mathbf{m})^2 \quad (15)$$

with exchange stiffness constant $A_{\text{ex}} = \frac{2J_{\text{ex}}}{a}$ where a is the lattice constant and J_{ex} is the exchange integral. Naturally, the value and form of that constant will depend on the crystal lattice itself. The exchange interaction favours alignment of spins, but its nature is short-range. An interesting situation arises when the exchange interaction starts to compete with the dipole interaction (magnetostatic) because the dipole interaction, though weaker, has a longer range, potentially dominating in sufficiently large samples. This competition is, in part, responsible for the magnetic domain configuration. Another use case where dipole interaction plays a major role is when multiple magnetic devices are placed in a close mutual vicinity; we discuss an example of such a circumstance in [Dipolar coupling](#) where we measure the synchronisation capacity of two MTJs placed at a sequentially longer distance. In any case, the exact shape of the dipole interaction for an arbitrary system is complicated, but Newell et al.³⁰ derived the analytical form of the macromagnetic demagnetising tensor. In micromagnetic calculations, when spanned on a regular grid, the demagnetising field can be computed across the entire configuration; there are a couple of efficient methods that reduce the complexity from $\mathcal{O}(n^2)$ to $\mathcal{O}(n \log n)$ by clever use of the Fourier transform, symmetry, and grid padding³¹.

In many systems with multiple FM layers, interlayer exchange coupling (IEC) becomes relevant. IEC is a function of the thickness of the nonmagnetic (NM) layer and encompasses both the effects related to the confinement of Fermi surface electrons in the NM itself and the spin-dependent scattering at the FM/NM interfaces³². The bilinear constant J_1 can follow the RKKY-like oscillatory behaviour, although due to aliasing the true period may be lost in the experiment. One simple model places the origin of the standard IEC oscillations in quantum wells³³, where the quantum well resonance mode periodically crosses the Fermi energy as the thickness of the spacer layer varies³⁴. The so-called quadratic term originates from both intrinsic and extrinsic factors, although the latter is taken to have a more significant influence. Extrinsic factors are typically attributed to interfacial roughness: tiny fluctuations in the thickness of the spacer layer, interfacial defects that become scattering centres, or interfacial atomic mixing. Both bilinear and biquadratic terms are generally combined into the following energy surface

²⁹ M. Donahue and D. Porter, “Exchange energy formulations for 3D micromagnetics”.

³⁰ Newell, Williams, and Dunlop, “A generalization of the demagnetizing tensor for nonuniform magnetization”.

³¹ Abert, Bruckner, et al., “A full-fledged micromagnetic code in fewer than 70 lines of NumPy”; Miltat and M. J. Donahue, “Numerical Micromagnetics”.

³² Tsymbal and Žutić, *Spintronics handbook. Volume 2*.

³³ M. Stiles, “Interlayer Exchange Coupling”; Bruno, “Interlayer Exchange Interactions in Magnetic Multilayers”.

³⁴ The electrons reflect from both interfaces in a quantum well – this is the aforementioned model for the confinement of the Fermi surface. Classically, this leads to a standing wave, ergo a resonance mode. Varying the thickness causes a shift in energy and, hence, an oscillatory crossing of the Fermi energy

expression:

$$\mathcal{F}_{\text{IEC}}^* = -J_1 \mathbf{m}_i \cdot \mathbf{m}_j - J_2 (\mathbf{m}_i \cdot \mathbf{m}_j)^2 \quad (16)$$

The $*$ denotes that the energy is in J/m^2 and not J/m^3 units, and in macro-magnetic models it is rescaled by the FM thickness to arrive at the correct dimensions. We note that (16), or at least its bilinear part, is often applied even when the coupling is of non-oscillatory character and has slightly different origins as those outlined above, yet it follows the dependence on the thickness of a spacer material.

As we discuss later in more detail in [Spin-Orbit torque](#), a broken inversion symmetry at the interface results in the promotion of the spin-orbit interaction, and this in turn may also lead to the emergence of the Dzyaloshinskii–Moriya energy term:

$$\mathcal{F}_{\text{DMI}}^* = -\mathbf{D} \cdot (\mathbf{m}_i \times \mathbf{m}_j) \quad (17)$$

where $\mathbf{D}$ is the DMI vector and $\mathbf{m}_{i/j}$ corresponds to the magnetisation sites. If the asymmetry arises exclusively due to the interface, we may talk about the DMI vector pointing in the direction perpendicular to the interface normal. Then, in field terms, the DMI can be modelled as an in-plane field. The sign of the constant $\mathbf{D}$ determines the chirality of the domain wall and the direction of its movement under the SHE field; this concept will be made clearer in the context of the equations discussed in the [Domain dynamics](#) section.

Non-conservative torque terms

While static analysis of the LLG equation still plays an important role in determining magnetic parameters from experimental data, the dynamic effects appearing in torque terms are arguably more interesting and broaden the applications of spintronics devices. As previously discussed, two key effects – STT and SOT – appear almost identical within the formulations given by equations: (10) and (7). One can write $H_{\text{DL/FL}}$ amplitudes in terms of the a_j and ϵ terms and vice versa. However, their origin, mechanics, and consequences for the experimental reality are different and, therefore, require some degree of distinction in the simulation process.

Spin Transfer torque

We start with a discussion of STT as it has been the cornerstone of spintronics devices for almost three decades since it was first described by Slonczewski in 1996³⁵. There are two components to understanding the spin transfer torque: one that describes the passing of the spin current through an FM, and another that concerns the behaviour at the NM/FM interface³⁶ (the following paragraph closely follows Sect. 3 of that work). Mechanically, the idea is simple: an incoming spin current, for example along the $\hat{x}$ axis,

³⁵ Slonczewski, “Current-driven excitation of magnetic multilayers”.

³⁶ Ralph and M. Stiles, “Spin transfer torques”.

causes a torque transverse to the magnetisation of the FM layer, meaning that, to some degree of approximation, there is no transverse angular momentum flowing away from that FM layer. Analysis of the interfacial behaviour reveals that the transverse component of the incoming spin current is absorbed at the interface. In a simple approximation, we may say that the spin coming from NM to FM sees an energy split between the majority and minority bands, which are separated by some energy difference. First, this interfacial band mismatch is responsible for the absorption of the spin-angular momentum component transverse to the FM. Second, because of the exchange energy difference, the spins will oscillate, which in turn leads to dephasing at the interface. The result of that dephasing is that the spin current that leaves the FM is, for the most part, collinear with the FM. The spin current injected into an NM/FM interface is usually achieved by affixing another, preceding FM layer, usually named "a reference layer" with magnetisation pinned by synthetic antiferromagnet (SAF)³⁷ that, through strong coupling, prevents the reference layer from changing its magnetisation orientation.

Spin-Orbit torque

To introduce the SOT, we first consider the spin Hall effect family, with particular focus on Anomalous Hall Effect (AHE), pure spin Hall effect (SHE) and inverse Spin Hall effect (ISHE)³⁸. In heavy metals such as platinum or tungsten, we refer to a "plain" SHE where the transverse spin current arises in the absence of the magnetic field³⁹. In contrast to the ordinary Hall effect, SHE does not involve transverse charge accumulation.

The origin of SHE divides into intrinsic and extrinsic factors. The intrinsic mechanism depends on the band structure and is typically attributed to the deflection caused by the coherence induced by the external electric field. The electrons acquire an additional velocity component, $\frac{d\langle \mathbf{r} \rangle}{dt}$ that depends on the Berry curvature of the Bloch state, $\mathbf{b}_n$, and is perpendicular to that electric field, $\mathbf{E}$:

$$\frac{d\langle \mathbf{r} \rangle}{dt} = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} + \frac{e}{\hbar} \mathbf{E} \times \mathbf{b}_n \quad (18)$$

where $\mathbf{k}$ is the momentum and ε_n is the band energy. The extrinsic mechanisms are usually subdivided into skew-scattering and side-jumping. Skew-scattering, first described by Smit⁴⁰, tends to dominate in nearly perfect crystals⁴¹. The chiral scattering of the electrons from impurities is caused by spin-orbit interaction leading to asymmetric left-handed and right-handed (with respect to the magnetisation) transition probabilities for a scattered electron, resulting in the current flow perpendicular to both the electric field and the magnetisation direction (AHE) or spin current polarisation (SHE).

However, the side-jumping mechanisms are often defined as the remaining contribution to the SHE/AHE conductivity after the skew-scattering and intrinsic factors have been accounted for. Typically, a semi-classical argument for side-jumping is attributed to Berger⁴², and explains how a Gaussian

³⁷ SAF is a system created by putting together FM layers with their magnetisations in an anti-parallel alignment, thus mimicking AFM in effect.

³⁸ Inoue and Ohno, "Taking the Hall Effect for a Spin"; Sinova, Valenzuela, et al., "Spin Hall effects".

³⁹ Hirsch, "Spin Hall Effect"; Dyakonov and Perel, "Current-induced spin orientation of electrons in semiconductors".

⁴⁰ Smit, "The spontaneous hall effect in ferromagnetics II".

⁴¹ Sinova, Valenzuela, et al., "Spin Hall effects".

⁴² Berger, "Emission of spin waves by a magnetic multilayer traversed by a current".

wavepacket undergoes a displacement transversal to its momentum upon encountering a potential gradient induced by a spherical impurity. In those cases, the governing spin-orbit Hamiltonian is usually given by⁴³:

$$\mathcal{H}_{\text{SO}} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{\partial V}{\partial t} S_z L_z \quad (19)$$

where S_z and L_z are the z component of the spin and orbital angular momentum, respectively. In a phenomenological picture, when an in-plane charge current flows in the HM, the SHE generates a transverse pure spin current $\mathbf{j}_s$, which is usually described with the following expression:

$$\mathbf{j}_s = \theta_{\text{SH}} \left(\frac{\hbar}{2e} \boldsymbol{\sigma} \times \mathbf{j}_c \right) \quad (20)$$

where $\mathbf{j}_c$ denotes charge current, $\boldsymbol{\sigma}$ the polarisation of the spin current and θ_{SH} is the spin Hall angle defined as a ratio of spin Hall conductivity σ_{SH} to electrical conductivity σ , $\theta_{\text{SH}} = \frac{\sigma_{\text{SH}}}{\sigma}$. Since SHE leads to a transverse spin current flow, the spin current is absorbed at the HM/FM interface, and its transverse component dephases within the FM, exerting a torque on the FM magnetisation. However, creating an HM/FM interface has the additional effect of breaking the inversion symmetry, which leads to the Rashba-Edelstein effect (REE). REE causes net spin accumulation at the interface and exerts a torque on the FM via the exchange interaction, distinct from the spin-transfer torque, if the net spin polarisation at the interface is misaligned with the FM magnetisation.

In the literature, one frequently associates the damping-like torque with SHE and the field-like torque with REE and, while that is ultimately a good approximation, it presents a somewhat incomplete picture. For example, Amin and Stiles⁴⁴ show a HM thickness dependence of τ_{DL} , τ_{FL} torque amplitudes, broken down by the underlying effect (bulk SHE or REE). REE tends to give more or less constant values of both torques, with a dominant contribution from τ_{FL} , excluding very thin HM films. In contrast, when the SHE is the main source of torque, the damping-like part dominates and displays a saturating increase with the HM thickness. At the same time, the field-like torque contributes less, but also increases in magnitude in a similar fashion. Notable are the different signs between the SHE and Rashba contributions for the field-like torque. This has also been experimentally observed for the damping torque and is attributed, for example, to increased oxidation⁴⁵, which causes Rashba to dominate over the SHE. The discussion of the differences between SHE and REE and their torque contributions is challenging because existing experiments offer limited means to differentiate these effects clearly. Furthermore, the exact values ascribed to field-like and damping-like, notwithstanding their origin (as they are summed either way in the LLGS model), are also experimentally determined for the most part.

⁴³ Sinova, Valenzuela, et al., “Spin Hall effects”.

⁴⁴ Amin and M. D. Stiles, “Spin transport at interfaces with spin-orbit coupling”.

⁴⁵ Qiu, Narayanapillai, et al., “Spin-orbit-torque engineering via oxygen manipulation”; An, Kageyama, et al., “Spin-torque generator engineered by natural oxidation of Cu”.

Numerical solutions to the LLGS equations

The LLGS equation is typically solved by numerical integration, although there are Monte Carlo solvers for atomistic versions of the equation⁴⁶. In CMTJ, the fixed-step Runge-Kutta 4 (RK4) is the default deterministic solver. Other choices include the Dormand-Prince, DP5(4), method for adaptive step integration, which is a fifth-order method with a fourth-order error estimate⁴⁷, and stochastic solvers: Euler-Heun and Heun. For most applications, we stick to fixed-size methods for the following reasons. First, the fixed step makes it trivial to compute the signal spectrum, which is the most common downstream operation performed after the simulation. Second, the accuracy of the solution does not outweigh the increase in computational complexity. If necessary, the step size can be simply reduced in the RK4 method to retain a higher degree of precision.

⁴⁶ Evans, Fan, et al., “Atomistic spin model simulations of magnetic nanomaterials”.

⁴⁷ Dormand and Prince, “A family of embedded Runge-Kutta formulae”.

0							
1/5	1/5						
3/10	3/40	9/40					
4/5	44/45	-56/15	32/9				
8/9	19372/6561	-25360/2187	64448/6561	-212/729			
1	9017/3168	-355/33	46732/5247	49/176	-5103/18656		
1	35/384	0	500/1113	125/192	-2187/6784	11/84	
	35/384	0	500/1113	125/192	-2187/6784	11/84	0
	5179/57600	0	7571/16695	393/640	-92097/339200	187/2100	1/40

Table 1: Butcher tableau for Dormand-Prince method.

Higher-order methods are usually given in the form of a Butcher tableau, such as the one we provide for DP5(4) in Tab.1. In this table, the rows are indexed by i , and the columns by j . Leftmost column coefficients are denoted by c_i , the values in the penultimate (second to last) row are referred to as b_i , and the bottommost one as b_i^* . The latter are used for error estimate in the adaptive methods. The slope k_i of an RK method with s stages is defined as:

$$k_i = f(t_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{i,j} k_j) \quad (21)$$

where $i = 1, \dots, s$, f is the differential equation we wish to integrate and h is our step. t_n is the time at n th step and y_n is the value of the integral calculated at n th step. DP5(4) has $s = 7$. The generalised form of the numerical solution is then:

$$y_{n+1} = y_n + h \sum_{i=1}^s k_i b_i \quad (22)$$

Consequently, the error estimate would be the difference between two approximations at the same step y_{n+1} and y_{n+1}^* , but y_{n+1}^* is calculated with the b^* coefficients instead of the b coefficients:

$$e_n = y_{n+1} - y_{n+1}^* = h \sum_{i=1}^s k_i (b_i - b_i^*) \quad (23)$$

What does the error estimate bring to the table? Apart from some useful knowledge of how well we integrate, it is used to guide step size. For example, in DP5(4), an adjustment ratio to the step size could be of the following form:

$$r = q \left(\frac{1}{\text{err}} \right)^{\frac{1}{5}}, \quad \text{with} \quad \text{err} = \left\| \frac{e_n}{\text{atol} + \text{rtol} \max(|y_n|, |y_{n+1}|)} \right\| \quad (24)$$

where q is the constant safety factor, rtol is the relative error tolerance, and atol is the absolute error tolerance. The update rule is then $h' = \min(h_{\min}, \max(h_{\max}, rh))$ where h is the base step, and we make sure that the new time step is within acceptable limits, $h' \in (h_{\min}, h_{\max})$. The solver also determines whether to accept or reject a step; the step is rejected when $\text{err} > 1$, and the time step is reduced until $h_{\min}$ is reached.

Stochastic forms of Landau-Lifshitz-Gilbert-Slonczewski equation

There are a couple of established methods for solving stochastic differential equations numerically; among the most prevalent are the Euler Heun and stochastic Heun methods, or the Runge-Kutta methods⁴⁸. Many methods cause drift of the magnetisation norm⁴⁹, so in our implementations we renormalise the magnetisation vector after each step to enforce $|\mathbf{m}| = 1$. Attempting to solve stochastic LLGS equations with standard methods typically results in an incorrect distribution of the noise (this problem becomes pronounced when simulating the $1/f$ noise). Specifically from a numerical point of view, because the normal schemes dictate samples to be drawn at each advancement of the time step, while in the stochastic version the sample is drawn once and then shared between intermediate approximations. We further note that in this scheme we can advance our approximations of the stochastic part without having to consider the remaining, coupled layers, as in our setting the noise vector generated in the layer is independent of the one generated for any other. A stochastic formulation of LLGS takes the form of a Stratonovich SDE:

$$dX_t = f(X_t, t)dt + g(X_t, t) \circ dW_t \quad (25)$$

where $f(X_t, t)$ is the deterministic part of the equation and $g(X_t, t)$ is the stochastic part of the equation. dW is a Wiener increment. The symbol $\circ$ denotes the Stratonovich product, which distinguishes (25) from Ito's SDE. For the Itô integration, coefficients are evaluated at the left endpoint of the interval and in Stratonovich at the midpoint. Unlike classical Riemann integrals, the stochastic integral depends on that choice. In the particular context of the sLLGS equation, it is convenient to define the two parts f and g as operators acting on different terms of the effective field. More specifically, we first define an operator $\tilde{\mathbf{M}}_t$ acting on some field term $\mathbf{H}_t$ as follows:

$$\tilde{\mathbf{M}}_t(\mathbf{H}_t, \eta_1, \eta_2) = \eta_1 \mathbf{m}_t \times \mathbf{H}_t + \eta_2 \mathbf{m}_t \times (\mathbf{m}_t \times \mathbf{H}_t) \quad (26)$$

⁴⁸ Mackevičius, *Introduction to Stochastic Analysis*; Rößler, “Runge-Kutta Methods for the Strong Approximation of Solutions of Stochastic Differential Equations”.

⁴⁹ Ament, Rangarajan, et al., “Solving the stochastic Landau-Lifshitz-Gilbert-Slonczewski equation for monodomain nanomagnets”.

with η_1, η_2 being the scalar constant that scales the field-like or damping-like portion of the equation. In our case, we will implicitly define $\mathbf{f}_t(\mathbf{m}_t)$ as a proper function acting on the torque and effective fields:

$$\mathbf{f}_t(\mathbf{m}_t) = \frac{-\gamma_0}{1 + \alpha_G^2} [\tilde{\mathbf{M}}_t(\mathbf{H}_{\text{eff},t}, 1, \alpha_G) + \tilde{\mathbf{M}}_t(\mathbf{H}_{\text{torque},t}, -\eta_{\text{FL}}, \eta_{\text{DL}})] \quad (27)$$

where η_{FL} and η_{DL} play the role of the torque weighting terms, and depend on the LLGS formulation (in the sense of SOT or STT). As a form of notation abuse, we will talk about g as a plain $\tilde{\mathbf{M}}_t$ operator such that we involve the explicit Stratonovich notation: $\mathbf{g}_t(\mathbf{m}_t) \circ \Delta \mathbf{W}_t = \tilde{\mathbf{M}}_t(\Delta \mathbf{W}_t, 1, \alpha_G)$. We used the notation involving $\Delta \mathbf{W}$ instead of $d\mathbf{W}$ to denote the discretised motion. Because of that, we normalise by the integration step in the subsequently described solver schemes.

We will also assume that the samples from the stochastic process, $\Delta \mathbf{W}_t$ contain all the necessary scaling inside, so, for example, the thermal field can be written as:

$$\mathbf{H}_T(t) = \sigma \Delta \mathbf{W}_t = \sigma(t) \sqrt{h} \boldsymbol{\xi}_t \quad (28)$$

where $\boldsymbol{\xi}_t \in \mathbf{R}^3 \sim \mathcal{N}(0, \mathbf{I}_3)$ ⁵⁰ and σ denote the standard deviation of the thermal process^{51,52}:

$$\sigma(t) = \sqrt{\frac{2\alpha_G k_B T(t)}{\mu_0 M_s V \gamma_0}} \quad (29)$$

where V is the volume of the cell (layer) and $k_B T(t)$ is the thermal energy of the system⁵³. When this term is multiplied by $\sqrt{\Delta t}$ in the solver, it retains the same units as the non-stochastic terms when they are multiplied by Δt . In the context of $\tilde{\mathbf{M}}_t(\Delta \mathbf{W}, 1, \alpha_G)$, the damping term is sometimes discarded, due to its smaller contribution compared to the direct term⁵⁴. In the following, we give a brief description of two methods available in CMTJ for stochastic integration.

Euler-Heun scheme

Aptly named, it combines the first-order approximation (Euler) for the non-stochastic part and the second-order approximation (Heun) for the stochastic part. Following the convention of marking f_t as marking the n^{th} step of the non-stochastic LLGS and g_t to mark the n^{th} step of the stochastic LLGS, we can denote the update scheme as:

$$\mathbf{m}_{t+1} = \mathbf{m}_t + \mathbf{f}_t(\mathbf{m}_t) \Delta t + \frac{1}{2} [\mathbf{g}_t(\mathbf{m}_t) + \mathbf{g}_{t+1}(\hat{\mathbf{m}}_{t+1})] \circ \Delta \mathbf{W}_t \sqrt{\Delta t} \quad (30)$$

where we denoted the integration time step as Δt . Implicitly, both $\mathbf{f}_t$ and $\mathbf{g}_t$ also depend on time due to the presence of drivers controlling various dynamic aspects of the system, but for the sake of notation clarity, we omit that. The intermediate update $\hat{\mathbf{m}}_{t+1}$ is then given by:

$$\hat{\mathbf{m}}_{t+1} = \mathbf{m}_t + \mathbf{g}_t(\mathbf{m}_t) \circ \Delta \mathbf{W}_t \sqrt{\Delta t} \quad (31)$$

⁵⁰ a multivariate Gaussian distributed random vector. Here, we make a transition from W being a generalised Brownian process to a Wiener process.

⁵¹ Brown, “Thermal Fluctuations of a Single-Domain Particle”.

⁵² We cite the standard form here, but the author thanks Professor Jack Sankey for the discussion and the showing how the factor 4, instead of 2, could arise from equipartition derivation.

⁵³ the time dependence is given here explicitly, as the package allows us to determine the temperature changes over time.

⁵⁴ Kubo and Hashitsume, “Brownian Motion of Spins”.

Stochastic Heun

Compared to the Euler-Heun scheme, the stochastic Heun adds the second order also to the non-stochastic part of the equation. Concretely, the update is given by:

$$\mathbf{m}_{t+1} = \mathbf{m}_t + \frac{1}{2}[\mathbf{f}_t(\mathbf{m}_t) + \mathbf{f}_{t+1}(\hat{\mathbf{m}}_{t+1})]\Delta t + \frac{1}{2}[\mathbf{g}_t(\mathbf{m}_t) + \mathbf{g}_{t+1}(\hat{\mathbf{m}}_{t+1})] \circ \Delta \mathbf{W}_t \sqrt{\Delta t} \quad (32)$$

with the intermediate estimate:

$$\hat{\mathbf{m}}_{t+1} = \mathbf{m}_t + \mathbf{f}_t(\mathbf{m}_t)\Delta t + \mathbf{g}_t(\mathbf{m}_t) \circ \Delta \mathbf{W}_t \sqrt{\Delta t} \quad (33)$$

Free energy models

In this section, we detour from the LLGS approach to magnetisation dynamics to comment on the techniques that focus on gradient optimisation, particularly the optimisation of the free energy of the system. These methods are also implemented in the CMTJ package and provide an alternative insight into the behaviour of the system, especially in the context of the resonance frequency. Sometimes, avoiding the explicit computation of dynamics and eloping into the energy domain gives numerical benefits such as stability – for example, systems with high IEC would require very small integration steps for dynamics simulation, while the energy model may be less demanding in the optimiser step. Further, visualising energy landscapes, like the one we show in Fig.3 can tell us more about available systems states in general, and the minima indicate stable positions across multiple realisations. Naturally, the energy model comes at the cost of impossibility of simulating interesting phenomena with nonharmonic input such as CIMS. We begin with the introduction of the Smit-Beljers (SB) model and then hint at spherical LLG solutions, which do not require time-dependent integration to obtain the stable state and the resonance frequency of the system. The expression for the free energy of a layer defined as in the SB model⁵⁵ is usually given by:

$$\mathcal{E}_i = -\mu_0 M_{s,i} \mathbf{m}_i \cdot \mathbf{H}_{\text{ext}} + \frac{\mu_0 M_{s,i}^2}{2} (\mathbf{m}_i \odot \mathbf{m}_i) \hat{\mathbf{N}}_i - K_{u,i}^{\text{PMA}} m_{z,i}^2 - K_{u,i}^{\text{IMA}} (\mathbf{m}_i \cdot \mathbf{K}_{\text{dir},i})^2 \quad (34)$$

where $\mathbf{m}$ is the unit magnetisation vector in the spherical coordinates, M_s is the magnetisation saturation, K_u^{PMA} is the perpendicular anisotropy component, $\mathbf{K}_{\text{dir}}$ is the in-plane direction of the in-plane anisotropy component with a value of K_u^{IMA} , $\mathbf{H}_{\text{ext}}$ is the applied magnetic field. The total free energy $\mathcal{F}$ is the sum over all layers of N , including the coupling energy between the neighbouring layers, and a simple dipole interaction defined through a tensor $\hat{\mathbf{N}}^{\text{dip}}$:

$$\mathcal{F} = \sum_{i=1}^N [\mathcal{E}_i + \sum_{j,j \neq i}^N \frac{\mu_0 M_{s,i} M_{s,j}}{2} \mathbf{m}_i^T \hat{\mathbf{N}}_{ij}^{\text{dip}} \mathbf{m}_j] - \sum_{k=1}^{N-1} [J_{1,k} (\mathbf{m}_k \cdot \mathbf{m}_{k+1}) + J_{2,k} (\mathbf{m}_k \cdot \mathbf{m}_{k+1})^2 + \mathbf{D}_k \cdot (\mathbf{m}_k \times \mathbf{m}_{k+1})] \quad (35)$$

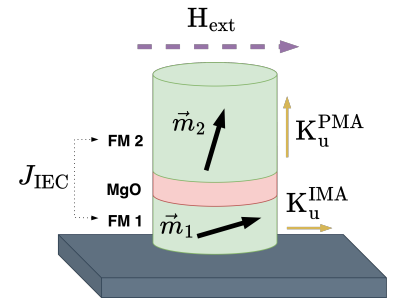


Figure 2: Individual magnetic contributions illustrated on an example MTJ. The anisotropy values are defined per layer, whereas the interlayer exchange coupling is defined per each neighbouring pair of the ferromagnetic layers.

⁵⁵ Baselgia, Warden, et al., “Derivation of the resonance frequency from the free energy of ferromagnets”; Rodríguez-Suárez, Rezende, and Azevedo, “Ferromagnetic resonance investigation of the residual coupling in spin-valve systems”.

with t_i denoting the thickness of the i^{th} layer. J_1 and J_2 are the values of the linear and quadratic IEC values between the k^{th} and $k+1^{\text{th}}$ layers. Likewise, $\mathbf{D}_k$ denotes the interlayer DMI vector for the interaction between the same layers⁵⁶. Individual contributions are explained in Fig. 2.

As we have mentioned in [Energy density contributions](#), the entire free energy expression (35) can be converted to an effective field that acts on each individual layer, $\mathbf{H}_{\text{eff}}$.

First, the equilibrium state is computed using a gradient descent method, in the form of Adam, a momentum-based optimiser⁵⁷. Then, to compute the ferromagnetic resonance, we construct a dynamical Smit-Beljers matrix with the use of a Hessian matrix:

$$\mathcal{M}_{i,j}(\omega) = \frac{\partial \mathcal{F}}{\partial \mathbf{v}_i \mathbf{v}_j} + \zeta_{[j/2]}(U_{2N} - L_{2N}) \quad (36)$$

where $\mathbf{v} = [\theta_1, \phi_1, \dots, \theta_N, \phi_N]$ is the vector of the spherical coordinates of the N layers. As notation shorthand, we incorporate U_{2N} and L_{2N} matrices, which are upper and lower shift matrices, respectively, constructed as $U_{i,j} = \delta_{i+1,j}$ and $L_{i,j} = \delta_{i,j+1}$ with δ denoting the Kronecker delta. $\zeta_k = i \frac{\omega}{\gamma} M_s^k \sin \theta_k t_k$ is the imaginary factor for the k^{th} layer where ω marks the resonance frequency of the system in radians, t_k is the thickness of the k^{th} layer, and γ is the gyromagnetic factor.

Algorithm 1: High level overview of the algorithm for computing the resonance frequency and the equilibrium position.

Result: $\mathbf{r}$, vector containing the resonance frequencies.
Result: $\mathbf{v}^* = \Theta^*, \Phi^*$, equilibrium state for each layer.
Data: $\mathbf{v}$ vector of all layers and their parameters
 // Construct free energy vector $\mathcal{F}$ using (35).
 // Find energy minimum using gradient descent
 $\mathbf{v}^* = \Theta^*, \Phi^* \leftarrow \text{AdamGradientDescent}(\mathcal{F}(\mathbf{v}), \nabla_{\mathbf{v}} \mathcal{F}(\mathbf{v}))$
 // Construct dynamical matrix with (36)
 $\mathcal{M}(\omega) \leftarrow \text{ConstructHessian}(\mathcal{F}, \mathbf{v}^*)$
 // Perform LU decomposition of the $\mathcal{M}$ matrix
 $\mathbf{L}, \mathbf{U}, \mathbf{P} \leftarrow \text{LU}(\mathcal{M})$
 // $\mathbf{P}$ is the row permutation matrix
 $\det \mathcal{M} \leftarrow \det \mathbf{P} \det \mathbf{U}$
 // Find roots $\mathbf{r}$ of the determinant expression.
 $\mathbf{r} \leftarrow \text{FindRoots}(\det \mathcal{M})$

The real positive roots of the determinant $\det \mathcal{M}|_{\mathbf{v}^*}$ correspond to resonant frequencies for the equilibrium state $\mathbf{v}^*$. We note that for weakly coupled layers, that is, for small values of J_1 (J_2), usually on the order of $\mu\text{J}/\text{m}^2$ or less, (36) can be approximated with a single-layer determinant solution:

$$\left(\frac{\omega}{\gamma}\right)^2 = \frac{1}{M_s^2 \sin^2 \theta} \left(\frac{\partial^2 \mathcal{F}}{\partial \theta^2} \frac{\partial^2 \mathcal{F}}{\partial \phi^2} - \frac{\partial^2 \mathcal{F}}{\partial \theta \partial \phi} \right) \quad (37)$$

⁵⁶ Arregi, Riego, et al., “Large interlayer Dzyaloshinskii-Moriya interactions across Ag-layers”.

⁵⁷ Kingma and Ba, *Adam*.

This approximation introduces a small error, but vastly improves the speed of computation, especially if the number of layers is large. The pseudocode in Alg.1 outlines the individual high-level steps necessary to calculate the ferromagnetic resonance at a given applied field.

The bulk of the algorithm's time is occupied by two components: computing the determinant and finding the roots of the determinant. The former can be quickly computed by first decomposing the matrix using the LU decomposition⁵⁸ and then computing a determinant of the resultant upper triangular matrix. However, finding roots poses a greater challenge. First, for $N \leq 2$, the returned roots are given by analytical formula. For other cases, they are computed numerically using Powell's hybrid method, implemented in the MINPACK library⁵⁹ (the SCIPY⁶⁰ module uses the same implementation). As it returns only a single root per call, we discretise the search space $[0, f_{\max}]$ into k smaller regions over which the root-finding functions are being called. On the other hand, due to the implementation of the Adam gradient descent algorithm, convergence to the energy minimum is very fast, even for larger N , and the root finding algorithm usually becomes the main bottleneck of the entire procedure. One strategy for physics-guided optimisation is to intentionally decouple selected layers where possible. This means either fixing the direction of the magnetisation vector or setting some of the IEC constants to 0 which eliminates the corresponding off-diagonal (latter) or both diagonal and off-diagonal (former) terms.

To ensure better convergence and to increase the chance of finding the global minimum instead of a local one, the initial magnetisation at the start of the simulation is knocked off the initial condition by a small random perturbation; in dynamical simulation, the same effect can also be achieved by adding some white noise via the temperature field. Yet, reaching global minimum is not guaranteed, as illustrated by the example simulation in Fig.3 – consecutive gradient descent steps are shown for two different starting conditions. Another advantage of this method is rather practical in nature, and when computing the main resonance spectrum or equilibrium, we do not need to be concerned with precise parameter selection, such as the integration step in the dynamics simulation, as the defaults of the computational parameters in CMTJ are suitable for a wide range of systems. Finally, from the point of view of simulation design, the SB model gives a simple way to define the antiferromagnet (AFM) that has a net-zero internal magnetisation. This cannot be done as easily in the dynamics model without modification, as the field contributions, such as interlayer exchange coupling or anisotropy fields, require normalisation by a M_s quantity. Modelling SAF is still possible by setting up two explicit layers of the compensating magnetic moment. Another example of the application of the SB model, this time including the resonance spectra, is described later in [Bayesian optimisation](#).

⁵⁸ Boyd and Vandenberghe, *Convex optimization*.

⁵⁹ More, Garbow, and Kenneth E. Hillstom, *User Guide for MINPACK-1*.

⁶⁰ Virtanen, Gommers, et al., "SciPy 1.0".

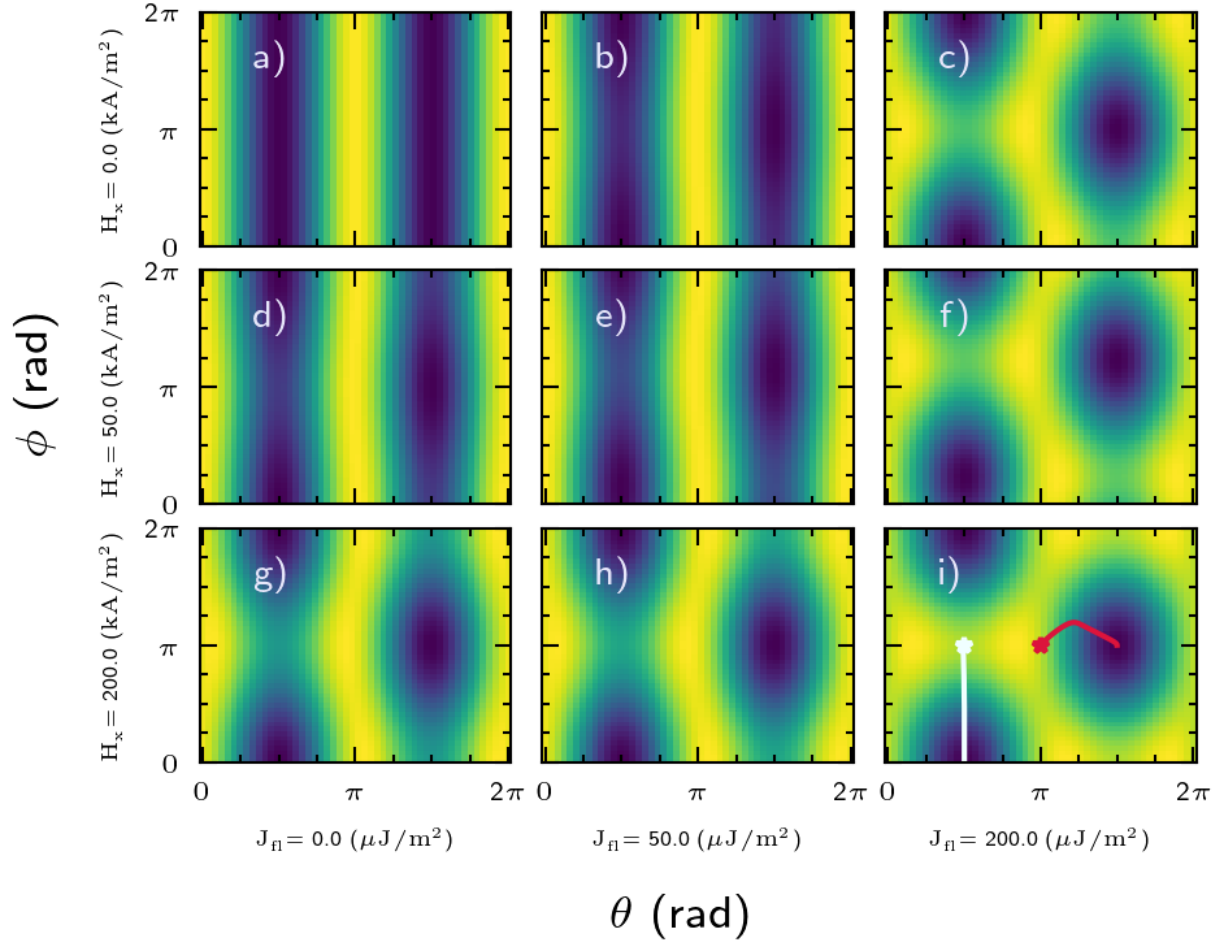


Figure 3: Energy landscapes for different values of the IEC and field magnitudes applied in the x direction for a sample structure with two FM layers. The darker the colour, the lower the value of the energy. The last panel, (i), shows two choices of initial conditions and the resulting gradient descent trajectories which are represented by the white and red lines. The star indicates the starting position. We see that increasing the coupling forces the system to be more stable in the minimum it selects. Increasing the field, as expected, has a similar effect.

Landau-Lifshitz-Gilbert-Slonczewski in spherical coordinates

A result similar to that presented by the SB method can be obtained by expressing the LLG equation using the spherical coordinates given in a general form for N layers as:

$$\mathbf{v} = \frac{\gamma_0}{(1 + \alpha_G^2)} \begin{pmatrix} \frac{1}{M_{s,1}} \left(-\frac{1}{\sin \theta_1} \frac{\partial \mathcal{F}}{\partial \phi_1} - \alpha_G \frac{\partial \mathcal{F}}{\partial \theta_1} \right) \\ \frac{1}{M_{s,1} \sin \theta_1} \left(\frac{\partial \mathcal{F}}{\partial \theta_1} - \frac{\alpha_G}{\sin \theta_1} \frac{\partial \mathcal{F}}{\partial \phi_1} \right) \\ \dots \end{pmatrix} + \boldsymbol{\tau} \quad (38)$$

where $\boldsymbol{\tau}$ denotes torque terms. Given the spherical coordinates of N layers, we may find a stable solution by first finding the energy minimum according to the procedure previously outlined for the SB model and then solving the eigenvalue problem for the LLG Jacobian:

$$\mathbf{D}[f(\mathbf{v})] = \omega \mathbf{I} \quad (39)$$

where ω are the eigenvalues and we denoted the RHS of the (38) as $f(\mathbf{v})$. Taking the imaginary part of ω yields the resonant frequencies of the system. An additional advantage of this approach is demonstrated by the possibility of adding torque terms to the RHS of (38). This model was used in⁶¹ where additional torque terms were included in the numerical analysis. In this model, one can also include the VSD computation assuming that under a small oscillating voltage signal V_{AC} , the magnetisation follows and oscillates around the stationary point $\mathbf{v}_0$ with a small amplitude $\delta \mathbf{v}$.

$$(\omega \mathbf{I} - \mathbf{D}_{\mathbf{v}}[f(\mathbf{v}, V_{AC})]) \delta \mathbf{v}(t) = \mathbf{D}_{V_{AC}}[f(\mathbf{v}, V_{AC})] \delta V_{AC}(t) \quad (40)$$

To obtain the linearised solution $\delta \mathbf{v}(t)$ we can invert the LHS matrix:

$$\delta \mathbf{v}(t) = (\omega \mathbf{I} - \mathbf{D}_{\mathbf{v}}[f(\mathbf{v}, V_{AC})])^{-1} \mathbf{D}_{V_{AC}}[f(\mathbf{v}, V_{AC})] \delta V_{AC}(t) \quad (41)$$

The derivative respective to exciting signal, here the voltage, necessitates that some term in $f(\mathbf{v}, V_{AC})$ depends on V_{AC} . Usually this is done through a torque with $\boldsymbol{\tau}(V_{AC})$ term, but it can be placed in the $\mathcal{F}$ term; for example, in voltage-controlled magnetic anisotropy (VCMA) systems, one can set the anisotropy energy dependent as $K_u + V_{AC} \delta K_u$ ⁶².

Domain dynamics

Classically, the dynamics of the domain wall is derived from the Lagrange-Euler (LE) equations, rather than the LLGS equation; this formalism was first introduced by Döring⁶³ and later expanded with damping dissipative terms by Gilbert⁶⁴. Similarly to the LLGS equation, the Lagrangian formulation is divided into conservative energy and non-conservative (dissipative) terms, wherein the latter is introduced into the picture through the Rayleigh dissipation function $\mathcal{R}$ – in the short derivation that follows we will only include the

⁶¹ Ogrodnik, Grochot, et al., “Study of Spin–Orbit Interactions and Interlayer Ferromagnetic Coupling in Co/Pt/Co Trilayers in a Wide Range of Heavy-Metal Thickness”; Ogrodnik, Antonio Vetrò, et al., “Field- and temperature-modulated spin diode effect in a GMR nanowire with dipolar coupling”.

⁶² Nozaki, Shiota, et al., “Electric-field-induced ferromagnetic resonance excitation in an ultrathin ferromagnetic metal layer”.

⁶³ Döring, “Über die Trägheit der Wände zwischen Weißschen Bezirken”.

⁶⁴ Gilbert, “Classics in Magnetism A Phenomenological Theory of Damping in Ferromagnetic Materials”.

damping term, but torque from the STT or the SHE are often enclosed in that term as well. The profile of a Bloch domain wall can be represented as the magnetisation angle with respect to the easy axis:

$$\theta(x, t) = 2 \arctan \left(\exp \left(-\frac{x - X(t)}{\Delta} \right) \right) \quad (42)$$

where Δ is the width of the domain wall and $X(t)$ is the time-dependent position of the domain wall. However, since for the LE in addition to a position coordinate we need to have a conjugate momentum as well, we use the out-of-plane angle magnetisation $\phi(x, t)$ as such. This quantity is fixed to a domain wall and hence depends only on time $\phi(x, t) = \phi_0(t)$ as the magnetisation precesses. At this point, we are ready to compute the equations of motion for the Lagrangian $\mathcal{L}$ defined as an integral over the entire space of the Lagrangian density $L = K - \varepsilon$:

$$\mathcal{L} = \int d\Omega K - \varepsilon \quad (43)$$

with:

$$K = \frac{M_s}{\gamma} \dot{\phi} (1 - \cos \theta) \quad (44)$$

where we use a dot notation to indicate time-derivative and we include the conservative ε energy terms. These energy terms are of the same type as those described in [Free energy models](#). After defining the aforementioned Rayleigh dissipative equation:

$$\mathcal{R} = \frac{1}{2} \frac{\alpha_G M_s}{\gamma} (\dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2) \quad (45)$$

The two equations of motion for a 1 dimensional case are then given by the LE application:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} + \frac{\partial \mathcal{R}}{\partial \dot{q}_i} = 0 \quad (46)$$

where $q_i = \{X, \phi\}$. As a result, we obtain sets of two equations⁶⁵ describing the velocity of the domain wall $\dot{X}$ and the rate of change of the in-domain angle $\dot{\phi}$:

$$\begin{aligned} (1 + \alpha_G^2) \dot{X} &= \Delta (\Gamma_A + \alpha_G \Gamma_B) \\ (1 + \alpha_G^2) \dot{\phi} &= -\alpha_G \Gamma_A + \Gamma_B \end{aligned} \quad (47)$$

where Δ is the domain width, Γ_A contains effective field terms and Γ_B contains force dissipation terms:

$$\begin{aligned} \Gamma_A = \gamma_0 \left(-\frac{1}{2} H_k \sin 2\phi - \frac{\pi}{2} H_y \cos \phi + \frac{\pi}{2} H_x \sin \phi + \frac{\pi}{2} Q H_{DMI} \sin \phi + \right. \\ \left. \frac{2J_{IEC}}{\mu_0 M_s t_{FM}} \sin(\phi - \phi') \right) + \frac{b_j}{\Delta} \end{aligned}$$

⁶⁵ Thiaville, Rohart, et al., “Dynamics of Dzyaloshinskii domain walls in ultrathin magnetic films”; Martinez, Emori, et al., “Current-driven dynamics of Dzyaloshinskii domain walls in the presence of in-plane fields”; Alejos, Raposo, et al., “Current-driven domain wall dynamics in ferromagnetic layers synthetically exchange-coupled by a spacer”; Yang and S. Parkin, “Novel domain wall dynamics in synthetic antiferromagnets”.

$$\Gamma_B = \gamma_0 \left(Q(H_z + H_{th} + H_p) + \frac{\pi}{2} Q H_{SHE} \cos \phi - \zeta \frac{\pi}{2} H_R \cos \phi \right) + \zeta \frac{b_j}{\Delta}$$

with H_R as Rashba term, H_{SHE} spin Hall term, H_p , pinning field term, H_{th} thermal field term. b_j is the STT coefficient and ζ is the nonadiabatic parameter of the STT. ϕ' denotes the angle of the domain wall of the other coupled layer. $Q \in \{-1, 1\}$ parameter denotes whether the DW is down-up or up-down, respectively. The schematic distinction between the Bloch and Néel domain walls is shown in Fig.4.

Numerical library design

In this section, we comment on the design principles for the CMTJ library that implements the numerical methods described throughout this section. Modern computing libraries aim to combine speed with a flexible interface. The user or programming interface should be intuitive yet extensible enough to maintain its relevance in a dynamically changing landscape of sprouting programming frameworks, styles, and modules. One great example is the NUMPY library⁶⁶ which despite the rapid proliferation of PYTHON retained a widespread influence on computational programming in this language. The success of such libraries stem from their previously mentioned characteristics: speed and flexibility – on the one hand, the underlying code is written in pure C for maximum performance of the vectorised function execution⁶⁷, on the other hand, the library exposes pythonic⁶⁸ interface that feels native to the language. NUMPY has been so effective that numerous other libraries (SCIPY, PANDAS, or TORCH just to name a few) either directly mimic its interface or ensure compatibility with NUMPY objects and functions. The CMTJ is designed in a similar fashion, combining the performance in C and ensuring interoperability with modern PYTHON. The first goal can be achieved via the PYTHON application interface, a relatively low-level interface that exposes C objects directly in PYTHON. However, since it is a basic interface, it introduces significant overhead and tends to insert a PYTHON-specific dependencies into the C code. This makes it challenging to maintain pure C components, resulting in high coupling, and reduced cohesion^{69,70}. Another library, PYBIND11, offers much more flexibility and minimises the coupling between C and PYTHON-specific parts. It requires, at minimum, a single additional file in which the C functions and objects are mapped to the PYTHON interface. This approach enabled us to maintain a clear separation, allowing users to import headers directly from C++, or use the PYTHON interface. Additionally, a similar mechanism for exposing the C++ code is provided by the BOOST library⁷¹ – which also supports direct use of NUMPY objects from C++ without implicit conversion. The VISM⁷² application utilises the BOOST library and the PYQT⁷³ interface to visualise magnetic multilayers. The following publication describes in greater detail the physics that can be reproduced by the CMTJ library. Since that publication, the pack-

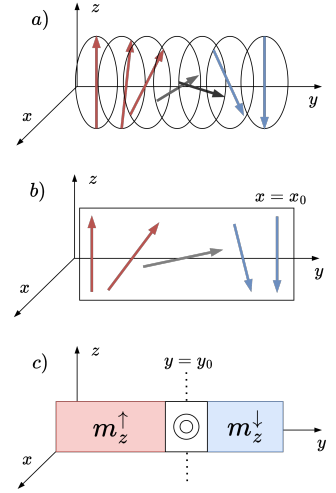


Figure 4: Two different domain wall types. (a) In the Bloch domain wall the rotation of the magnetisation is not constrained by a plane. On the other hand, the Néel domain wall (b) is characterised by a rotation in plane, here $x = x_0$. (c) Schematic view of the Néel domain wall used for simulations, the position of the domain wall is marked by $y = y_0$.

⁶⁶ Harris, Millman, et al., “Array programming with NumPy”.

⁶⁷ Vectorisation is a method wherein through loop avoidance a sequence of operations can be executed in a wavefront parallel manner as per the single instruction multiple data (SIMD) model.

⁶⁸ Although this expression may be considered colloquial, it accurately describes a manner in which code is written. Here, it pertains to the use of native semantics and programming models in PYTHON as opposed to patterns imported from other languages such as C, C++ or JAVA.

⁶⁹ Both cohesion and coupling are being used as technical terms from the realm of software engineering, see the reference.

⁷⁰ Martin, *Clean code*.

⁷¹ *Boost C++ Libraries*.

⁷² Mojsiejuk, Kulig, et al., “Visualization for Micromagnetics With Synchronized Plotting”.

⁷³ *PyQt5 Reference Guide — PyQt Documentation v5.15.7*.

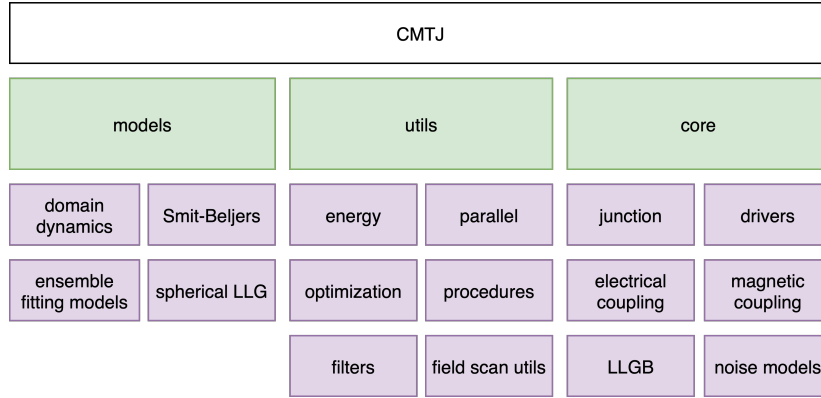


Figure 5: Outline of the CMTJ package library and its decomposition into submodules.

age has been expanded to include the Smit-Beljers models (as described in [Free energy models](#) and [Landau-Lifshitz-Gilbert-Slonczewski in spherical coordinates](#)), domain wall dynamics ([Domain dynamics](#)), Landau-Lifshitz-Bloch, and a variety of optimisation tools pertaining to those described in [Bayesian optimisation](#). Currently, version 1.9.0 of the core library (excluding examples, graphical interfaces, and additional models) contains approximately ~ 5500 lines of PYTHON code and ~ 4600 lines of C++ code. The division of the main library into submodules is given in Fig.5. Additionally, we offer a simple web-based user interface and a large language model agentic system to assist users with simulations. More details in [Additional Tools and Interfaces for CMTJ](#).

Chapter summary

In this chapter, we provided an overview of the numerical techniques implemented in the CMTJ library. The library represents the primary technical contribution of this thesis and offers the spintronics community accessible numerical techniques that do not require a powerful machine to run. Furthermore, the tools described in this section are essential for analysing and interpreting the subsequent results presented in this thesis.

Modelling spin Hall devices

This section introduces general modelling techniques used in the analysis and simulation of spin Hall devices and their associated experimental measurements. Key examples include harmonic Hall voltage detection, current-induced magnetisation switching (CIMS), spin diode ferromagnetic resonance (SD-FMR), pulse-induced magnetometry (PIMM), and R(H) loops. Specifically, the aforementioned techniques can be simulated with the CMTJ package, as detailed in [Pub. 2: Open-source macromagnetic package](#). For experimentalists, the ability to simulate these methods offers valuable insights into observed phenomena and parameter variations, particularly in large-scale parameter scans demonstrated throughout this thesis. The main challenge in reproducing the experimental techniques lies mostly in the complexity of measurement methods, which may involve complex post-processing and filtering procedures.

We begin this section with a brief characterisation of the fabrication process that leads, among other devices, to spin Hall bars. Then, we touch on the spin Hall effects in these devices, expanding the previous discussion from [Spin-Orbit torque](#) with details relevant to this particular chapter. The following subsections are arranged into two case studies: we begin by describing FMR spectrum analysis methods and combine them with harmonic Hall detection to investigate the Ta/CoFeB system, as described in [Pub. 1: Numerical model for the harmonic Hall voltage detection](#). We show how, with the use of simulation, we are able to extrapolate the experimental study with insights about the influence of field-like and damping-like torques on the observed harmonic voltage components. In the second part, we combine R(H) loops with CIMS to explain the interesting asymmetry of SOT switching under field reversal in Co/Pt/Co systems. Details of that sample can be found in⁷⁴. For completeness, in Appendix [Sample fabrication process](#) we include a description of some of the fabrication processes used in the production of the experimental samples discussed in this and the next chapter.

Magnetoresistance in spin Hall bars

The key measurable quantities of the device can be described with the most fundamental one, the resistance model. The baseline for the analysis of SHE

⁷⁴ Grochot, Ogrodnik, et al., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”; Ogrodnik, Grochot, et al., “Study of Spin–Orbit Interactions and Interlayer Ferromagnetic Coupling in Co/Pt/Co Trilayers in a Wide Range of Heavy-Metal Thickness”.

devices in this work is established on the grounds of the SMR-corrected equation for the longitudinal R_{XX} and transverse R_{XY} resistance of FM / HM due to Kim et al.⁷⁵:

$$R_{XX} = R_{xx0} + (\Delta R_{AMR} m_x^2 + \Delta R_{SMR} m_y^2) \quad (48)$$

$$R_{XY} = R_{xy0} + \frac{\Delta R_{AHE}}{2} m_z + \frac{w}{l} (\Delta R_{SMR} + \Delta R_{AMR}) m_x m_y \quad (49)$$

where w is the width of the sample and l is the length of the sample.

As indicated in the above equations, there are contributions of three primary resistance effects: anisotropic magnetoresistance (AMR), spin Hall magnetoresistance (SMR), and anomalous Hall effect resistance (AHE). The AMR arises because of spin-dependent scattering in FM – when the direction of the current is parallel to the magnetisation, the cross-section of spin scattering is the largest. Fig.6 illustrates the effects discussed in [Spin-Orbit torque](#) and shows how R_{XX} and R_{XY} are measured.

SMR is a consequence of two effects that manifest in the HM and on the FM/HM interface. First, the longitudinal charge current induces an SHE in the HM. Then, as the transversal current reaches the interface, diffuses through the interface, and exerts a torque on the FM layer if the diffusing spins are perpendicular to the magnetisation or if the spin current carriers are collinear with the magnetisation, it deflects back into the HM. The latter case leads to spin accumulation and ISHE⁷⁶ in which the spin current is converted back to the charge current, increasing the total longitudinal current in FM, thereby reducing its longitudinal resistance. In contrast, the former reduces the spin accumulation and thus the charge current, increasing the resistance.

Finally, AHE was briefly discussed in the [Non-conservative torque terms](#) section. As the current flows through the FM layer, the spin-dependent scattering and intrinsic factors lead to transverse spin and charge accumulation, which in ferromagnets is naturally asymmetric because of the imbalance of the majority and minority electrons. The dependence of $m_x m_y$ in transversal expression (49) is often attributed to the mixing of SHE and AHE⁷⁷ – initially, the longitudinal charge current in the FM induces the spin current in the direction perpendicular to both the magnetisation and the current itself, that is, $\mathbf{m} \times \mathbf{j}_c$. This spin current then translates into the charge current in the direction $\mathbf{m} \times \mathbf{m} \times \mathbf{j}_c$. At the same time, the transversal spin current (in the z direction) originating from plain SHE in the HM causes the charge current flow in the $\mathbf{m} \times \mathbf{p} \times \mathbf{j}_c$ ⁷⁸. Therefore, for those accompanying effects to manifest in the transversal magnetoresistance measurement, the magnetisation should have some x and y components such that the entire chain of the described derivative mechanisms takes place. This mixing is of rather small magnitude.

⁷⁵ Kim, Sinha, et al., “Layer thickness dependence of the current-induced effective field vector in TaCoFeBIMgO”.

⁷⁶ Saitoh, Ueda, et al., “Conversion of spin current into charge current at room temperature”.

⁷⁷ Taniguchi, “Magnetoresistance generated from charge-spin conversion by anomalous Hall effect in metallic ferromagnetic/non-magnetic bilayers”.

⁷⁸ this expression, assuming a current along x -axis and spin polarisation along y -axis, reduces to $\mathbf{m} \times \hat{\mathbf{z}}$ where $\hat{\mathbf{z}}$ is the unit vector along z axis

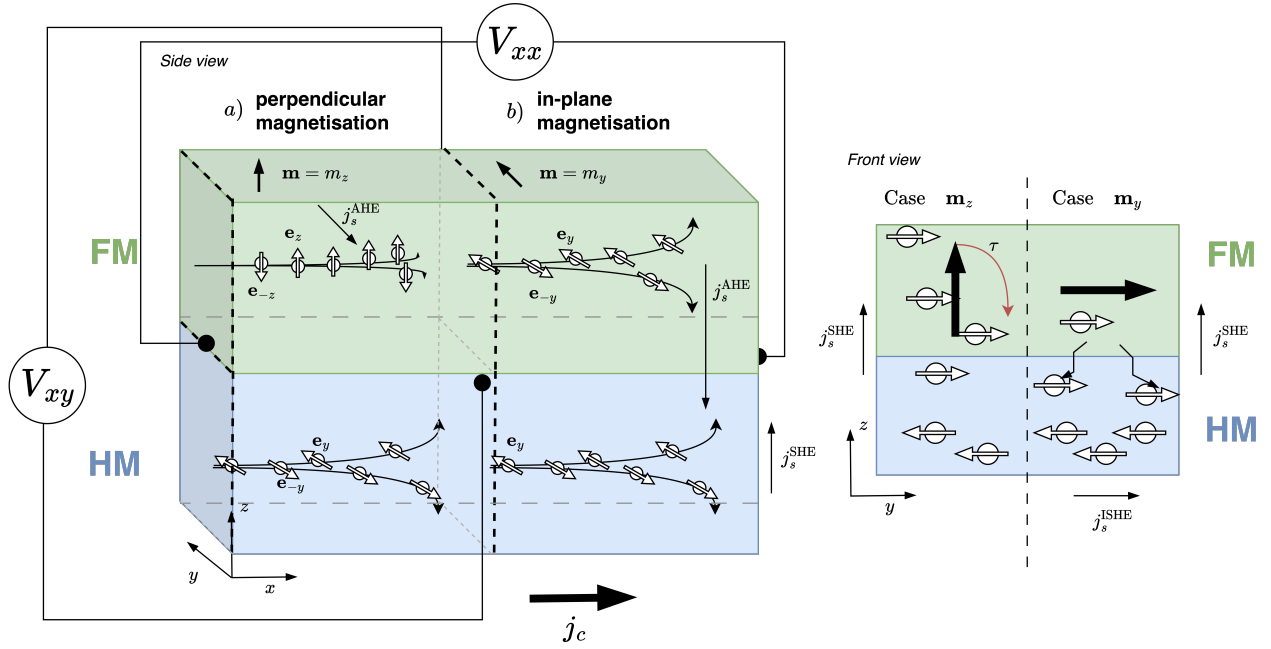


Figure 6: Selected effects in the Hall device for longitudinal V_{xx} and transverse V_{xy} arrangements for the voltage measurement and two cases of the magnetisation m . The charge current flows in the HM (blue). The vertical black dashed line divides the two cases of FM (green) magnetisation – along the z axis (left) and along the y axis (right). Depending on this arrangement, the AHE-induced current can flow into the FM.

Electrical modelling of Spin Orbit Torque Ta/CoFeB bilayer system

Next, we examine FMR by current rectification and harmonic Hall voltage detection methods in the context of the HM/FM bilayer Ta/CoFeB device. Each section includes remarks pertaining to more general cases, in order to show that the outlined simulation methods are widely applicable.

Ferromagnetic Resonance Spectrum Analysis

There are two main methods that are usually used to obtain ferromagnetic resonance spectra⁷⁹: SD measurement or PIMM. Both methods are based on the dynamics of the system, but respond to different excitations. PIMM, in particular, can be viewed as a time-domain impulse response measurement of a spintronic system: the magnetisation vector is rocked out of its equilibrium with a short impulse, effectively a current impulse, but in fact it may happen indirectly through a resulting Oersted field impulse. Excluding the extreme damping cases, the magnetisation vector begins to relax towards the oscillation at natural frequency, which changes with the external field's magnitude or its applied angle. SD is similar in this regard to PIMM, but is typically considered as the frequency-domain method, where the dynamics is forced with the injection of a microwave sinusoidal current. The full spectrum can

⁷⁹ Ziętek, Cecot, et al., “Magnetization dynamics of NiFe film and anisotropic magnetoresistance device”.

be obtained either by fixing the frequency and sweeping with the magnetic field, or vice versa, i.e. applying a fixed field while varying the generator frequency. The former has an experimental advantage in that the transmittance of the system does not change during the sweep, since the feeding excitation is kept constant (as opposed to continuous or spurious input frequency changes). However, regardless of the method, the final result should be approximately the same: a dispersion relation showing the main modes of oscillation over a range of scanned parameters (for the most part, it is a field magnitude or applied angle).

The basic set of simulated fits related to the VSD simulation has been described in detail for the Ta/CoFeB bilayer for both R_{xx} and R_{xy} configurations in [Pub. 1: Numerical model for the harmonic Hall voltage detection](#), but here we wish to elaborate on the idea mentioned in that work. We aim to solve the inverse problem: identifying the parameters set that reproduce a given experimental line. In our case, we might be interested in reproducing the main resonance lines of some device. To do that, we can perform an iterative procedure in which we make educated guesses about likely parameters that could lead to a particular experimental result. This procedure is manual, but an optimisation technique can be used to automate and speed up the process. We now briefly describe the Bayesian optimisation process and discuss how it can be applied to fitting the spectral data.

Bayesian optimisation

If the target function is complex and its derivative is not available, then zero gradient optimisation methods can be employed to efficiently find a (near-)global optima. One such method is Bayesian optimisation⁸⁰. Suppose that we wish to find a global minimum of a function f whose explicit form we do not know and which is costly to compute. In Bayesian optimisation, we place a Gaussian process ($\mathcal{GP}$) prior on f and then optimise an acquisition function $\alpha(x)$ built from the posterior predictive to select the next x . Thus, the optimisation will alternate between two steps: (i) fit the $\mathcal{GP}$ to the current observations, (ii) select the next candidate x_c by maximising the acquisition function, and then evaluate $f(x_c)$. The procedure is then repeated with $(x_c, f(x_c))$ added to the observation set $\mathcal{D}$. Sometimes, when the observation of $f(x)$ is noisy, we model the observations as $y(x) = f(x) + \varepsilon$ with $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$. In the case of Bayesian optimisation, the most common choice is to have f sampled from a Gaussian process:

$$f(x) \sim \mathcal{GP}(m(x), k(x, x')) \quad (50)$$

i.e., $\mathcal{GP}$ is a distribution over functions, and for each x it defines the Gaussian parameters: the expected value, $m(x) = \mathbb{E}[f(x)]$, and the variance. Taking the zero mean, $m(x) = 0$, simplifies the downstream expressions and can be achieved by renormalising the data. The kernel $k(x, x')$ defines the covariance

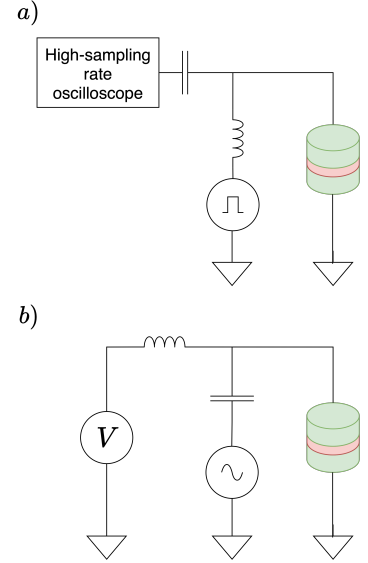


Figure 7: Setups of the experimental methods: schematics of (a) PIMM experiment and (b) the VSD-FMR experiment.

⁸⁰ Brochu, Cora, and Freitas, *A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning*.

between the samples taken from the domain of f and is typically defined on a radial basis, parameterised over $\Theta = (\eta, \lambda)$ such that:

$$k_{\Theta}(x, x') = \eta \exp\left(-\frac{1}{2} \frac{\|x - x'\|^2}{\lambda^2}\right) \quad (51)$$

The set of parameters Θ is learnt during the training procedure. We construct the marginal likelihood $p(y|X)$, defined over the observed data y , given the inputs X :

$$p(y|X) = \int p(y, f|X) df = \int p(y|f, X) p(f|X) df \quad (52)$$

In this expression, we identify the likelihood $p(y|f, X)$ and a Gaussian process prior, $p(f|X) = \mathcal{N}(m(X), \mathbf{K}_{\Theta}(X, X))$, where $\mathbf{K}_{\Theta}$ is now a $N \times N$ matrix, with $N = |X|$, $[\mathbf{K}_{\Theta}]_{ij} = k_{\Theta}(x_i, x_j)$. The fitting procedure seeks to find:

$$\Theta^*, \sigma_{\epsilon}^* = \operatorname{argmax}_{\Theta, \sigma_{\epsilon}} \log p(y|X) \quad (53)$$

and is optimised numerically. However, the posterior predictive $f(x)|\mathcal{D}$ for the function values at any point x is also Gaussian, and its two statistics, mean and variance, are computed from closed-form expressions⁸¹:

$$\mu(x, \Theta) = m(x) + \mathbf{k}_{\Theta}^T \mathbf{K}_y^{-1} \mathbf{y} \quad (54)$$

$$\sigma^2(x, \Theta) = k_{\Theta}(x, x) - \mathbf{k}_{\Theta}^T \mathbf{K}_y^{-1} \mathbf{k}_{\Theta} \quad (55)$$

where $\mathbf{k}_{\Theta} = [k_{\Theta}(x, x_1), \dots, k_{\Theta}(x, x_N)]$, $\mathbf{y} = [y(x_1) - m(x_1), \dots, y(x_N) - m(x_N)]$ and $\mathbf{K}_y = \mathbf{K}_{\Theta}(X, X) + \sigma_{\epsilon}^2 \mathbf{I}$

Fitting a Gaussian process under the set of N observations constitutes the first of two steps of global optimisation of f . In the next step of the procedure, we balance the exploitation of high-confidence regions against the exploration of high-variance regions. Regulating this balance is done via the acquisition functions, of which two are the most common: expected improvement and upper confidence bound (UCB). In our experiments, we predominantly use UCB, but modern methods combine multiple acquisition functions and then maximise over the Pareto front⁸²:

$$\alpha_{\text{UCB}}(x|\mathcal{D}_n) = \mu(x, \Theta) + \sqrt{\beta} \sigma(x, \Theta) \quad (56)$$

where $\mathcal{D}_n$ denotes the dataset observed so far: $[(x_1, y(x_1)), \dots, (x_N, y(x_N))]$. β parameter controls the trade-off between exploitation and exploration by promoting a large mean or a large variance. The next candidate for the evaluation is thus given by:

$$x_c = \operatorname{argmax}_x \alpha_{\text{UCB}}(x|\mathcal{D}_n) \quad (57)$$

When fitting any experimental result, we keep in mind the problem of the multiplicity of solutions. Potentially, the space of systems that have the exact

⁸¹ Bishop, *Pattern recognition and machine learning*.

⁸² Cowen-Rivers, Lyu, et al., *HEBO Pushing The Limits of Sample-Efficient Hyperparameter Optimisation*.

same set of minima (parameters) is infinite, and similar sets of parameters may lead to the same results. Therefore, to fit a resonance line, we first solve the linear assignment problem per field index H_k :

$$P^* = \min_P \sum_i^T \sum_j^S C_{ij} P_{ij} \quad \text{s.t.} \quad \sum_i P_{ij} = 1, \sum_j P_{ij} = 1, \quad P_{ij} \in \{0, 1\} \forall i, j \quad (58)$$

with T as the number of target frequencies and S as the number of candidate frequencies per field index H_k . The cost function is defined as $C_{i,j} = |\mathbf{f}_{i,\text{target}} - \mathbf{f}_{j,\text{candidate}}|$ and P_{ij} is the assignment of i^{th} target frequency value to j^{th} simulated frequency. For our optimisation metric, we take the maximum error of the optimal assignment for each field index k :

$$\epsilon_k = \max\{C_{ij} : P_{ij}^* = 1\} \quad (59)$$

This arrangement of the cost function not only makes it a worst-case estimator, but also allows us to avoid having to determine the source of the resonance layer, thus making our system somewhat spatially invariant⁸³. The final value of the cost function that enters the Bayesian optimisation is given by mean squared error (MSE):

$$\text{MSE} = \frac{1}{K} \sum_k^K \epsilon_k^2 \quad (60)$$

where K is the total number of field-scan steps.

This procedure was used in the investigation of the experimental samples of Ta(2)/CoFeB(5)/W(0-10)/CoFeB(1)/MgO(2)/Ta(1) (thicknesses in nm) over a range of W thicknesses. The fitting procedure was first performed under the assumption that there is a transition from the effective in-plane anisotropy of the thinner CoFeB layer to the perpendicular anisotropy as the thickness of the W decreases. The initial set of parameters⁸⁴: M_s , $K_u^{\text{PMA,top}}$, $K_u^{\text{IMA,bottom}}$ and antiferromagnetic coupling constant J parameters, was seeded for the thickest W of 9.74 nm by Bayesian optimisation within reasonable boundary conditions. The fittings for consecutively smaller thicknesses were tuned only in J and K_u , with upper bounds inherited from the system with the next thickest W. The final result of this procedure is shown against the experimental data in Fig. 8. The SB model, described in the [Free energy models](#) section, is particularly suited for such a fitting, as it is able to give direct frequency values that can be easily inserted into the cost function. In contrast, the dynamic LLGS model would require automatic frequency extraction from the spectrum, which is prone to numerical noise, especially if the spectrum is multimodal. The Bayesian optimisation procedure outlined in this section was used to seed a good initial set of parameters for most of the simulations described in the subsequent chapters.

⁸³ A simple example of this is to imagine a weakly-coupled system with two FM layers with reasonably different magnetic parameters. We expect 2 frequencies for each field, one per layer. During the simulation, we should also obtain 2 frequencies, provided that they are not degenerate. We need not concern ourselves with the geometry of a system because if the parameters of the upper and lower layers are flipped, the resonance spectrum coming from the simulation would be exactly the same, and so should be the cost function

⁸⁴ Here the top layer had a perpendicular anisotropy and the bottom layer had the in-plane anisotropy.

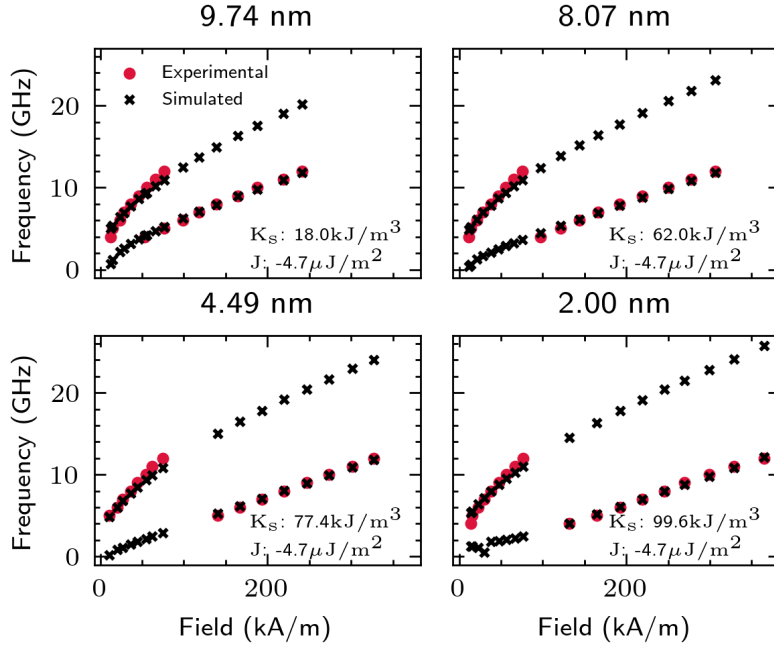


Figure 8: Ferromagnetic resonance fits to the experimental data on Ta(2)/CoFeB(5)/W(0-10)/CoFeB(1)/MgO(2)/Ta(1) wedge samples. The lower resonance line comes from the thinner layer, and it slowly decreases as the thickness decreases; this is primarily caused by the increase of the perpendicular anisotropy component of that layer. Fits were carried out using the SB model.

Harmonic Hall voltage detection

One of the key parameters in optimising SOT devices is the spin Hall angle. The determination of that parameter tells us how well a given system converts the charge current into the spin current, and therefore it is critical for energy-efficient fast memory applications. Switching dynamics is typically driven by extrinsic stimuli, most often current injection. Hence, it must be governed by the torques, both the damping and the field-like. One way to measure the efficiency of both torques occurs through harmonic Hall voltage detection. First, we define two quantities: damping- and field-like spin torque efficiencies (alternatively, effective spin Hall angles), $\xi_{\text{DL/FL}}$ respectively:

$$\xi_{\text{DL/FL}} = \frac{2e\mu_0 M_s}{\hbar} \frac{t_{\text{FM}} H_{\text{DL/FL}}}{j_c} \quad (61)$$

where $\mu_0 M_s$ is the magnetisation saturation, t_{FM} is the thickness of the ferromagnetic layer, and j_c is the charge current density flow in the heavy metal. What we ultimately aim to measure are the two quantities, the magnitudes of the torques $H_{\text{DL/FL}}$. These are extracted by fitting the first- and second-harmonic responses of the system under sinusoidal excitation with the current input. Each of these responses is measured in two arrangements, one called longitudinal (L) with the field applied along the direction of the current flow, the x axis, and the other transversal (T) where we apply the field along the y axis (see Fig. 1 in [Pub. 1: Numerical model for the harmonic Hall voltage detection](#)). This results in four measurement curves, each of which is used

in the fitting procedure. Specifically, we should fit to the low-field region, where the first harmonic response will have a quadratic form and the second harmonic will have a linear form. Thus, we have the following:

$$H_{DL} = -\frac{2}{\zeta} \frac{\rho_L \pm 2\kappa\rho_T}{1 - 4\kappa^2} \quad (62)$$

where κ is the ratio of the planar Hall effect to AHE resistance, $\rho_{L/T} = \partial V_{2\omega} / \partial H_{\text{ext}}^{L/T}$ and $\zeta = \partial^2 V_{\omega} / \partial H_{\text{ext}}^2$. The latter two parameters come from fitting the harmonic response in the process in which we obtain the slope of the linear region and the coefficient of the quadratic function. As noted earlier, the determination of field-like and damping-like torques can be done in a number of other ways, for example through the analysis of the SOT-FMR as in the work of Skowroński et al.⁸⁵. Nguyen et al.⁸⁶ provide a good review of the available methods.

The work [Pub. 1: Numerical model for the harmonic Hall voltage detection](#) demonstrates an end-to-end process where simulation has been paired with the experiment – starting from magnetoresistance fits, through VSD-FMR fits and culminating with fitting the harmonic Hall voltage detection curves. Finally, the simulation is used to extrapolate the results and present the dependence of the harmonic Hall voltage measurements on the torques: H_{DL} and H_{FL} , M_s and the anisotropy constant K_u .

⁸⁵ Skowroński, Karwacki, et al., “Determination of Spin Hall Angle in Heavy-Metal/Co – Fe – B -Based Heterostructures with Interfacial Spin-Orbit Fields”.

⁸⁶ Nguyen and Pai, “Spin-orbit torque characterization in a nutshell”.

Electrical modelling of ferromagnetically coupled Co/Pt/Co system

In this section, we continue our study of spin-Hall devices, this time focussing on the trilayer system Co/wedge Pt/Co. The following sections contain selected results from the work Grochot, Ogrodnik, et al. (“[Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system](#)”) and expand on them. Before that is discussed in detail, we begin with a general overview of R(H) and CIMS methods; in the latter we use, as illustrative examples, an extrapolated numerical sample.

Current Induced Magnetisation Switching

We now give a brief account and a general overview of the CIMS, to form a basis for a later discussion in the context of the perpendicular-magnetised Co/Pt/Co system and its interesting behaviour. In CIMS we attempt to flip the state of the magnetisation along a specific axis, for example, z axis, such that if the initial magnetisation vector was aligned along the $-z$ axis, then after a current impulse it flips to point along the $+z$ axis. The duration and shape of the impulse impact the result; shorter impulses give steep relationships, which have a single maximal (minimal) switching current, whereas longer impulses (in the infinite limit, simply an applied current density) saturate critical current densities at large absolute values of the externally applied

magnetic field. The procedure used to simulate CIMS related phenomena is described in Alg.2.

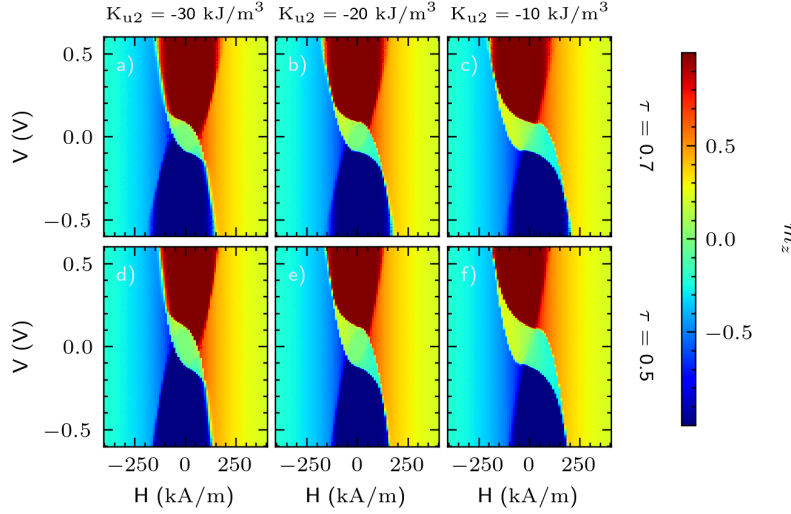


Figure 9: CIMS stability diagrams – an averaged m_z component as a function of torque τ , external magnetic field, applied voltage (current), and K_2 , the quadratic anisotropy constant. Top row, $\tau = 0.7$, bottom $\tau = 0.5$, left-to-right has an increase in K_2 which skews, rotates and narrows the region where $m_z = 0$. The plots were produced for the MTJ structure SAF/FeCoB/MgO/FeCoB. Parameters: $\mu_0 M_s = 1.12$ T, and perpendicular anisotropy constant $K_{u,1} = 563$ kJ/m³. The temperature was set to 300 K and the simulation was averaged over 50 realisations.

The standard stability diagram is produced by averaging the magnetisation component along the switching axis over a fixed time window $[t_{\text{relax}}, T]$ after discarding the initial relaxation period, t_{relax} (T is the total simulation time)⁸⁷. We look for the regions of high and low resistance as a function of the current density. In the picture, high-resistance states indicate that the maximum resistance was observed when scanning the current density in one way (from negative to positive values, or vice versa); the converse case applies to low-resistance states. As there is no need to compute a frequency spectrum, cal-

⁸⁷ Strelkov, A. Timopheev, et al., “Stability phase diagram of a perpendicular magnetic tunnel junction in noncollinear geometry”; A. A. Timopheev, Sousa, et al., “Respective influence of in-plane and out-of-plane spin-transfer torques in magnetization switching of perpendicular magnetic tunnel junctions”.

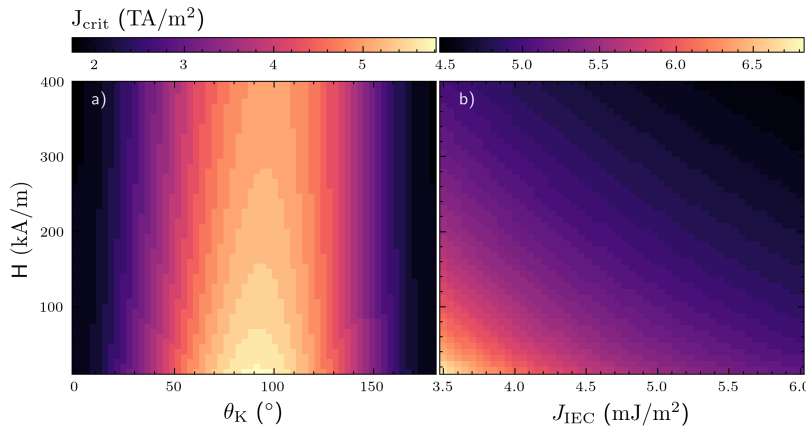


Figure 10: Critical current density as a function of the field vs anisotropy angle (a) and the field vs the IEC constant (b). Figure shown on JEMS 2022.

culating the switching diagram is much more efficient with the adaptive step

Algorithm 2: Procedure for simulating CIMS

Result: Steady state resistance vector $\mathcal{R}$

$\mathcal{R} \leftarrow \{\}$

$j_{\min} \leftarrow$ minimum current density

$j_{\max} \leftarrow$ maximum current density

$\mathbf{H}_{\text{ext}} \leftarrow$ external applied field

$S \leftarrow$ ferromagnetic system

$T \leftarrow$ simulation time

for j **in** $[j_{\min}, j_{\max}]$ **do**

$S.\text{setCurrentDensityFunction}(j \exp\{-t/\tau_p\})$

$S.\text{setExternalField}(\mathbf{H}_{\text{ext}})$

$\mathbf{m} \leftarrow S.\text{runSimulation}()$

 // Take an average over relaxed $\mathbf{m}$ as a steady state of the magnetisation

$\langle \mathbf{R} \rangle \leftarrow \text{computeResistance}(\langle \mathbf{m} \rangle_{[t_{\text{relax}}, T]})$

$\mathcal{R} \leftarrow \mathcal{R} \cup \langle \mathbf{R} \rangle$

end

methods, as described in [Numerical solutions to the LLGS equations](#). A typical diagram based on sample buffer / SAF / FeCoB(1) / MgO(1) / FeCoB(1.3) / W(0.25) / FeCoB(0.5) / cap⁸⁸ is shown in Fig.9. Similarly to Strelkov et al.⁸⁹, we check the impact of changing the secondary quadratic anisotropy component on the shape of the $m_z = 0$ region. The STT formulation used is a bit different from the one shown in (7), using explicit linear and square voltage dependence in damping-like and field-like torques, respectively:

$$\mathbf{T}_{\text{torque}} = \mathbf{T}_{\text{DL}} + \mathbf{T}_{\text{FL}} = -\gamma a_{\parallel} V \mathbf{m} \times (\mathbf{m} \times \mathbf{p}) + \gamma a_{\perp} V^2 \mathbf{m} \times \mathbf{p} \quad (63)$$

where V is the applied voltage, $\mathbf{p}$ is the polarisation vector and $a_{\parallel}, a_{\perp}$ are the phenomenological transport parameters typically derived from free-electron, tight-binding or first-principles models of the MTJs⁹⁰.

Many modern designs favour SOT switching instead of STT switching due to issues connected to Joule heating, and, as we indicated in the earlier chapters, from a simulation point of view, these turn out to be equivalent up to a choice of a parameter. Theoretical aspects of the dependence of switching currents in HM/FM systems are reasonably well understood (Lee et al.⁹¹), and for instance, for an in-plane field H_x , the critical current threshold is given by:

$$j_c \propto \frac{2e}{\hbar} \frac{M_s t_{\text{FM}}}{\theta_{\text{SH}}} \left(\frac{H_k}{2} - \frac{H_x}{\sqrt{2}} \right) \quad (64)$$

where H_k denotes the effective anisotropy field. However, this relation does not hold when there is strong coupling, and thus numerical simulations are required for most cases. To illustrate the point and show how complicated the situation may become under large coupling in Fig.10 which presents an

⁸⁸ at the moment of writing, the article is in review

⁸⁹ Strelkov, A. Timopheev, et al., “Stability phase diagram of a perpendicular magnetic tunnel junction in noncollinear geometry”.

⁹⁰ Wilczyński, Barnaś, and Świrkowicz, “Free-electron model of current-induced spin-transfer torque in magnetic tunnel junctions”; Chshiev, Manchon, et al., “Analytical description of ballistic spin currents and torques in magnetic tunnel junctions”.

⁹¹ K.-S. Lee, S.-W. Lee, et al., “Threshold current for switching of a perpendicular magnetic layer induced by spin Hall effect”.

example trilayer (FM/HM/FM) switching mechanism as a function of the field and anisotropy angle θ_{K_u} (a) or exchange coupling constant between the two layers J_{IEC} (b). Here, particularly for (b), we can deduce, through a mix of parameter fitting and function guessing, that the dependence of the critical current on the system parameters could be proportional to (up to a shared offset constant):

$$j_{\text{crit.}} \propto j_0 \exp\{-aJ_{\text{IEC}} \sinh(bH_{\text{ext}})\} \quad (65)$$

where j_0 , a and b are the fitting constants, dependent on the intrinsic parameters of the system. The expression can be obtained by producing the slices of the map from (b), i.e. $j_{\text{crit}}(J_{\text{IEC}})$ for all fields and observing a clear exponential and $\sinh$ behaviour, and the latter can be deduced after plotting the fitting parameter as a function of H_{ext} .

Another non-trivial point is that of geometry. In⁹² we investigated a α -W/CoFeB stack where the signs of H_{FL} and H_{DL} could take negative values. When the impulse pulse is sent through the HM layer, the resulting Oersted field can hamper the switching, i.e. increase the magnitude of the critical current. Fig. 11 illustrates that classical geometry. However, if the sign of H_{FL} is negative, it effectively aligns with the Oersted field and therefore can result in overall reduced critical currents. We modelled the impact of the Oersted field using a simple relation (orientated along the negative y -axis to comply with the convention in Fig. 11):

$$H_{\text{Oe}, -y} = \sigma_{\text{Oe}} \frac{j(t)t_{\text{HM}}}{2} \quad (66)$$

where j is the current density, t_{HM} is the thickness of the HM layer, and σ_{Oe} is the scaling factor that corrects for the rough macro-spin Oersted field estimate.

In this switching geometry ($y \rightarrow -y$) with effective in-plane anisotropy, and no bias field, we require an additional symmetry-breaking term along the x axis; otherwise no stable or deterministic torque will be exerted with current flowing in the x axis (which fixes the polarisation vector along the $+y$ axis, $\hat{\mathbf{e}}_y$). To this end, we use in-plane demagnetisation terms. Starting from the LLG equation in the form of:

$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} - \gamma H_{\text{FL}} (\mathbf{m} \times \hat{\mathbf{e}}_y) - \gamma H_{\text{DL}} \mathbf{m} \times (\mathbf{m} \times \hat{\mathbf{e}}_y) \quad (67)$$

we analyse the stability condition $\frac{\partial \mathbf{m}}{\partial t} = 0$, and compute torque components at equilibrium⁹³:

$$0 = \frac{\partial \mathbf{m}}{\partial t} = T_{\text{eff}} + T_{\text{FL}} + T_{\text{DL}} \quad (68)$$

where $T_{\text{eff}} = \mathbf{m} \times \mathbf{H}_{\text{eff}}$ contains $\mathbf{H}_{\text{eff}} = (-H_d^x, -H_d^y - H_{\text{Oe}}, H_k - H_d^z)$, with the demagnetisation fields H_d^i for each component x, y, z , the Oersted field H_{Oe} , and the perpendicular magnetic anisotropy field H_k . Using $\mathbf{m} = (\cos \phi \sin \theta, \sin \theta \sin \phi, \cos \theta)$, and observing that switching occurs

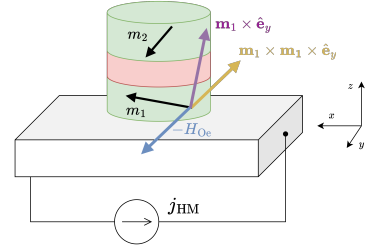


Figure 11: Sketch of a typical switching geometry. Note that H_{Oe} is drawn with the opposite sign to the damping-like torque.

⁹² Cierpiat, Grochot, et al., “Spin-Orbit torque in α -W-Based Magnetic Tunnel Junction”.

⁹³ K.-S. Lee, S.-W. Lee, et al., “Threshold current for switching of a perpendicular magnetic layer induced by spin Hall effect”.

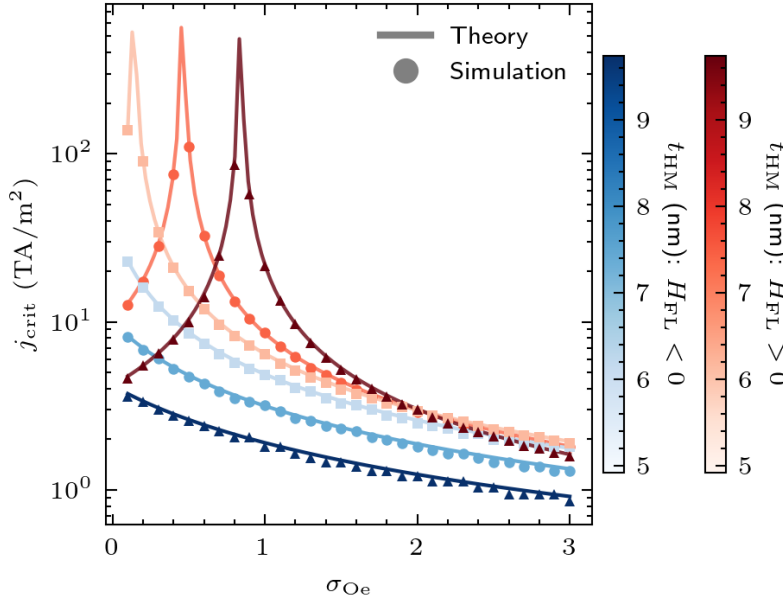


Figure 12: Theoretical (solid line) and simulated (markers) results for three sample thicknesses of W. Blue colour scale illustrates the case when $H_{FL} < 0$, and red when $H_{FL} > 0$. Values for j_{HM} , H_{FL} and t_{HM} were taken from the experiment. In each case, at $\sigma_{Oe,crit}$ and $H_{FL} > 0$, the Oersted field begins to dominate over H_{FL} . Since the Oersted field does not compete with $H_{FL} < 0$, there is no inflexion point and the current densities are lower overall. The change of peaks depending on W is not always linear, because the increase in the current (and thus the Oersted field) is not linear in the same way as the increase of H_{FL} .

mainly in-plane, that is, $\theta \approx \pi/2$ we arrive at the approximate equilibrium equation:

$$(H_{FL} + H_{Oe} + H_d^y) \cos \phi - H_d^x \sin \phi = 0 \quad (69)$$

The damping-like torque is not present in (69), suggesting that the switching in this geometry is driven primarily by field-like torque. After taking the derivative and making trigonometric substitution, we obtain the solution to the quadratic equation for $\sin \phi$:

$$\sin \phi = \pm \frac{H_d^x}{\sqrt{(H_d^x)^2 + (H_d^y + H_{FL} + H_{Oe})^2}} \quad (70)$$

Substituting (70) it back into (69), and setting $H_{Oe} = jH_{Oe}^j$ and $H_{FL} = jH_{FL}^j$, we arrive at the threshold current after solving for $j = j_{th}$:

$$j_{th} = \frac{\pm H_d^x - H_d^y}{H_{FL}^j + H_{Oe}^j} \quad (71)$$

Clearly, competition arises when the field-like torque in (71) changes sign. In our simple Oersted field model, the inflexion point of this competition occurs at the singularity $\sigma_{Oe,crit}$:

$$\sigma_{Oe,crit} = -\frac{2H_{FL}^j}{t_{HM}} \quad (72)$$

Fig.12 shows the simulated and computed threshold currents for the competing and non-competing cases of field-like torque, clearly indicating that

a non-competing case of $H_{FL} < 0$ yields order of magnitude smaller critical currents. Three thicknesses of HM were considered, demonstrating the shifting of the critical point, σ_{Oe} .

In the subsequent discussions, we omit the impact of the Oersted field on the switching currents either because of its additive nature (in qualitative sense it compensates the increase or decrease in torques) or because it cancels out in the overall geometry.

R(H) loops

$R(H)$ loops are the most basic tools that provide fundamental insight into the systems. The direction of the applied external field and the resulting shape of the $R(H)$ curve reveal the AMR, AHE and SMR factors, or the magnetic anisotropy energy. In the latter case, if the field is applied along the easy axis, the $R(H)$ curve exhibits a more "square"-like shape. In contrast, a smooth, continuous transition from one boundary-resistance state to another is a testimony to a large anisotropy in that direction. Any horizontal shifts may indicate the presence of some internal bias field, for example, coming from the exchange bias contribution.

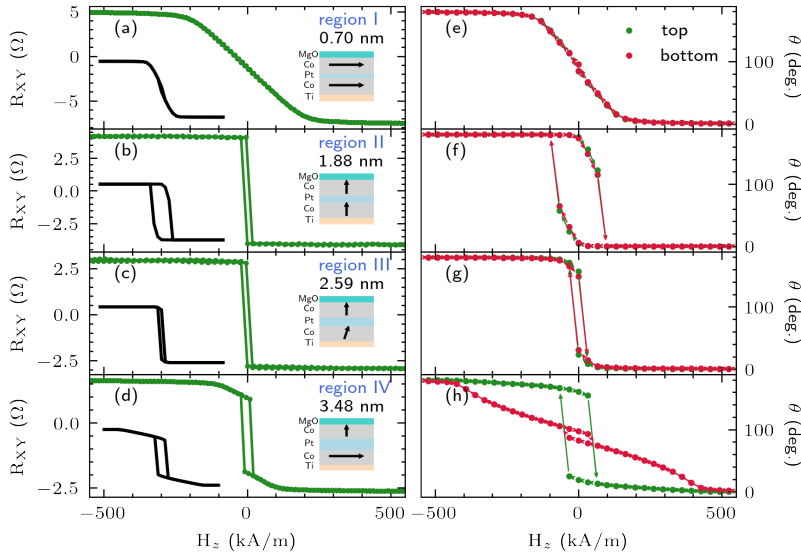


Figure 13: Study of AHE loops for 4 different thickness regions of the Pt (it is given by the inlaid thickness in nm) for the Co(1)/Pt(0-4)/Co(1) sample. Left, (a-d) – black curves in the inset correspond to the simulated results, whereas the green line represents the experimental data. The inset pictures of the Co/Pt stack illustrate the effective anisotropies of each FM layer. A clear transition to strong perpendicular anisotropy of the top Co layer is visible as we move from region I to region III. In region IV the IEC is very weak, almost negligible, so the bottom Co layer, being decoupled from the top one, stays in plane. Right, (e-h) simulation of the θ magnetisation coordinate of the top (red) and bottom (green) layers, corresponding to black insets in (a-d). As the thickness of the Pt spacer increases, the top layer switches with a larger field than the bottom one: the strong coupling field no longer enforces mutual and symmetric switching.

A notable application of $R(H)$ modelling is found in the case of the coupled thin Co layers (each having 1 nm thickness) separated by a Pt spacer that changes from 0 to 4 nm. The detailed description of the fabrication procedure is given in Grochot et al.⁹⁴ and Ogrodnik et al.⁹⁵ In such a system, the coupling between the two ferromagnets is varied with the thickness of the Pt layer; however, we found also that the anisotropy varies with that thickness, and appears to be crucial components in understanding the phenomenon of

⁹⁴ Grochot, Ogrodnik, et al., "Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system".

⁹⁵ Ogrodnik, Grochot, et al., "Study of Spin–Orbit Interactions and Interlayer Ferromagnetic Coupling in Co/Pt/Co Trilayers in a Wide Range of Heavy-Metal Thickness".

multilevel switching that we discuss later in the text.

A study of the Co/wedge Pt/Co system begins with the AHE loops, that is, the $R(H)$ loops with the external field applied along the z axis, as they mainly measure the m_z component of the magnetisation; see Eq.(49). We will vary selected parameters to investigate possible explanations for the shape transition of the AHE loops in the second (moderate coupling between to Co layers) and third (weak coupling) regions of the Co(1)/Pt(0-4)/Co(1) sample (thicknesses given in nm); the particular characteristics of each region are given by Ogrodnik et al.⁹⁶ First, we present the simulation results for the base case that agree with the observed experimental values, as shown in Fig.13, where the simulated loops are placed as insets. The hysteresis is given for an external perpendicular field, H_z , taken for 4 different thicknesses of Pt. The thicker the Pt layer, the lower the IEC value, which corresponds to the J parameter, which means that the two layers are progressively weakly coupled. Regions II and III are characterised by the largest perpendicular anisotropy in the top layer. Hence, under the large J regime, the two layers will switch simultaneously in fully perpendicular loops.

⁹⁶ Ogrodnik, Grochot, et al., “Study of Spin–Orbit Interactions and Interlayer Ferromagnetic Coupling in Co/Pt/Co Trilayers in a Wide Range of Heavy-Metal Thickness”.

Fig.13(e-h) also gives magnetisation angles θ of the top and bottom layers for the corresponding AHE loops. The transition from (a-c) to (d) reveals a plausible reason behind the bending of the loop, which may be explained by the difference in switching fields between the top and the bottom layers; this is caused by a much smaller coupling value that no longer enforces symmetric switching. Those results parametrically match the experimental case and will later be used for the CIMS simulations.

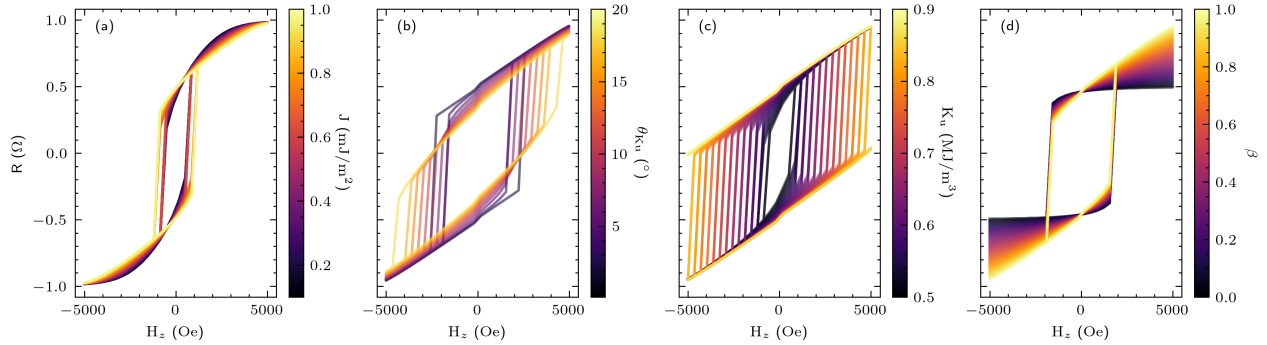


Figure 14: Effects of variation in 4 parameters on AHE loops. (a) IEC constant J , (b) anisotropy axis angle $\theta_{K_{u,1}}$, of the top layer, (c) anisotropy constant $K_{u,1}$ of the top layer and (d) the AHE asymmetry parameter β . Relating the behaviour from this plot to Fig.13 we see that there are multiple underlying parameters that could explain the bending of the hysteresis in this system. From Fig.13 (f) we see strong perpendicular anisotropy of the top layer, while the bottom goes strongly in-plane. The widening of the hysteresis can also be explained by larger in-plane anisotropy.

Further investigation of the origins of loop deformation is conducted by varying key simulation parameters, as shown in Fig.14. There, the following parameters were changed: factor β , $K_{u,1}$ (the anisotropy axis), $\theta_{K_{u,1}}$ (the angle of the anisotropy respective to the positive z axis), and J (the IEC

constant). β parameter determines the balance between the top and bottom layers in the resistance summation (75), and its significance is discussed in detail in later section. At first glance, the effects of varying β and J appear similar, but in fact the latter causes the AHE loop to bend more, rather than just rotate. Therefore, the change in shape and bending of the loop near the switching field in region IV may be attributed to a small IEC value. Likewise, a stronger rotation of the same loop may be caused by a greater influence of the interface mixing, leading to greater interfacial asymmetry and hence to a greater β factor.

Multilevel switching in Co/Pt/Co systems: numerical analysis

A phenomenon called multilevel switching (MLS) is observed in Co/wedge Pt/Co thin-wedge systems with strong ferromagnetic interlayer coupling through the Pt layer when subjected to a CIMS experiment⁹⁷. Under certain conditions, such as appropriately large perpendicular anisotropy, the top and bottom layers experience strong opposite spin-orbit torques induced by the current impulse in the heavy metal that separates the two FM layers. If there exists an asymmetry between the two Co layers, for example, due to different interfacial mixing of the heavy metal with the ferromagnets⁹⁸, then we may observe a separation of standard CIMS hysteresis. Representative results are shown in Fig. 15 (a, d, g); the middle panel is omitted from this discussion for now. The key characteristics of this switching behaviour are as follows:

1. the decrease in the width of the hysteresis, and so the critical switching currents, with the increase in thickness of Pt,
2. the apparent vertical gap between the hysteresis performed under the positive external applied field and the negative one,
3. the squishing of the hysteresis height (peak-to-peak resistance) with the decrease in thickness of Pt.

To better understand the physical origin of this behaviour, we start with a simplified algebraic model that considers the additive contributions of the top and bottom layer AHE terms. From (49) we exclude the mixing term $m_y m_x$ due to the vanishing amplitude of m_y in the studied system; this also brings more clarity to the consecutive discussion. First, consider the total transverse resistance as the sum of contributions from the top and bottom layers:

$$R_{XY} = R_{xy0}^{(1)} + R_{xy0}^{(2)} = \Delta R_{AHE}^{(1)} m_z^{(1)} + \Delta R_{AHE}^{(2)} m_z^{(2)} \quad (73)$$

with superscripts indicating the top (1) and bottom (2) layer quantities. For a moment, we ignore $R_{xy0}^{(1,2)}$ quantities as they present a constant offset irrespective of the magnetisation state. If we start with a standard bilayer hysteresis under the switching current, we can make a symmetric argument that the switching current sweeping from $j_{\max}$ to $j_{\min}$ at H_x is simply a reflection

⁹⁷ Grochot, Ogrodnik, et al., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”.

⁹⁸ Ogrodnik, Grochot, et al., “Study of Spin–Orbit Interactions and Interlayer Ferromagnetic Coupling in Co/Pt/Co Trilayers in a Wide Range of Heavy-Metal Thickness”.

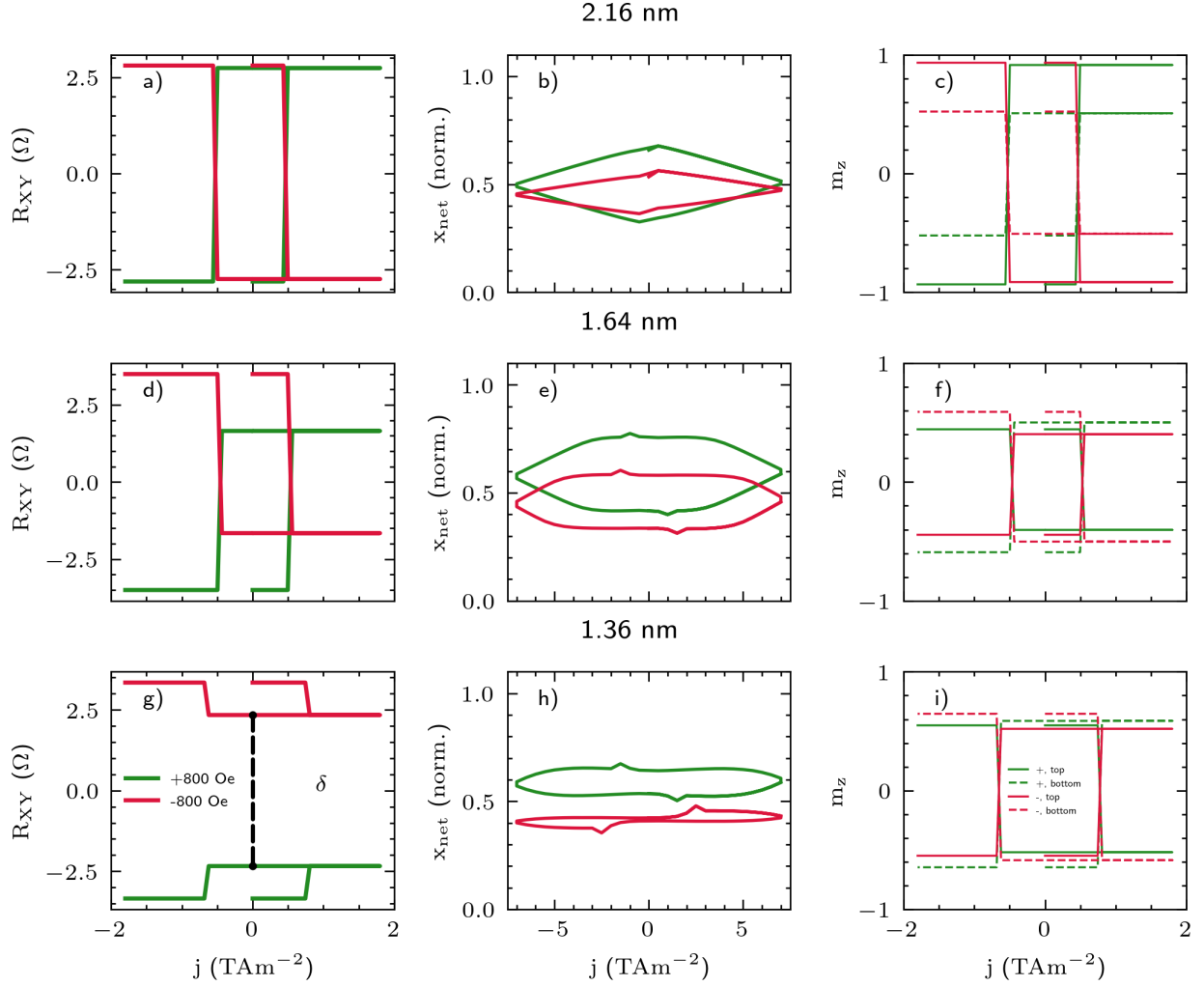


Figure 15: Macromagnetic and domain wall models with asymmetric AHE resistance switching hysteresis $R_{XY}(j)$ under field reversal regime. The left-hand side panel presents the macromagnetic switching model, whereas the middle-panel side model gives the domain wall model simulation, with y-axis denoting the displacement of the domain wall. We see a similar behaviour of state overlap as the Pt thickness decreases (coupling increases) in both cases. The right-hand side panel shows the m_z states during the switching procedure, as shown in (a, d, g). The figure taken from (Grochot, Ogrodnik, et al., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”) shows purely simulation results.

with respect to the y axis when we sweep under $-H_x$ and, indeed, that is the case when we inspect the critical current (j_c) behaviour introduced by Lee et al.⁹⁹, mentioned earlier. We note that this formula (64) pertains to the bilayer FM/HM systems and hence has a primarily illustrative purpose in this discussion because of the strong coupling field in the system – we indicate this approximation with the use of the $\propto$ symbol. The reason why we roughly hold to that approximation in the subsequent argument is that the experimental critical current thresholds as shown in¹⁰⁰ indeed exhibit a similar switching model, up to a value of the offsetting field, a case that we consider more in detail in a later discussion. Under this symmetric switching argument, we define an MLS gap δ_{MLS} as:

$$\delta_{\text{MLS}} = R_{\text{XY}}^+ - R_{\text{XY}}^- = \Delta R_{\text{AHE}}^{(1)} (m_{z,+}^{(1)} - m_{z,-}^{(1)}) + \Delta R_{\text{AHE}}^{(2)} (m_{z,+}^{(2)} - m_{z,-}^{(2)}) \quad (74)$$

Here, we denoted $R_{\text{XY}}^{+/-}$ as the hysteresis resistance under positive field and negative field, respectively. To obtain $\delta_{\text{MLS}} \neq 0$ we have $\Delta R_{\text{AHE}}^{(1)} \neq \Delta R_{\text{AHE}}^{(2)}$, since under symmetric j_c we assumed $m_{z,+}^{(i)} - m_{z,-}^{(i)} = 0, i = \{1, 2\}$. Note that we inspect the case of field reversal, in which the response is symmetric about the y axis, so there is no change of sign between $m_{z,-}^{(i)}$ and $m_{z,+}^{(i)}$. This suggests that the MLS gap arises from the asymmetries in AHE resistance between layers. To incorporate this into the model, we introduce a weighting factor, β , that captures the imbalance in the interfacial contributions of AHE and / or the electrical connection:

$$R_{\text{XY}} = R_{\text{xy0}}^{(1)} + R_{\text{xy0}}^{(2)} + \frac{1}{2} \kappa \Delta R_{\text{AHE}} (m_z^{(1)} + \beta m_z^{(2)}) \quad (75)$$

where the superscript refers to the top (1) or the bottom layer (2). The parameter β ranges from 0 exclusive (asymmetric interfaces) to 1 inclusive for entirely symmetric interfaces. Second, the parameter κ corrects for the amplitude of hysteresis in macromagnetic simulations. Equation (75) is modified from Kim et al.¹⁰¹ where in the approximation we again neglected $\Delta R_{\text{SMR}_{\text{xy}}}$ and $\Delta R_{\text{AMR}_{\text{xy}}}$ due to their small values in the experiment. Fig. 15 leans on the idea of the AHE resistance asymmetry by introducing the interfacial asymmetry parameter β as outlined above – β approaches one as the Pt layer increases in thickness. Clearly, it can provide an adequate level of agreement with the experiment compared to the experimental data¹⁰². The estimate for the size of the MLS gap based on the β factor is shown in Appendix [Estimate of the MLS gap](#).

In addition to the AHE asymmetry, another contributing factor is the asymmetry arising from interfacial DMI effects. We mentioned in sections [Energy density contributions](#) and [Non-conservative torque terms](#), that strong interfacial asymmetry induces a myriad of effects, one of them being the DMI effect described in an earlier chapter. From the experiment, the measured DMI field in the studied sample appears to be the strongest in the III region, and due to interfacial characteristics, the H_{DMI} field points along the

⁹⁹ K.-S. Lee, S.-W. Lee, et al., “Threshold current for switching of a perpendicular magnetic layer induced by spin Hall effect”.

¹⁰⁰ Grochot, Ogrodnik, et al., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”.

¹⁰¹ Kim, Sheng, et al., “Spin Hall Magnetoresistance in Metallic Bilayers”.

¹⁰² Grochot, Ogrodnik, et al., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”.

x axis, the same as the applied external field. Hence, we could modify our previous expression (64) for the critical current:

$$j_c \propto \frac{2e}{\hbar} \frac{M_s t_{\text{FM}}}{\theta_{\text{SH}}} \left(\frac{H_k}{2} - \frac{H_x \pm H_{\text{DMI}}}{\sqrt{2}} \right) \quad (76)$$

which has the effect of modulating the H_x field depending on the direction of the applied field. Including the DMI asymmetry between the two interfaces modifies the in-plane field, widening or narrowing the hysteresis loop depending on its alignment relative to the applied field. Typically, the DMI values in Co/Pt systems are of the order of 1 mJ/m^2 , although there appears to be some variation in reporting these numbers in the literature¹⁰³.

¹⁰³ Kuepferling, Casiraghi, et al., “Measuring interfacial Dzyaloshinskii-Moriya interaction in ultrathin magnetic films”.

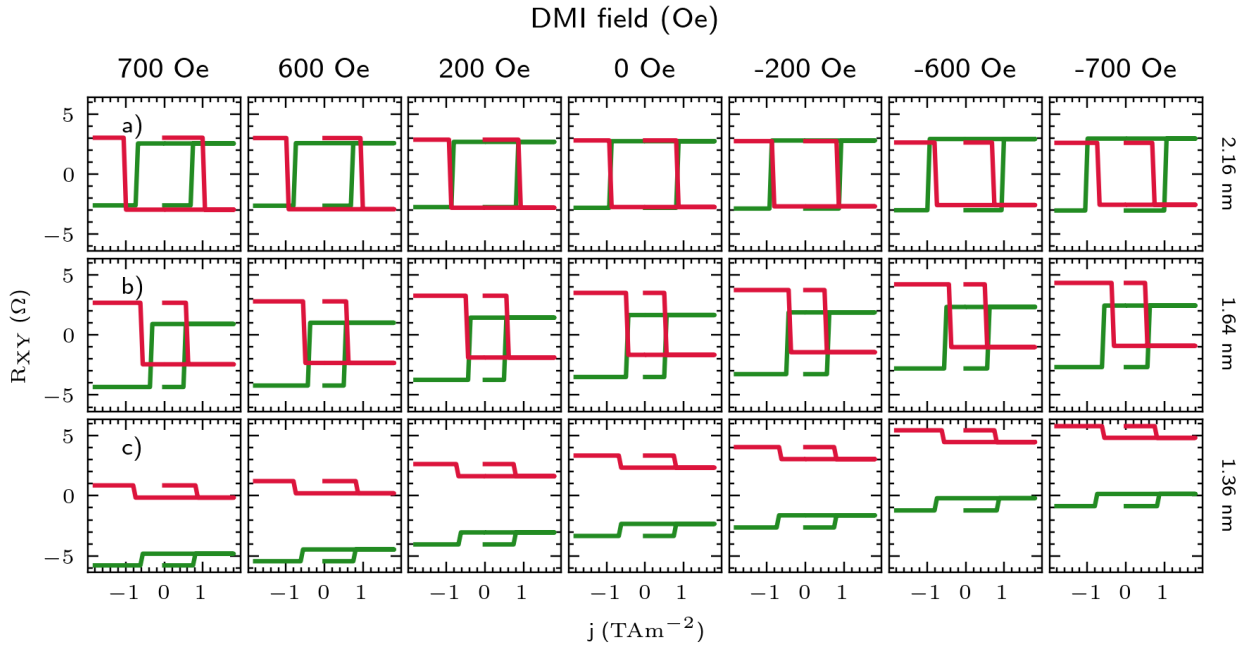


Figure 16: Simulated effect of the DMI field on hysteresis loops at different Pt spacer thicknesses during CIMS. (a) Pt thickness of 2.16 nm, (b) 1.64 nm, (c) 1.36 nm. All parameters, other than the H_{DMI} magnitude along x direction, were kept the same as in the previous simulations. As before, red colour denotes the hysteresis under -800 Oe while the green one under 800 Oe.

In Fig. 16, we can observe how the DMI field aids the switching mechanism. If it is in the same (opposite) direction as the applied field, the DMI field facilitates (opposes) switching, which manifests itself with a narrower (wider) hysteresis. There is also the question of the vertical drift of the hysteresis when substantial asymmetry is present; Fig. 16(b, c). This drift persists even if we disable m_x, m_y from R_{XY} calculation, suggesting this is solely due to m_z behaviour. In particular, inspecting torque equilibria (68), we notice that H_{DMI} appears in the z component of the torque, as it is set along the x axis. The DMI field will tend to reduce the m_z component if positive, specifically for the bottom layer, which has a much lower perpendicular anisotropy;

the top layer with strong PMA is not affected by the drift. However, when both the R_{XY} of the top and bottom layers are added in series, that small drift is amplified, especially for thinner Pt layers, which are parametrised to weaker PMA in the model.

Altogether, the DMI alone does not influence the gap (see that in Fig. 16, at $H_{DMI} = 0$ the gap is still visible, and is unaffected in size otherwise). However, the DMI component does introduce a different type of asymmetry, the asymmetry between the switching currents for the positive and negative fields, but does very little to meaningfully affect the size or the behaviour of the gap.

To account for the MLS gap itself, we consider one more alternative mechanism that bases the existence of the MLS gap on the strength of the coupling field and appropriate relative positioning of $m_z^{(1)}$ and $m_z^{(2)}$, but assumes equal β factors for both layers. The idea here is as follows: in the strong coupling regime, we want the two anisotropy fields to force the z components of the magnetisation close to each other, which maximises the coupling field strength. According to the coupling formula (16), if two z are imbalanced, that is, one is small and the other is large, the product will likely be small, but when those two are of similar magnitude, the coupling field acting on both will be rather large. Therefore, in the simulations we devise the following method to test this hypothesis: we set the coupling high (in the range of 3 – 6 mJ/m²) and set the perpendicular anisotropy of the top layer at K_{off} . The bottom layer anisotropy is then defined relative to the top layer anisotropy, such that: $K_{bottom} = K_{off} - \Delta K$, with positive ΔK . Here, we assume, as per the parameters in Ogrodnik et al.¹⁰⁴, that the top layer has strictly perpendicular anisotropy with the bottom layer being much smaller, to the extent that it can be effectively in-plane, if needed. We can now scan with the value of ΔK to obtain Fig. 17 and Fig. 18. Here, we define the field reversal gap, or shift, as $\delta' = |\min(R_{XY}^+) - \min(R_{XY}^-)|$, which means that if δ' is larger than the height of the hysteresis, then there is no overlap between the two hysteresis loops under field reversal. This is in effect equivalent to δ_{MLS} .

Taken together, our results suggest that both the interfacial AHE asymmetry (through the β factor) and the anisotropy configuration jointly contribute to the emergence of the field-reversal hysteresis gap. In the article, Grochot et al.¹⁰⁵ considered a narrower range of parameters, mainly the variation in the anisotropy, which excluded the latter option, as it requires a larger anisotropy gap between the two Co layers.

Multilevel switching with domain wall model

The multilevel switching can be reproduced with the domain wall dynamics model we described in [Domain dynamics](#). Because of the large spin-orbit coupling at the interfaces with the HM, there is a reasonably large DMI.

¹⁰⁴ Ogrodnik, Grochot, et al., “Study of Spin–Orbit Interactions and Interlayer Ferromagnetic Coupling in Co/Pt/Co Trilayers in a Wide Range of Heavy-Metal Thickness”.

¹⁰⁵ Grochot, Ogrodnik, et al., “Influence of ferromagnetic interlayer exchange coupling on current-induced magnetization switching and Dzyaloshinskii–Moriya interaction in Co/Pt/Co multilayer system”.

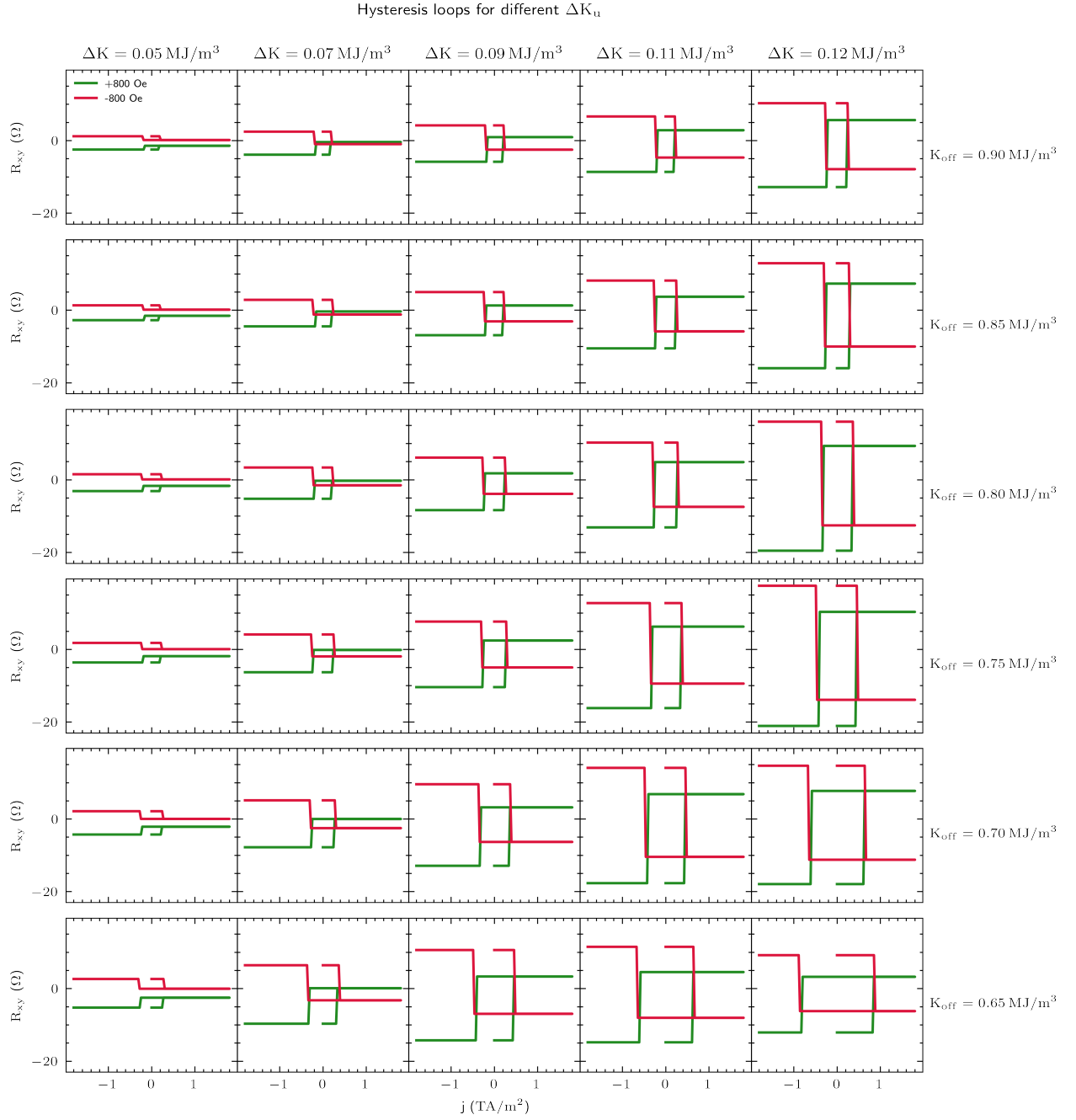


Figure 17: Effect of scanning with ΔK for different values of the top layer perpendicular anisotropy K_{off} . This is an alternative way to achieve MLS, avoiding the introduction of an interfacial asymmetry variable, which was required for Fig.15

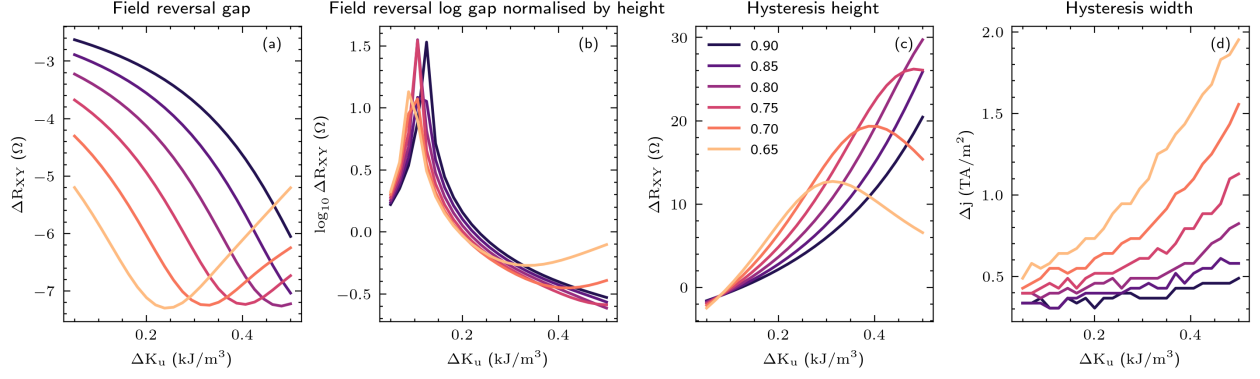


Figure 18: Effect of scanning with ΔK on hysteresis parameters, presented for different values of the top layer perpendicular anisotropy K_{off} . (a) field reversal gap defined as $|\min(R_{XY}^+) - \min(R_{XY}^-)|$, and normalised by the positive field hysteresis height in (b). (c) hysteresis height (taken from the positive field hysteresis) and d) hysteresis width (taken from the positive hysteresis field). Note that if the field reversal gap is normalised (b), it gives rise to an interesting non-linearity – the magnitude here denotes the effective resolution of the gap, that is, it peaks where the gap is the largest relative to the height of the hysteresis. The wiggly nature of (c) is due to the granularity of the current scan, and hence the switching currents are not always selected with the highest precision.

We now return to the middle side of Fig. 15 which presents a side-to-side comparison between the two switching models, where for the domain wall model we used the displacement on the strip of the domain as an indicator of the m_z component, the model derives from (47). Summing the contributions of the two layers, we reproduce the result from the classical macromagnetic simulation. A proper square-like hysteresis loop of the system is possible; however, it requires an additional field component or clipping. When the domain reaches an edge of the device, we have to either numerically clip the x component to contain the domain within the sample or introduce an edge potential that acts as a stopping force as the domain approaches the edge. Only the asymmetric AHE hypothesis was modelled, as other mechanisms are not readily compatible with the domain wall dynamics.

Chapter summary

This chapter summarises the research on spin Hall bars, in particular, a study on two systems: the CoFeB/Ta bilayer device and the coupled HM/FM Co/wedge Pt/Co systems which take advantage of the spin Hall effect and IEC. We presented a wide range of electrical detection techniques, outlining how they were implemented in CMTJ. For the coupled device, we also analysed an interesting phenomenon of the multilevel switching, proposing two viable hypotheses that could explain it, at least numerically: one relies on the asymmetry in the AHE resistance of the two layers, while the other is more organic and arises through the asymmetry in the perpendicular anisotropy of Co layers. Arguably, these two mechanisms may coexist and are indistinguishable in simulation. Regarding the application of multilevel switching,

it could be perceived as a variation of multibit cells, similar to¹⁰⁶, particularly if the gap separation can be controlled through a careful fabrication process. Then, given sufficient resolution between levels (i.e. the gap is wide enough), four resistance states per device could be distinguished. Finally, the phenomenon of multilevel switching warrants supplementary research to determine whether it can be reproduced with different FM and/or HM materials. Similarly, in the simulation domain, the topic could be further explored in a more granular fashion using the micromagnetic approach.

¹⁰⁶ Rzeszut, Skowroński, et al., “Multi-bit MRAM storage cells utilizing serially connected perpendicular magnetic tunnel junctions”.

Modelling magnetic tunnel junctions

This chapter focuses on magnetic tunnel junctions, and is structured into two main sections: one addressing the electrical coupling of the in-series connected MTJs, and the other the modelling of $1/f$ noise. After a brief characterisation of an MTJ, we investigate a desynchronisation phenomenon observed experimentally in such systems and discuss how it manifests when there is a notable parameter dispersion between two connected devices. In the second section, we consider MTJs within a stochastic framework, highlighting the capabilities of CMTJ to simulate stochasticity, particularly composite magnetic noise in MTJs. Both sections share a common focus on the device itself and the modelling approach used in CMTJ.

Magnetic Tunnel Junctions

Modern magnetic tunnel junctions are composed of two FM layers, typically made of CoFeB, or Fe layers separated by an oxide, typically MgO. The operation of such a device relies on the quantum-mechanical tunnelling of the electrons from one FM layer to another through the insulating oxide barrier. Tunnelling depends on the matching of the majority and minority bands.

W. Butler showed from DFT calculations¹⁰⁷ how symmetry-dependent spin filtering leads to giant tunnelling magnetoresistance (TMR) along high-symmetry interfaces¹⁰⁸. In summary, the symmetry group in the Brillouin zone along [001] is $4mm$, with the cubic crystal direction [001] denoted as Δ . This group has four representations (two one-dim and two two-dim), of which the symbols of particular significance are Δ_1 (spd)¹⁰⁹, Δ_5 (p_x, p_y, d_{xy}), and Δ'_2 (d_{xy}). These form a specific band structure along the Δ line $\Gamma[000] \rightarrow H[001]$ in which they turn out to be the only bands that cross the Fermi level. In particular, in a spin-resolved band structure, one can see that Δ_1 crosses the Fermi level only for the majority carriers and has the slowest decay rate. Therefore, if two Fe electrodes are in parallel, the majority spin Δ_1 continues through the barrier from one electrode to the other. When the two electrodes are in opposite magnetisation, there are no Δ_1 states available to carry the tunnelling current. This is enough to account for the giant TMR in FM/MgO/FM structures (other bands, Δ_5 and Δ_2 have Tunnelling Density of States (TDOS) that decay orders of magnitude faster in

¹⁰⁷ Butler, X.-G. Zhang, et al., “Spin-dependent tunneling conductance of Fe | MgO | Fe sandwiches”.

¹⁰⁸ in the original work it was Fe/MgO [001] which we follow here as well

¹⁰⁹ the brackets indicate the basis

the direction of the opposite electrode). The picture of the highly symmetric crystalline MgO barrier can be contrasted with that of the amorphous one of the Al-O barriers, where other Bloch states also carry the tunnelling current, effectively reducing the total spin polarisation and causing incoherent tunnelling. In fact, some of the first significant TMR ratios at room temperature were demonstrated by Miyazaki and Tezuka¹¹⁰ on the amorphous barrier junctions Fe/Al₂O₃/Fe, and amounted to 18%. In 2004, Parkin et al.¹¹¹ and Yuasa et al.¹¹², independently, replaced that amorphous barrier with magnesium oxide and showed TMR ratios of 220% in Fe/MgO/Fe MTJs at room temperature. Later, in 2008, Ikeda et al. reported a record-breaking TMR ratio of 604% at room temperature for the CoFeB/MgO/CoFeB pseudo-spin valve structure¹¹³.

Drawing from the conclusions above, we would ideally like any tunnel barrier to be as thin as possible, which would mean the strongest tunnelling current and the smallest resistance due to the higher Δ_1 TDOS at the opposing electrode. However, when we make the barrier too thin, we at the same time remove the symmetric bands, which perform spin filtering, i.e. the discrepancy between the majority Δ and minority Δ , meaning the majority spin carriers and the minority spin carriers; existence of which is indispensable to the TMR effect.

An important trend in modern MTJ design tends to lean towards fabrication of the perpendicular anisotropy MTJs¹¹⁴. In a general case, we have two components of the magnetisation energy representing the interplay between the magnetic anisotropy energy and the demagnetisation energy. We could write it down in a simplified form as¹¹⁵:

$$E = -N \frac{M_s^2}{2\mu_0} V + K_{\text{perp}} V \quad (77)$$

with M_s expressed here in Tesla, V as the volume, N being the demagnetisation factor (in a simplified expression of that of (34)), and K_{perp} denoting the perpendicular magnetic anisotropy energy density, expressed in J/m³. Given the expression (77), we can also consider the stability of MTJ. The energy barrier between the parallel and antiparallel states, which keeps the magnetisation in a given state, is given by $\Delta = E/k_b T$, where k_b is the Boltzmann constant, and T is the temperature. The reason why perpendicular MTJs are desired is that there exists an asymmetry between the energy barrier that keeps the state stable, E_b^{stab} and the barrier that is required during current-induced switching, the switching current being proportional to a switching energy barrier E_b^{sw} : $I_c \sim \alpha E_b^{\text{sw}}$ ¹¹⁶. In the in-plane case, the in-plane magnetic anisotropy is the stabiliser of the state, whereas the demagnetisation energy is the one that has to be overcome for switch. On the other hand, in the perpendicular case, the demagnetisation and magnetic anisotropy energy work along the perpendicular direction, so $E_b^{\text{sw}} = E_b^{\text{stab}}$. The critical current for switching the in-plane case is thus larger than the one usually required to switch a

¹¹⁰ Miyazaki and Tezuka, "Giant magnetic tunneling effect in Fe/Al₂O₃/Fe junction".

¹¹¹ S. S. P. Parkin, C. Kaiser, et al., "Giant tunnelling magnetoresistance at room temperature with MgO (100) tunnel barriers".

¹¹² Yuasa, Nagahama, et al., "Giant room-temperature magnetoresistance in single-crystal Fe/MgO/Fe magnetic tunnel junctions".

¹¹³ Ikeda, J. Hayakawa, et al., "Tunnel magnetoresistance of 604% at 300K by suppression of Ta diffusion in CoFeB/MgO/CoFeB pseudo-spin-valves annealed at high temperature".

¹¹⁴ Ikeda, Miura, et al., "A perpendicular-anisotropy CoFeB-MgO magnetic tunnel junction"; Yakata, Kubota, et al., "Influence of perpendicular magnetic anisotropy on spin-transfer switching current in CoFeB/MgO/CoFeB magnetic tunnel junctions".

¹¹⁵ Igarashi, Jinnai, et al., "Temperature dependence of the energy barrier in X/1X nm shape-anisotropy magnetic tunnel junctions".

¹¹⁶ J. Hayakawa, Ikeda, et al., "Current-Driven Magnetization Switching in CoFeB/MgO/CoFeB Magnetic Tunnel Junctions".

perpendicular junction. How can we achieve a perpendicular junction experimentally? It turns out that making the FM layers (CoFeB) thinner orients the magnetisation from the in-plane to the out-of-plane (perpendicular) direction, but only to some extent¹¹⁷. However, making the layers too thin may eventually result in a superparamagnetic state. Depending on whether the sample was deposited and annealed (1.65 nm - 1.52 nm), mid-range thicknesses appear adequate. As seen in (77), the magnetic anisotropy energy can also be regulated by volume; thus, the diameter of the junction plays a crucial role in the thermal stability of the perpendicular MTJ¹¹⁸. With that, we can manipulate the demagnetisation energy by engineering an adequate demagnetisation tensor, rather than simply manipulating the interfacial, i.e., perpendicular anisotropy¹¹⁹. Here, the problem is that if we make the diameter smaller, the interfacial anisotropy term drops (assuming that the demagnetisation stays the same), and the barrier decreases. Therefore, we have indeed achieved better switching at the cost of lower stability. However, one can engineer the demagnetisation tensor differently by adjusting the thickness-to-diameter ratio, which, when done properly, maintains low switching currents and a larger energy barrier.

There is yet another flavour of MTJs, the stochastic MTJs (sMTJs), where one tunes the energy barrier to achieve fast fluctuation switching and small relaxation time, which translate to fast computation. Kanai et al.¹²⁰ showed that having in-plane MTJs (IMA-MTJs) as opposed to perpendicular MTJs (PMA-MTJs) seems beneficial for probabilistic bit (pbit) applications, because the time constants of the in-plane can be two orders of magnitude lower than for PMA-MTJs, although the energy barrier was set to be the same for those two. This is because in PMA-MTJs $\Delta \propto H_k^{\text{eff}}$ ¹²¹ with a trade-off of $\nabla E \propto H_k^{\text{eff}}$, while in IMA-MTJs $\Delta \propto H_{k,\text{in}}$ ¹²² but $\nabla E \propto H_k^{\text{eff}}$, with H_k^{eff} being the effective anisotropy field. ∇E denotes the energy gradient as a function of spatial coordinates. For the PMA-MTJs, we make a trade-off between setting the barrier high and making an easy path between two states, while in IMA-MTJs those two can be set independently.

In one of the following sections we discuss MTJs operating as spin-torque oscillators (STOs). To achieve stable auto-oscillation of the magnetisation in an MTJ, the current applied to the junction needs to be below the switching threshold but above a current value where the damping is compensated. If this condition is met, the resulting stable auto-oscillation of magnetisation induces resistance oscillation, and the system can act as an AC voltage signal generator in a GHz regime. Typically, STOs require the presence of the external magnetic field to tilt the free layer magnetisation relative to the magnetisation of the polarising (reference) layer, but zero-field operation is also possible as shown by Skowroński et al.¹²³ (canted PMA in the free layer, IMA reference layer) or Fang et al.¹²⁴ (IMA free layer and PMA reference layer). The critical current threshold for auto-oscillation in STOs with a PMA free layer, in the absence of field-like torque, can be given after Taniguchi et

¹¹⁷ Ikeda, Miura, et al., “A perpendicular-anisotropy CoFeB–MgO magnetic tunnel junction”.

¹¹⁸ Igarashi, Jinnai, et al., “Temperature dependence of the energy barrier in X/1X nm shape-anisotropy magnetic tunnel junctions”.

¹¹⁹ Jinnai, Watanabe, et al., “Scaling magnetic tunnel junction down to single-digit nanometers—Challenges and prospects”.

¹²⁰ Kanai, K. Hayakawa, et al., “Theory of relaxation time of stochastic nanomagnets”.

¹²¹ effective perpendicular anisotropy

¹²² in-plane anisotropy

¹²³ Skowroński, Stobiecki, et al., “Zero-Field Spin Torque Oscillator Based on Magnetic Tunnel Junctions with a Tilted CoFeB Free Layer”.

¹²⁴ Fang, Feng, et al., “Zero-field spin transfer oscillators based on magnetic tunnel junction having perpendicular polarizer and planar free layer”.

al.¹²⁵:

$$j_c = \frac{4\alpha e M_s t_{\text{FM}}}{\hbar P \lambda} (H_{\text{appl}} + H_{\text{K,eff}}) \quad (78)$$

where t_{FM} is the thickness of the free layer and $H_{\text{appl}}, H_{\text{K,eff}}$ are the external magnetic field applied along the z -axis and the effective PMA field, respectively.

Electrical coupling

Introduction to inter-device coupling

The coupling of spintronic devices is one of the fundamental mechanisms through which computation is carried out in a spintronic system. Common-place methods include coupling via the electrical connection of the MTJs, static coupling due to dipolar interaction, and coupling mediated through the propagation of the spin waves.

Electrical coupling has been extensively explored in a myriad of applications. First, Tsunegi et al.¹²⁶ experimentally scaled electrically coupled oscillators, demonstrating that networks of up to 8 STOs exhibit increased emitted power and Q factor. They also showed that the coupled STOs retain in-phase synchronisation over longer time scales, proving the robustness of the synchronised state against thermal fluctuations. In 2021, Sharma et al. demonstrated a series and a parallel STO array and proposed their use for WiFi band transmission and energy harvesting¹²⁷. Gibeault et al. presented the programmable electric coupling between stochastic MTJs¹²⁸ while Romera et al.¹²⁹ showed a practical implementation of electrically coupled STOs for a classification task.

Another class of solutions uses VCMA to control the strength of the coupling. Yun et al.¹³⁰ have designed a device based on the Pt/Co/GdO stack, where a gating region (a cobalt layer exposed to GdO) had a tunable anisotropy through oxygen ion migration in GdO. Such a mechanism has effectively coupled the competition between DMI (when the gated region is in-plane, causing the neighbouring regions with PMA to exhibit chiral texture) and tunable exchange coupling to the anisotropy of that gated region. The authors showed that it is possible to construct an Ising machine based on such a device.

The dipolar coupling, being a static interaction, is primarily dependent on the distance between the devices. Still, we can control how much it affects each device by manipulating with other field terms in the effective field. First, Kanao et al.¹³¹ demonstrated a basic case of reservoir computing with nanomagnets. The array of STOs connected to a linear layer with trainable weights was shown to perform simple short-term memory and parity check tasks. Nomura et al.¹³² included the VCMA control in a similar array of STOs, which opened the way to computing simple logic operations: AND/X-OR/OR.

¹²⁵ Taniguchi, Arai, et al., “Theoretical Study of Spin-Torque Oscillator with Perpendicularly Magnetized Free Layer”.

¹²⁶ Tsunegi, Taniguchi, et al., “Scaling up electrically synchronized spin torque oscillator networks”.

¹²⁷ Sharma, Mishra, et al., “Electrically connected spin-torque oscillators array for 2.4 GHz WiFi band transmission and energy harvesting”.

¹²⁸ Gibeault, Adeyeye, et al., “Programmable electrical coupling between stochastic magnetic tunnel junctions”.

¹²⁹ Romera, Talatchian, et al., “Binding events through the mutual synchronization of spintronic nano-neurons”.

¹³⁰ Yun, K.-J. Lee, and Lim, “Critical switching current density induced by spin Hall effect in magnetic structures with first- and second-order perpendicular magnetic anisotropy”.

¹³¹ Kanao, Suto, et al., “Reservoir Computing on Spin-Torque Oscillator Array”.

¹³² Nomura, Furuta, Tsujimoto, Kuwabiraki, Peper, et al., “Reservoir computing with dipole-coupled nanomagnets”; Nomura, Furuta, Tsujimoto, Kuwabiraki, Samura, et al., “Randomly generated node-state-update procedure for dipole-coupled magnetic reservoir computing with voltage control of the magnetism”.

Electrical coupling – experimental setup and observations

In this section, we explore the concept of electric coupling primarily within a simulation context, with a slight experimental backdrop. The discussion draws heavily from the work by Rzeszut, Mojsiejuk, et al. (“Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions”), originally published in 2023, but substantially revised thereafter. Relevant passages from that work are cited verbatim when appropriate; however, readers are encouraged to consult the original text for detailed implementation information.

Our study begins with an experimental setup of a basic injection locking system through an external generator signal. The sample is an MTJ Si /SiO₂ / buffer / (4) Ru / (6) IrMn / (2.5) CoFe / (0.8) Ru / (2.5) CoFeB / (1) MgO / (1.8) CoFeB / (1) MgO / (3) Ru / (5) Ta / (2) Ru / (3) Pt with bracketed thicknesses expressed in nanometers. The presence of Ru indicates that the reference CoFeB layer is strongly pinned to the SAF, as well as the MgO cap, which is known to enhance perpendicular magnetic anisotropy¹³³. A similar structure has been shown to produce a decent STO in the work of Skowroński et al.¹³⁴

First, the ability of the MTJ to synchronise needs to be validated. Therefore, junction parameters are fitted to the experimental FMR spectrum following the procedure described in [Bayesian optimisation](#) – result of that fit is presented in Fig.19a). Then, the same junction is synchronised to half of the generator frequency, which, following the experiment, was also 4 GHz – as per Fig.19b). The ratio $\Delta j / j$, that is, the ratio of AC density to DC density, plays a significant role in the injection locking simulation. As shown in Fig.20 the increase in the locking range correlates with the increase in that ratio. The minimal current modulation ratios required for injection locking (0.1-0.2) agree with theoretical observations¹³⁵. Having verified the basic synchronisation case, we are now ready to discuss the electric coupling where we will compare the numerical modelling with the experimental result. In contrast to dipole-based coupling, no magnetic effects participate in the coupling mechanisms of the oscillators that are electrically coupled. Although that dipole interaction is typically considered long-range separating the two oscillators apart with a distance of a couple μm is usually sufficient to isolate them magnetically – in the experiment it was taken to be at least 600 μm . A typical schematic illustrating possible electrical connections of the MTJ (both in series and in parallel) is given in Fig.21. From now on, given an in-series connection of two MTJs, we will refer to the first MTJ in the connection as *L* (left), and the second as *R* (right). Fig.22(a-c) illustrates the spectrum generated by *L* (a) and *R* (b) individually, when they were disconnected, and (c) shows their joint signal collected when measured in series. All subplots (a-c) share the same power scale. First, comparing (a) and (b), *L* has a much narrower oscillation linewidth than *R* throughout the external field scan. Second,

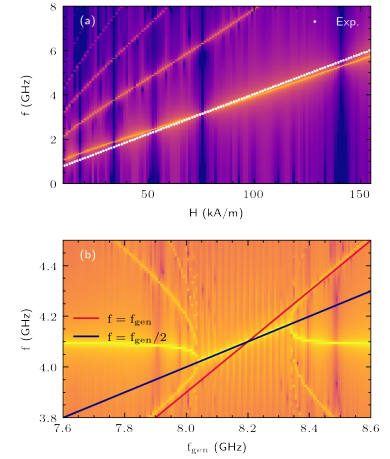


Figure 19: Simulation of the injection locking to the external generator signal. (a) Approximate fit to the experimental FMR. (b) The locking spectrum of the same MTJ. Synchronisation occurs at half the generator frequency.

¹³³ Kubota, Ishibashi, et al., “Enhancement of perpendicular magnetic anisotropy in FeB free layers using a thin MgO cap layer”; Diény and Chshiev, “Perpendicular magnetic anisotropy at transition metal/oxide interfaces and applications”.

¹³⁴ Skowroński, Chęciński, et al., “Microwave magnetic field modulation of spin torque oscillator based on perpendicular magnetic tunnel junctions”.

¹³⁵ Slavin and Tiberkevich, “Nonlinear Auto-Oscillator Theory of Microwave Generation by Spin-Polarized Current”.

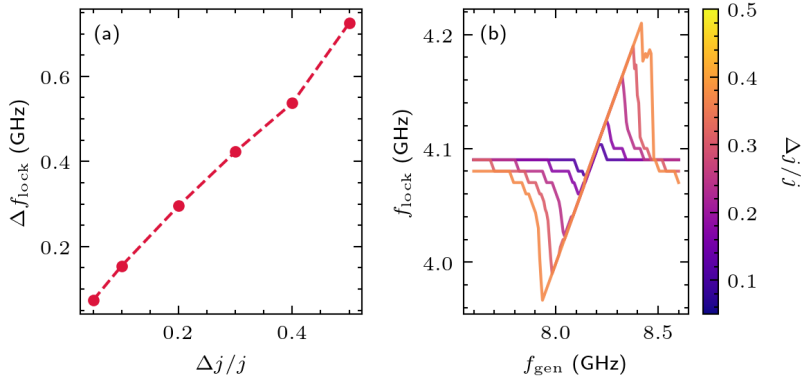


Figure 20: Dependency of the locking range on the amplitude of the excitation. The MTJ simulated here is the same as the one optimised in Fig.19. (a) Locking range bandwidth depending on the $\Delta j/j$ ratio. (b) Line of maximum resonance under different excitation amplitude $\Delta j/j$.

in the spectrum of R there is a well-defined oscillation line starting at 3 GHz at 80 kA/m.

This broad auto-oscillation pattern of R is retained in the in-series configuration S , shown in (c), although it becomes noticeably narrower compared to (b). In addition, the thin oscillation line starting at 3 GHz from (b) also appears in (c). Moreover, a distinct narrow spectral line emerging near 130 kA/m is observed in panel (c), which is absent in both individual spectra of L (a) and R (b).

Fig.22d) shows the lines of maximum power for each of the spectra, with an additional synthetic line created by averaging individual signals of L and R (grey line). In the region starting at about 135 kA/m L and R start to diverge strongly and at that point S closely follows R up to approximately 145 kA/m, beyond S diverges both from R and L (blue), as well as from their averaged signal (grey).

To clarify the relationship between L , R and S we fitted a trend line to L signal in Fig.22d), as it is the least affected by the in-series connection. A linear trend line is defined as: $f = kH + H_0$, where k is the slope, and H_0 is the intercept. Using that trend line, we subtract it from each of the main oscillating frequency lines in Fig.22d). The resulting characteristics visible in Fig.22e) are:

1. two points of divergence occur where R deviates from L , i.e. the red line moves away from zero. The first occurs at about 90 kA/m; a second, larger divergence appears at 130 kA/m, preceded by a brief synchronisation. This demonstrates that, individually, R and L do not oscillate with the same nominal frequencies in ranges (90, 125) and (130, 155) kA/m.
2. at 145 kA/m lines move further away from L -trend line (blue), including the signal S - $(L+R)/2$. This means that beyond 145 kA/m the maximum power signal of the in-series configuration no longer aligns with the individual or averaged responses of L and R .

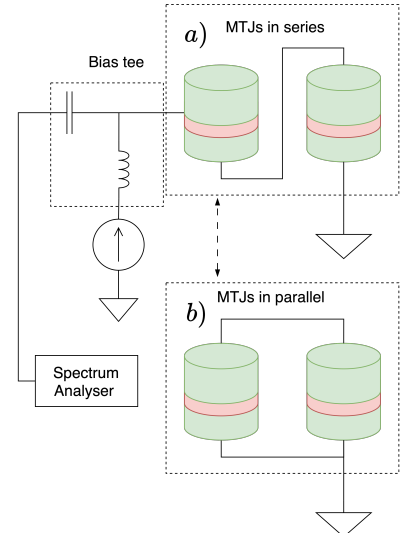


Figure 21: Measurement setup and available arrangements for electric coupling: (a) in-series coupling, and (b) parallel connection coupling.

Given these experimental observations, we can proceed to the numerical analysis of some of the synchronisation aspects observed in Fig.22.

Numerical modelling of electrical in-series coupling

The numerical reproduction of this experimental outcome derives from the work of Taniguchi et al.¹³⁶ where the authors introduce a simple model for electrical synchronisation in two configurations: in series and parallel. The total current fed to consecutive junctions $i + 1$ depends on the free magnetizations $\mathbf{m}$ and the reference layers $\mathbf{p}$ of the i_{th} and $i + 1_{th}$ junction:

$$j_c(t) = j_0(t) + \chi j_0(t)(\mathbf{m}_i \cdot \mathbf{p}_i + \mathbf{m}_{i+1} \cdot \mathbf{p}_{i+1}) \quad (\text{series}) \quad (79)$$

$$j_c(t) = j_0(t) + \chi j_0(t)(\mathbf{m}_i \cdot \mathbf{p}_i - \mathbf{m}_{i+1} \cdot \mathbf{p}_{i+1}) \quad (\text{parallel}) \quad (80)$$

where $j_0(t)$ is the value of the uncoupled current density and χ is the unitless coupling strength. Typically χ is constrained within the (0, 1) interval¹³⁷. In our simulations, we usually fix it to $\chi = 0.3$, but show that it can be as low as $\chi = 0.1$ under certain values of β (see the later discussion and Fig.26 for more details on the impact of χ and β). The situation originally considered in equation (79) supposes that j_c is the total current flowing in the circuit and j_0 is simply a theoretical baseline current. However, in the experiment, the voltage source response is not instantaneous as a result of the parasitic capacitance and inductance. Therefore, in the following analysis we assume that $j_c(t)$ is the current induced in the second (R) STO, while the input to the first MTJ, (L), is kept at $j_0(t)$. For completeness, we show in the Appendix, [Coupled current for the in-series configuration of STOs](#), that this assumption does not impact, up to a choice of constant χ , the result of the subsequent analysis. According to our assumption, as illustrated in Fig.23b,e,g), the peak associated with the first MTJ in the connection remains fixed while the resonance of the second junction is pulled toward it. This behaviour is the archetypal of injection locking scenarios. As a point of further note, we observe in Fig.23f) that the phase difference between two oscillating junctions seems to be approaching $\Phi_{\text{diff}} = 180$, indicating that $\chi > 0$ leads to in-phased synchronisation, while $\chi < 0$ aligns the frequencies, but causes out-of-phase oscillation. This is in contrast to the in-phase synchronisation shown in panel (c).

After examining a simple base case, we proceed to more complex conditions illustrated in Fig.22. The two MTJs of a connected pair are not identical, although they might have come from the same wafer. Therefore, in our discussion below, unlike prior studies¹³⁸, we assume that the connected devices are not identical and vary the anisotropy constant and magnetisation saturation to model the parameter dispersion. Taking anisotropy as an example: we denote the anisotropy of the left MTJ and the right MTJ by $K_{u,L}$, and $K_{u,R}$, respectively. The $K_{u,R}$ is then parametrized with a ΔK (a variation in

¹³⁶ Taniguchi, Tsunegi, and Kubota, “Mutual synchronization of spin-torque oscillators consisting of perpendicularly magnetized free layers and in-plane magnetized pinned layers”.

¹³⁷ Arun, Gopal, et al., “Influence of Field-Like Torque in Synchronization of Spin Torque Oscillators”; Taniguchi, Tsunegi, and Kubota, “Mutual synchronization of spin-torque oscillators consisting of perpendicularly magnetized free layers and in-plane magnetized pinned layers”.

¹³⁸ Arun, Gopal, et al., “Influence of Field-Like Torque in Synchronization of Spin Torque Oscillators”; Taniguchi, Tsunegi, and Kubota, “Mutual synchronization of spin-torque oscillators consisting of perpendicularly magnetized free layers and in-plane magnetized pinned layers”.

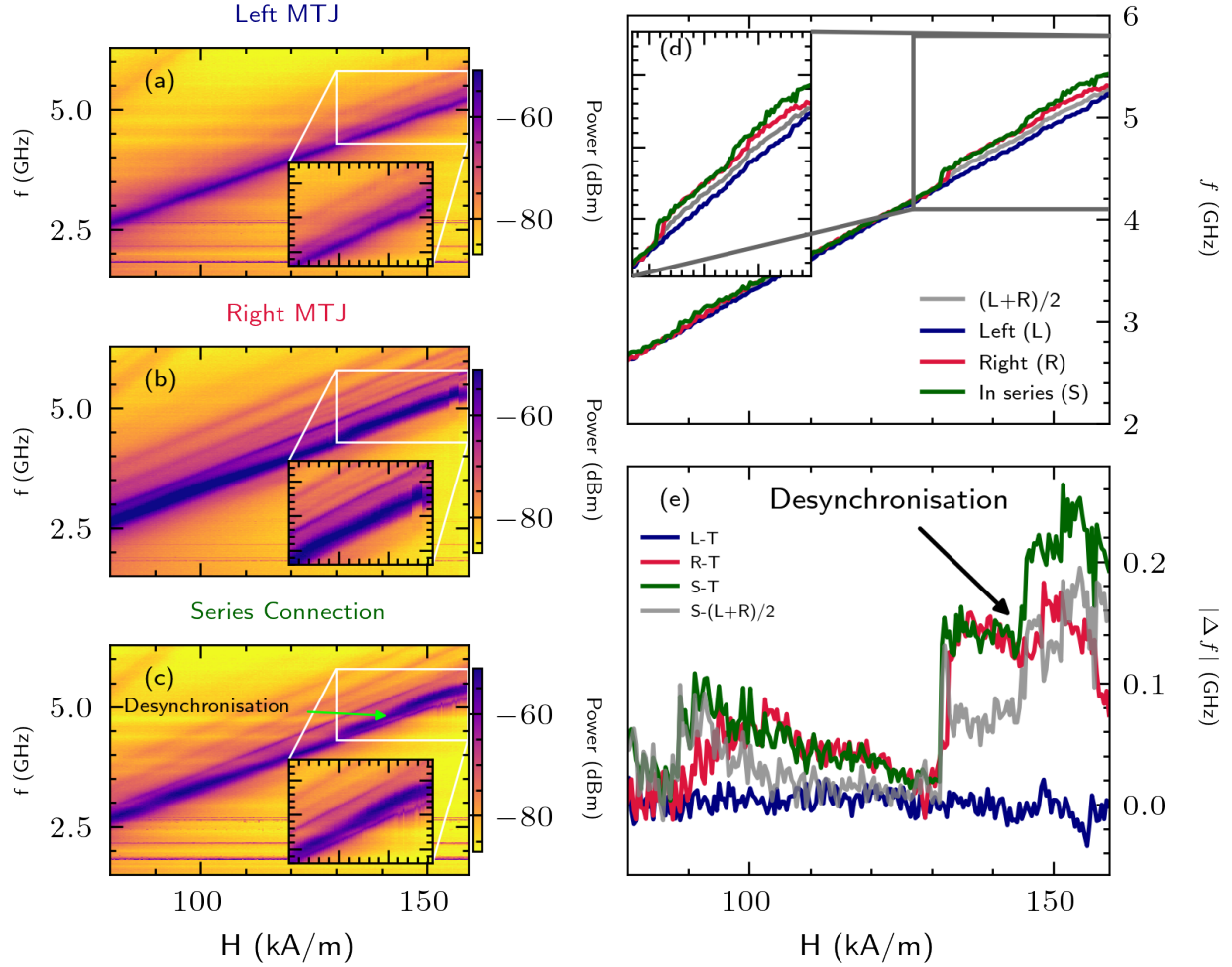


Figure 22: Experimental electrical frequency synchronisation and desynchronisation of two serially connected MTJs. The individual spectrum of left L (a), right R (b) MTJ individually and when connected in-series (c). (d) Main oscillating frequency of the L , R and in-series systems, with a zoom of the desynchronisation region. (e) the synchronisation and desynchronisation ranges of L and R and in-series (S) signal respective to the trend line (T) fitted to the L signal. L signal should, in theory, be least affected by the in-series electrical connection, and therefore is used as a reference. The arrow marks the spot where the R signal diverges from L , and S diverges both from L and R . As shown, up to about 145 kA/m, the S signal follows R closely and then settles to oscillate with its own distinct frequency. In the (d) and (e) panels, we include an average of L and R signals, $(L+R)/2$, for reference. In (e) that signal is subtracted from (S) for comparison. The figure and caption were adapted from Rzeszut, Mojsiejuk, et al. ("Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions").

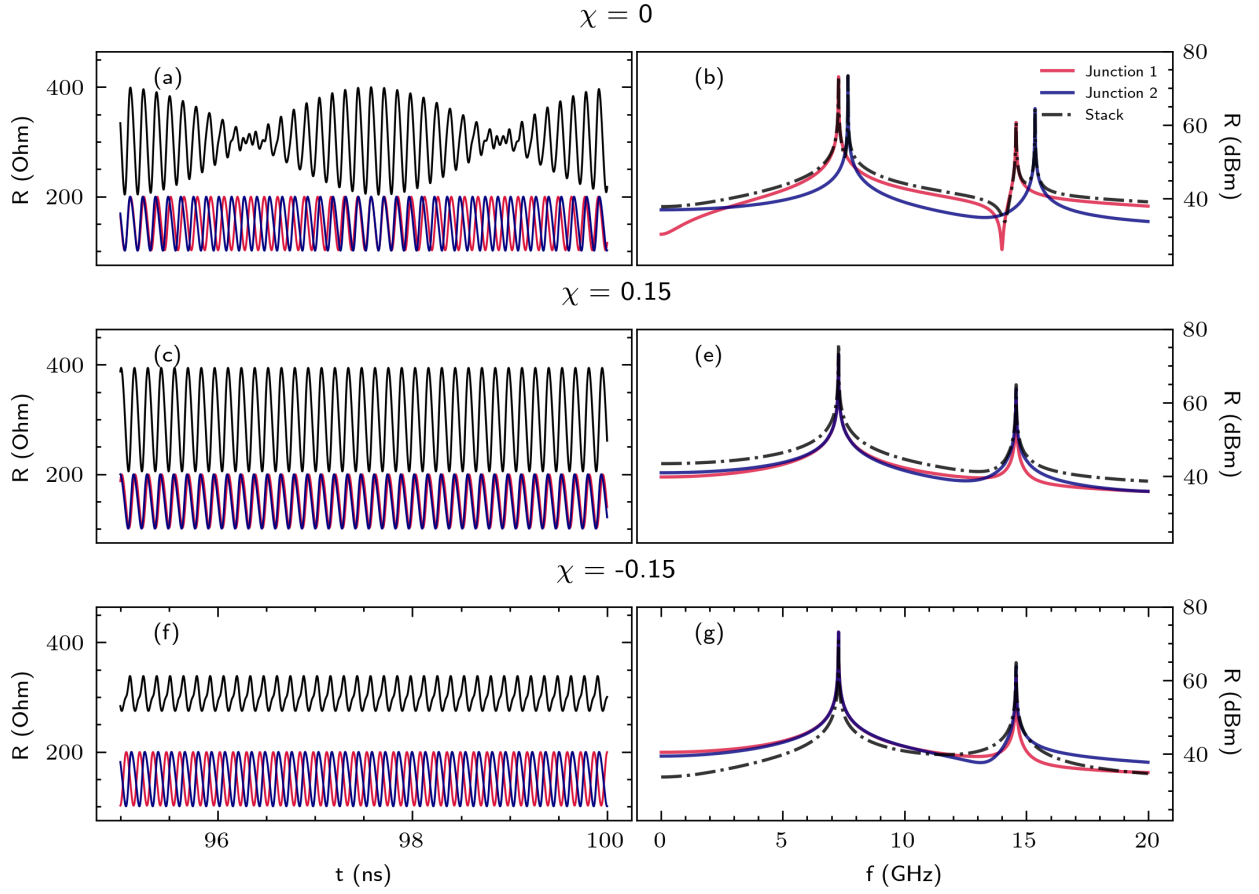


Figure 23: Three different coupling values for the in-series electric coupling. The left column shows the time series of serially connected MTJs and their individual time series. The right column presents the resonance spectrum of the stack and individual MTJs up to 20 GHz. Negative coupling causes phase synchronisation to settle at $\phi_{\text{diff}} = 180^\circ$, which may not be desirable, and the resulting resistance decreases. Comparing (b) with (e) and (g) we see that the blue spectrum of the second MTJ is *pulled* towards the resonance mode of the first MTJ which stays fixed. In that sense, electric coupling can be thought of as a case of injection locking.

magnetic anisotropy) parameter such that:

$$K_{u,R} = K_{u,L}(1 + \Delta K/100) \quad (81)$$

where the relative change in anisotropy ΔK is expressed in percentages and is allowed to vary between $(-10\%, 10\%)$. In other words, we keep the anisotropy of L fixed, and allow the anisotropy of R vary up to 10% respective to L . For assessing synchronisation quality, we use three metrics:

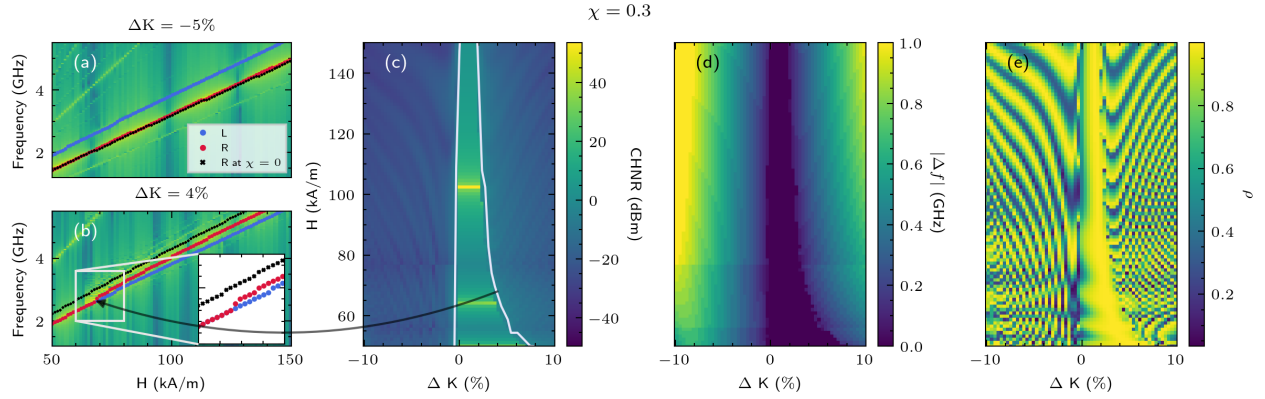


Figure 24: Simulated desynchronisation of serially coupled MTJs in function of the anisotropy change ΔK of the (R) MTJ in-series. Panels (a) and (b) show two sample spectra for R junction taken at $\Delta K = -5\%$ (a) and $\Delta K = 4\%$ (b). The arrow leads from the desynchronisation boundary at ≈ 68 kA/m and $\Delta K = 4\%$ in (c) to a precise place of desynchronisation in the spectrum of (b), with the desynchronisation moment placed in zoom in (b). (a-b) The blue marker follows the line of the main oscillating frequency of L , and the red marker tracks the one for R . The black dots show the main oscillating frequency line of R when the two MTJs are decoupled, i.e. $\chi = 0$. Otherwise, simulations performed assuming $\chi = 0.3$ and $\beta = 0.5$. (d) Frequency difference in (GHz) between the L and R junctions. For $\Delta K > 0$, i.e. $K_{u,R} > K_{u,L}$ there is a desynchronisation boundary where the L and R junctions start to fall out of synchronisation, i.e. leave the dark blue region (white line in (c) denotes that desynchronisation boundary H_{thres}). (c) illustrates that the dark-blue region from (d) is characterized by a large CHNR, supporting the evidence for strong synchronisation. The asymmetry between the frequency de-synchronisation fields for $\Delta K > 0$ and $\Delta K < 0$ arise from the particular arrangement of the (L) and (R) MTJs in-series, and is a direct consequence of smaller frequency changes due to current change. High order parameter values (e) confirm a good degree of synchronisation within the desynchronisation boundary. The figure and caption were adapted from Rzeszut, Mojsiejuk, et al. (“Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions”).

1. the cross-Harmonic-to-Noise (CHNR) ratio measuring spectral overlap between the two oscillating MTJs. The cross-Harmonic-to-Noise ratio is defined as:

$$\text{CHNR} = \frac{\sum_{\forall n > 0, n \in \mathbb{Z}} A_{nf_L}^R}{\sum_{f' \neq kf_L, \forall k > 1, k \in \mathbb{Z}} A_{f'}^R} \quad (82)$$

where f_L is the primary oscillating frequency of the first MTJ in-series. $A_{f_i}^R$ denotes the values taken from the frequency spectrum of the second MTJ in-series, that is, the amplitude at a frequency f_i .

2. the order parameter, which also quantifies the phase alignment. It serves as an additional measure of uniformity of synchronisation and is defined by the following equation¹³⁹:

$$\rho = \frac{1}{2} \left| \sum_i \frac{c_i}{|c_i|} \right| \quad (83)$$

¹³⁹ Kanao, Suto, et al., “Reservoir Computing on Spin-Torque Oscillator Array”; Acebrón, Bonilla, et al., “The Kuramoto model”.

where $c_i = m_x^i - im_y^i$ with m_x and m_y as the x and y components of the magnetization. The closer ρ approaches 1, the better the order of synchronisation.

3. and the absolute frequency difference between the dominant peaks of the two STOs: $|f_L - f_R|$

Having two junctions connected in-series, the magnetic field angle is set at $\theta = 25^\circ$, the same as in the experiment. For every field magnitude and ΔK value, we note the frequency difference of the primary modes between the first and second MTJ, which results in Fig.24d).

We observe that synchronisation occurs more easily when the anisotropy of the second MTJ is slightly larger ($\Delta K > 0$). However, beyond a threshold, increasing ΔK leads to desynchronisation, with the desynchronisation boundary influenced by the coupling constant χ . A similar desynchronisation boundary occurs if we move vertically, increasing the field. At some H_{thres} , marked with a white line in Fig.24c), there is a transition from the synchronised state to the desynchronised state. Fig.24c) shows the CHNR where the transition to the desynchronised state is connected with an abrupt nonharmonic oscillation of the second MTJ, which results in frequency splitting similar to the signal observed experimentally in Fig.22(c-d) – numerical equivalent presented in Fig.24b). As in the experiment, the main oscillating mode follows neither L nor R modes exactly. Finally, the order parameter is shown in Fig.24e), where for the synchronised region, we clearly observe swaths of large ρ values close to 1, which is in agreement with the results in Fig.24(c-d).

Following the analysis first shown for identical junctions by Arun et al.¹⁴⁰, we also investigate the influence of the field-like torque β scaling in the field-like torque term in our notation: $a_j \beta \tilde{\mathbf{M}}_l(\mathbf{p})$. Consistently with the aforementioned work, we observe that the presence of the synchronised state is essentially dependent on the strength of the β scaling. Fig.26 demonstrates how the desynchronisation threshold shifts for $\Delta K > 0$ both with the coupling strength χ and the field-like torque scaling β . There are two key observations from that figure: the first is that the induction of a larger field-like torque works in a similar fashion as increasing the coupling strength, i.e., it facilitates synchronisation, which results in broadening of the synchronised region, both across the field range (vertically) and also across the ΔK (horizontally), suggesting that one could be potentially compensated by the other. Secondly, we see that there is a distinct peak when β , which means that the largest field locking range does not need to occur at $\Delta K = 0$, which is when the two junctions are identical.

As evident from the discussion in [Introduction to inter-device coupling](#), VCMA seems to be an overarching mechanism to enhance coupling dynamics. Inspired by this, we used the existence of the desynchronisation threshold at a particular $K_{u,R}$ to induce the synchronised and desynchronised state be-

¹⁴⁰ Arun, Gopal, et al., “Influence of Field-Like Torque in Synchronization of Spin Torque Oscillators”.

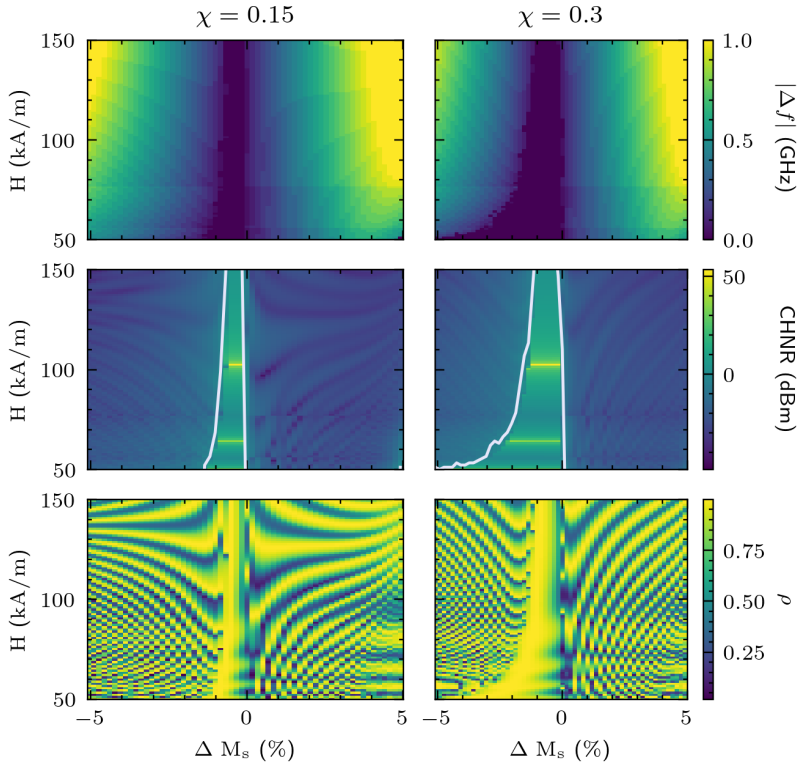


Figure 25: The impact of varying M_s and the coupling χ parameter. The synchronisation region grows with larger χ , but also expands for lower ΔM_s variations respective to L , as it has the exact opposite effect as increasing ΔK_u . ΔM_s is defined analogously to ΔK_u . The figure and caption were adapted from Rzeszut, Mojsiejuk, et al. ("Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions").

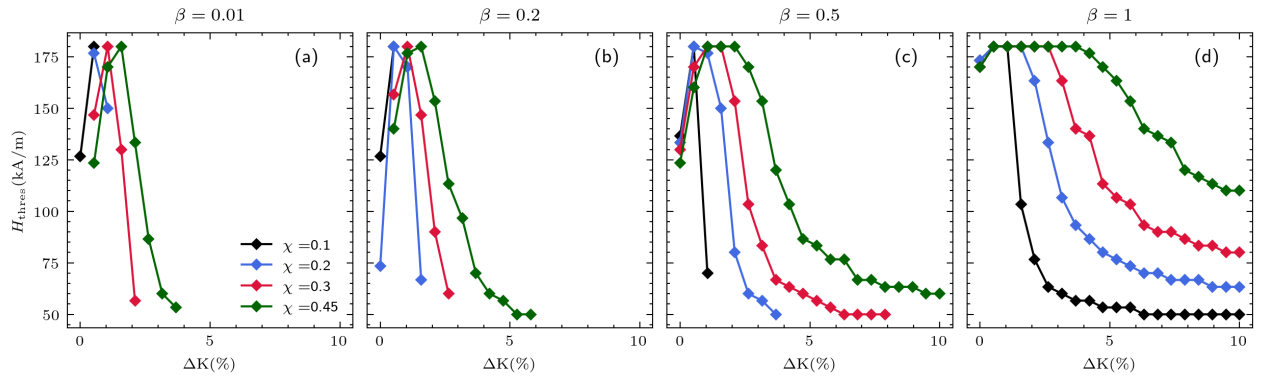


Figure 26: Effect of field-like torque scaling β and the magnitude of the electric coupling χ on the desynchronisation threshold H_{thres} in function of the anisotropy change ΔK of the (R) MTJ in-series. Case (a) corresponds to $\beta = \alpha_G$. A larger β widens the synchronisation range, similar to the effect of increasing the coupling constant χ . The external field range is capped at 175 kA/m. Plotted points denote only states that were synchronised at some field, a lack of a marker means that the state either did not start in a synchronised state at lower field values or it has already desynchronised. The figure and caption were adapted from Rzeszut, Mojsiejuk, et al. ("Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions").

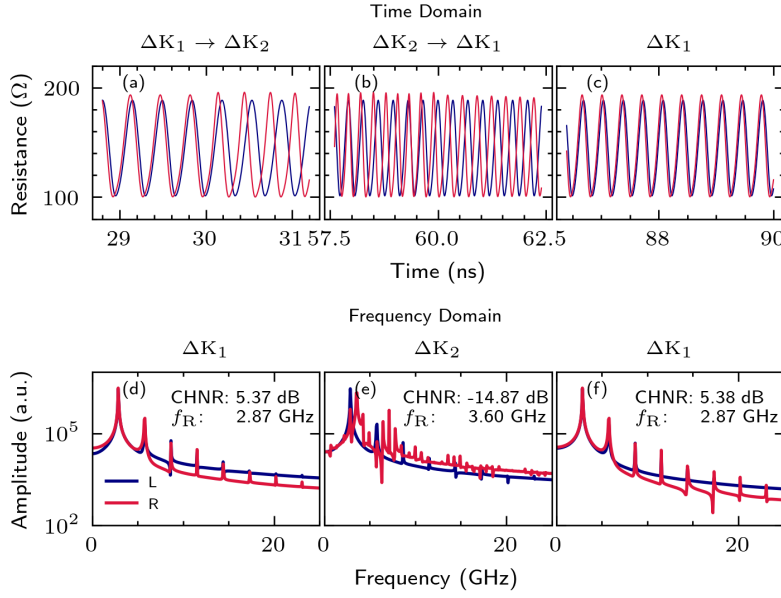


Figure 27: Simulated VCMA-controlled synchronisation of and in-series MTJ system. The VCMA controller switches from ΔK_1 to ΔK_2 first, then back to ΔK_1 . (a) shows the magnetoresistance during transition at 30 ns from ΔK_1 to ΔK_2 , (b) at 60 ns from ΔK_2 back to ΔK_1 and (c) gives last couple nanoseconds from a synchronised state in ΔK_1 after the final switch. Frequency spectra corresponding to states ΔK_1 , ΔK_2 and ΔK_1 (after the transition from ΔK_2) are shown in (d-f) respectively. Simulated for $\chi = 0.15$, $\Delta K_1 = 4\%$, $\Delta K_2 = 20\%$, $H_{\text{ext}} = 80 \text{ kA/m}$. The figure and caption were adapted from Rzeszut, Mojsiejuk, et al. (“Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions”).

tween two STOs coupled in the in-series configuration. Fig.27 illustrates this mechanism: the increase in anisotropy of the (R) MTJ from ΔK_1 to ΔK_2 causes the two STOs to desynchronise, but reverting the anisotropy back to ΔK_1 leads to a synchronised state again. Although the synchronised signal is easily detectable electrically because of an increase in amplitude, and a relatively small voltage is sufficient to switch the pair out of the synchronised state, the practical implementation of VCMA-based synchronisation control presents several challenges. The proposed structure is viable when the magnetisation dynamics is driven by a spin current that originates from spin-orbit coupling (SOT) rather than spin filtering (STT)¹⁴¹. In this configuration, an additional gate can be used to modulate the magnetic anisotropy via VCMA. Although devices based on ionic migration can exhibit significant VCMA¹⁴², they are limited by a lower modulation speed and degradation over time. In contrast, devices based on MgO/FM can operate at a rate below 1 ns¹⁴³.

Dipolar coupling

Another mode of interdevice coupling is due to dipolar coupling, which we indirectly compare to electrical coupling. As mentioned above, dipolar coupling is frequently the main mechanism used for simulation in reservoir computing¹⁴⁴. In those applications, a nanomagnet array is subjected to remagnetisation programming, often via setting the anisotropy. Then, the calculation is conducted after connecting the digitised magnetisation outputs with a synthetic neural network. For complex device geometries the dipolar interactions must be computed micromagnetically (*Dipolar coupling*), but for

¹⁴¹ Liu, Pai, et al., “Magnetic Oscillations Driven by the Spin Hall Effect in 3-Terminal Magnetic Tunnel Junction Devices”.

¹⁴² Bauer, Yao, et al., “Magneto-ionic control of interfacial magnetism”.

¹⁴³ Shiota, Nozaki, et al., “Induction of coherent magnetization switching in a few atomic layers of FeCo using voltage pulses”; Skowroński, Nozaki, et al., “Perpendicular magnetic anisotropy of Ir/CoFeB/MgO trilayer system tuned by electric fields”.

¹⁴⁴ Nomura, Furuta, Tsujimoto, Kuwabiraki, Peper, et al., “Reservoir computing with dipole-coupled nanomagnets”; Kanao, Suto, et al., “Reservoir Computing on Spin-Torque Oscillator Array”; Nomura, Tsujimoto, et al., “Reservoir computing with two-bit input task using dipole-coupled nanomagnet array”.

point dipoles we can use a macromagnetic approximation as an illustrative means of comparison with the electric coupling:

$$\mathbf{H}_{\text{dipole}} = 3 \frac{\mathbf{r}(\boldsymbol{\mu} \cdot \mathbf{r})}{|\mathbf{r}|^5} - \frac{\boldsymbol{\mu}}{|\mathbf{r}|^3} \quad (84)$$

where $\mathbf{r}$ is the distance vector spanning from the one device to another (centre to centre), $|\mathbf{r}|$ is its length and the quantity $\boldsymbol{\mu}$ is defined by the magnetisation $\mathbf{m}$

$$\boldsymbol{\mu} = \mu_0 \mathbf{M}_s V \quad (85)$$

where V is the volume of the ferromagnetic layer in the device.

In CMTJ, two devices can be coupled by any distance-based interaction function with the *GroupInteraction* class. For convenience, the library provides the basic dipolar approximations by estimating the dipolar tensor based on the device arrangement in space, but the user may define their custom interaction function.

For comparison with the electric coupling, we create two simulation setups using the same device parameters as the ones used for discussing electrical coupling. In the first setup, called *symmetric excitation*, the DC current is supplied to both STOs that differ slightly with the parameters. In the second, called *asymmetric excitation*, the current is supplied only to the STO (source), which allows us to observe the spectrum of the other MTJ undisturbed by its own auto-oscillation. Fig.28 presents the results of the symmetric and asymmetric excitation simulation setups as a function of the distance between two STOs and temperature. By comparing symmetric and asymmetric excitation, we observe additional frequency peaks permeating the spectra of both STOs when excited asymmetrically, in particular at $d = 100$ nm. At 300 nm, the unexcited MTJ practically loses the frequency component coming from the source. When the two STOs experience symmetric excitation, the frequency alignment is stronger and aligns the auto-oscillations of both STOs, even across the second harmonic at 150 nm. In both cases, we also run a temperature simulation with $T = 300$ K, averaged over 50 runs to see how selective the dipole excitation is when noise is present. The differences turn out to be relatively minor, with the exception of the spectra between $d = 100$ and $d = 150$ nm. In those two cases, we see that the further harmonics in *symmetric excitation* cease to appear in both STO spectra, while for *asymmetric excitation* the temperature eliminated the back-coupling of higher harmonics of the unexcited MTJ from the source spectrum. Another pronounced effect of temperature shows at $d = 300$ nm, *symmetric excitation*, where otherwise strong synchronisation would occur, but it diminishes completely at $T = 300$ K. Note that at a very close range, the system becomes stiff as the dipole excitation dominates, and the supplied current is no longer sufficient to excite neither of the junctions, cf. Fig.28 ($T = 0$ K at 50 nm for symmetric and asymmetric excitations). However, the introduction of temperature $T = 300$ K allows for a faint spectrum signal.

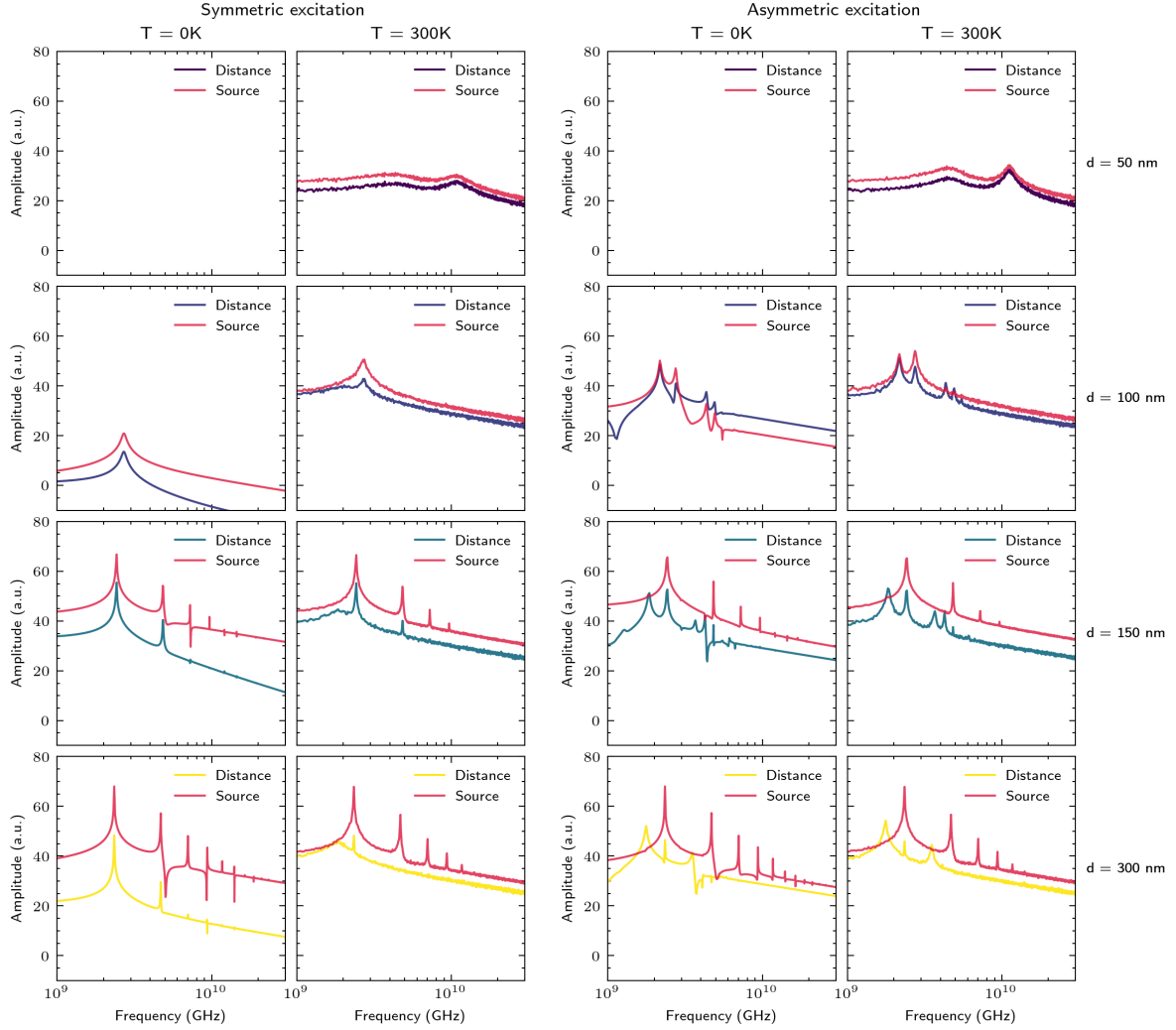


Figure 28: Comparison of dipole excitations as a function of temperature and distance. In symmetric excitation (left panel), the same current is supplied to both STOs. In asymmetric excitation (right panel) the current is supplied only to the first (source) STO. The source and distance STO differ with the anisotropy constant with the following relation $K_{\text{dist}} = 0.85K_{\text{source}}$. Note that at 50 nm and 0 K there is no effective excitation due to a very strong dipole coupling, which stiffens the system hence no spectrum is present.

Modelling correlated noise

Approaches to noise modelling

In addition to applications in storage and as oscillators, MTJs are widely used in sensing. We can construct TMR-based field sensors by leveraging two facts: (i) the magnetoresistance depends on the relative magnetisation angle between two layers, which is typically nonzero in the low-field regime, and (ii) the resistance-field relation, $R(H)$, is often linear in that low-field regime. Thus, in sensor development, achieving a high sensitivity is paramount. The voltage sensitivity in TMR sensors is typically defined as:

$$S = I_b \frac{dR}{dH} \quad (86)$$

where I_b is the bias current, and R is the measured resistance. Unfortunately, in the low-field regime, magnetic noise dominates electronic noise, the latter remaining relatively constant regardless of the applied field magnitude. Furthermore, this magnetic noise consists mostly of the $1/f$ type of noise which overpowers the noise coming from the thermal fluctuations in the low-frequency regime. The subject of magnetic noise in the sensor is a rapidly developing domain. Chęciński et al. demonstrated through a fitting procedure based on stochastic signal generation¹⁴⁵ that, to a good degree of precision, explains the RMS and the amplitude of composite white plus $1/f$ noise. However, in that work, the noise generator was used as an extrinsic signal and was not inserted into a magnetic simulation model. The question of direct inclusion of $1/f$ noise into a simulation warrants a discussion on practical application in numerical solvers such as those described in [Stochastic forms of Landau-Lifshitz-Gilbert-Slonczewski equation](#). Those schemes require a particular set of conditions for the stochastic part, specifically the samples drawn for $\Delta \mathbf{W}_t$. In classical examples $\Delta \mathbf{W}_t$ is drawn from the normal distribution and models the independent Brownian motion specifically. One, given that the $1/f^\alpha$ noise, where $\alpha = 0$ describes uncorrelated white noise and $\alpha = 2$ describes Brownian noise, we may argue that the process of generating the $1/f^\alpha$ noise is only different in the scaling of the multidimensional noise vector, but the underlying distribution still relies on initial sampling from $\mathcal{N}(0, \mathbf{I})$, as will be shown later. There is limited literature on $1/f$ noise applications as we attempted here, but there was some exploration in the context of the influence of such noise on the solutions of differential equations¹⁴⁶. We will only offer an empirical result arising from the implementation of the $1/f$ procedural generation into the magnetic solvers and consequently show that the resulting distributions of magnetisation under such inserted noise are indeed, to a large degree, consistent with the experimental observations (up to some scaling factor). Secondly, we want to touch on a point of physics, namely the assumption that the Wiener processes leading to the noise in separate layers are not correlated with each other. This becomes, in fact, a very

¹⁴⁵ Chęciński, Wiśniowski, et al., “Magnetic Noise Prediction and Evaluation in Tunneling Magnetoresistance Sensors”.

¹⁴⁶ Stoyanov, Gunzburger, and Burkardt, “Pink Noise, $1/f$ noise, and their effect on solutions of differential equations”.

convenient assumption, since correlated processes demand a different numerical treatment involving the correlation matrix¹⁴⁷. The locality of such a noise process may not be of extremely high concern in the macrospin perception of MTJs where a relatively thick oxide layer separates the two layers and thus the interlayer or magnetic coupling is weaker, but definitely requires further inspection if the algorithms described here were to be applied to the microspin simulations.

Empirical sensor field noise models were proposed in works by Jiang et al.¹⁴⁸, Nowak et al.¹⁴⁹ or Ozbay et al.¹⁵⁰ and provide a good baseline for experimental fits for the composite noise (white + 1/f):

$$S_v = \frac{(\alpha_{\text{mag}} \text{MSP} + \alpha) V_b^2}{\Omega f^\beta} + \mathcal{W} \quad (87)$$

where S_v denotes the voltage noise power, α is the electronic noise with units of m^3 , α_{mag} is the normalised 1/f magnetic noise, V_b is the bias voltage applied to the sensor, Ω is the volume of the sensing layer and f^β is the frequency exponentiated to a spectral component (we show the effect of having different exponents in the following sections). $\mathcal{W}$ represents the white noise component. The quantity $\text{MSP} = \frac{\Delta R}{R^2} \frac{dR}{dB}$ is called the magnetoresistance sensitivity product. The values of the α parameters are obtained through a fitting procedure. In the following paragraphs, we will consider only the effects of the magnetic noise, discarding the electrical noise components.

Simple model of 1/f noise

Egelhoff et al.¹⁵¹ attributed the existence of magnetisation hopping of domains between metastable states. In other words, the 1/f magnetic noise could be thought of in terms of multiple small magnetic domains fluctuating at relatively low frequencies. In contrast, thermal noise is white in nature, which means that its amplitude is constant for the entire spectrum of frequencies. A micromagnetic approach to white noise requires one seed and one random unit of vector sampling per magnetic site. But a similar approach for the 1/f noise would be more costly due to additional local computation, as will become evident from the algorithms that describe its procedural generation. Therefore, in lieu of the micromagnetic approach we will now entertain this idea of fluctuating domains in purely mathematical simulation, and by avoiding any computation of the sLLGS we hope to gain some insight into potential magnetic origins of the 1/f noise. Following Egelhoff's hypothesis, we first devise a randomly generated magnetic surface, that is, we create a set of magnetic domains of various sizes sampled from a distribution. The choice of the distribution is dictated primarily by a physical picture, domain imaging experiments often show not a uniform, but more of a gamma distribution of domain areas, which means skewing towards smaller domain areas¹⁵². However, ignoring this fact and selecting a uniform distribution of areas still produces the same result. After creating the magnetic structure, we now move

¹⁴⁷ Sauer, "Computational solution of stochastic differential equations".

¹⁴⁸ Jiang, Nowak, et al., "Low-frequency magnetic and resistance noise in magnetic tunnel junctions".

¹⁴⁹ Nowak, Weissman, and S. S. P. Parkin, "Electrical noise in hysteretic ferromagnet-insulator-ferromagnet tunnel junctions".

¹⁵⁰ Ozbay, Gokce, et al., "Low frequency magnetoresistive noise in spin-valve structures".

¹⁵¹ Egelhoff, Pong, et al., "Critical challenges for picoTesla magnetic-tunnel-junction sensors".

¹⁵² Egelhoff, Pong, et al., "Critical challenges for picoTesla magnetic-tunnel-junction sensors".

on to selecting the metastable oscillation patterns. In the simple model we discuss here, we pretend that all the magnetic contributions at play in the real device, i.e. the exchange, demagnetising, and anisotropy energies, lead to the result that the domains randomly change their orientation with some predefined period. Our previous assumption about the domain distribution proves to be convenient, as we are now able to posit that perhaps larger domains should be more stable than the smaller ones, hence having longer fluctuation periods than their smaller neighbours. In our model, this statement can take a functional form where $\tau_i \approx \lambda / \mathcal{A}_i$ which denotes a switching period τ_i of a domain i inversely proportional to its area $\mathcal{A}_i$ with a constant λ . Given the gamma distribution of $\mathcal{A}_i$, we also produce a somewhat inverted gamma-like distribution of τ_i . The constant λ here is only for the purpose of scaling the frequencies to the range that we can see in the final spectrum or in the time series. Having almost all pieces assembled, we discuss the simulation, where at each simulation step t we will check τ_i and for all domains for which we have $0 \equiv t \bmod \tau_i$, we will generate a random Gaussian vector $\zeta \sim \mathcal{N}(0, \sigma^2)$ where σ is some positive constant. It turns out that this procedure will result in a $1/f$ -like noise and Fig.29 gives the simulated picture.

In contrast, Fig.31 shows the experimental values obtained from the real sensors. From Fig.31 we also notice an extra factor at play, namely the characteristic corner point where the dominant $1/f$ noise transitions into the dominant white noise in the power spectrum. In our simple model, this can be accounted for in two ways. One is simply to generate a background white noise distortion for each site at each timestep, sampled similarly from a zero-mean Gaussian with σ' standard deviation $v \sim \mathcal{N}(0, \sigma'^2)$. The ratio of σ' to σ and any additional scaling in v determine whether the corner point moves up or down the spectrum. In the experiment, the simplified rule on how the corner sensor behaves for a sensor with strong perpendicular anisotropy is that the higher the sensitivity, the more the corner moves towards higher frequencies. For MTJ-based sensors with CoFeB electrodes, these relationships translate to anisotropy in an inverse way; a larger perpendicular anisotropy implies a lower sensitivity¹⁵³. Thus, for larger anisotropies, we may expect the corner point to be located at lower frequencies. A further point is the variability of the metastable switching. In the model, we can assume small random phase shifts, which can be summarised with a modification of the switching rule: $0 \equiv t \bmod (\tau_i + \delta_{i,t})$ where $\delta_{i,t}$ is a random instantaneous disturbance to the switching of the domain i at time t . We keep it small and on the order of 3-5. Yet another way to have a corner in the spectrum is to generate a set of background domains wherein each oscillates with a high frequency, or a frequency selected from uniform range. So, as shown in Fig.30 using the first of the solutions mentioned, we achieve the corner in the output spectrum, which brings us closer to the experimental result.

What we have essentially shown by this simple exercise is that the necessary components for $1/f$ noise originate in i) adequate modelling of the

¹⁵³ Wisniowski, Dabek, et al., “Effect of CoFeB electrode compositions on low frequency magnetic noise in tunneling magnetoresistance sensors”.

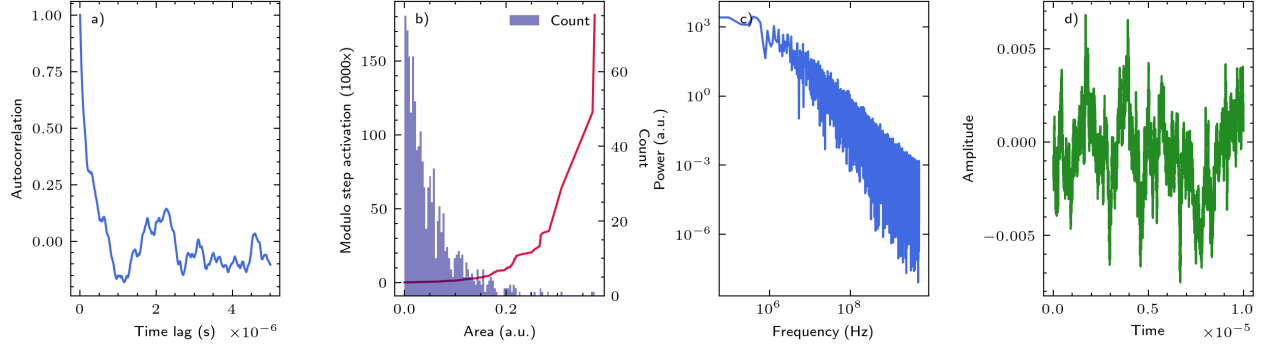


Figure 29: Result of the simplistic approach to simulating the domains. The behaviour of the autocorrelation (a) and $S(f)$ (c) strongly resembles what can be seen in the experiment. (b) the purple histogram denotes the distribution of the domain areas $\mathcal{A}_i$ in a sample, drawn from a Gamma distribution with parameters $a = 1, b = 0.05$ and the red line in the (b) modulo step denotes the activation period, which follows the inverted rule: $\tau_i \sim \lambda / \mathcal{A}_i$.

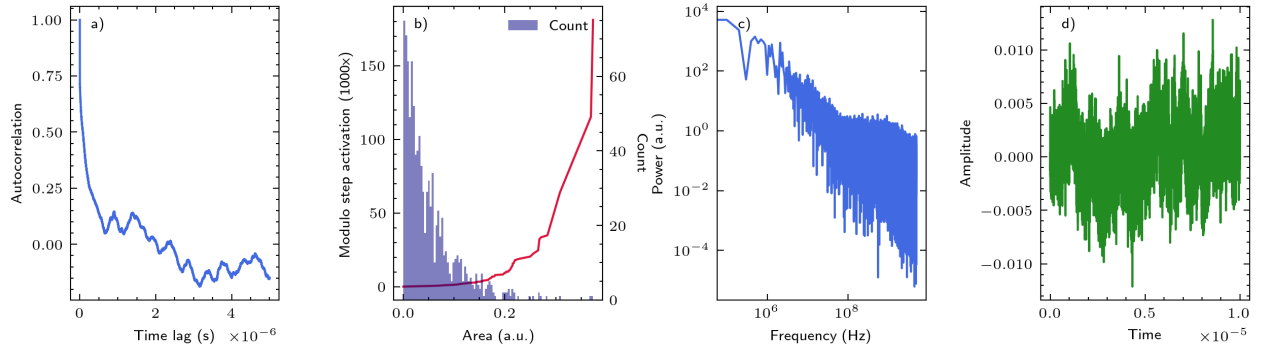


Figure 30: Result of the simplistic approach to simulating the domains, this time with the inclusion of the white noise. Specifically, (c) has the correct corner where the $1/f$ noise transitions into the white noise. Explanations of the panels follow from Fig.29. Noteworthy: even though we see the same distribution of the domains as in Fig.29, their volumes and their metastable switching periods (b), the autocorrelation drops and becomes less oscillatory (loses its detail and succumbs to dominant frequency).

metastable switching and ii) the thermal nature of the metastable fluctuation. This does not mean that the thermal effects themselves are directly responsible for the metastable switching of the domains, if that metastable switching indeed takes place, but rather that the mathematical nature of that fluctuation is similar.

Advanced algorithms for 1/f reproduction

We now discuss two known techniques that produce decent quality 1/f noise; most notably: the Voss-McCartney-Trammel (VMT)¹⁵⁴ algorithm and the Kasdin algorithm¹⁵⁵. The reason why we opt for an established algorithm in lieu of the procedure outlined in a paragraph above is that they reproduce a similar behaviour but with fewer parameters and have better properties in the time-domain, meaning that the samples produced by them yield more realistic autocorrelation.

Starting with the VMT algorithm, we define the three-dimensional random field:

$$\mathbf{H}_{1/f} = k\eta_{VMT}dW \quad (88)$$

where k is the scaling factor, and dW is the random Gaussian unit vector.

η_{VMT} will come from the VMT algorithm with the steps outlined in Alg.3.

The state vector is laid out such that the first element is the highest frequency noise component, n , the second appears with the probability p , at np , the third with p^3 at np^3 frequency, and so on. If p increases, then the frequencies are more clustered. A natural course of optimisation is to observe that in the second loop we need only to iterate over the unique realisations of the $T^{(k)}$ vector, which reduces the length of the subsequent inner loop, and hence the number of new pseudo-samples drawn diminishes. This is especially the case if $p > 0.5$. Otherwise, the cost of sorting may exceed the cost of a simple iteration. Furthermore, the probability that S_0 will change at each step i when the *else* statement omitted is still rather large, so skipping this clause may save extra time without the loss of generalisation.

Unlike the VMT algorithm, the Kasdin algorithm allows estimating $1/f^\alpha$ in the full range $\alpha \in [0, 2]$, $\alpha \in \mathcal{R}$. It can be elegantly described with a Z-transform system functional:

$$H^\alpha(z) = \frac{1}{(1 - z^{-1})^{\alpha/2}} \quad (89)$$

which can be rewritten using the fractional differencing theorem¹⁵⁶ to see the linear system:

$$H^\alpha(z) = \sum_{k=0}^{\infty} (-\alpha/2)_{(k)} (-1)^k z^{-k} \quad (90)$$

where $(-\alpha/2)_{(k)}$ is the falling fractional. We can convert it to the rising fractional using the identity $(-\alpha/2)^{(k)} = (-\alpha/2)_{(k)} (-1)^k$ leading to:

$$H^\alpha(z) = \sum_{k=0}^{\infty} (\alpha/2)^{(k)} z^{-k} \quad (91)$$

¹⁵⁴ Voss, ““1/f noise” in music”.

¹⁵⁵ Stoyanov, Gunzburger, and Burkardt, “Pink Noise, 1/f noise, and their effect on solutions of differential equations”; Kasdin, “Discrete simulation of colored noise and stochastic processes and 1/f^{alpha} power law noise generation”.

¹⁵⁶ Hosking, “Fractional differencing”.

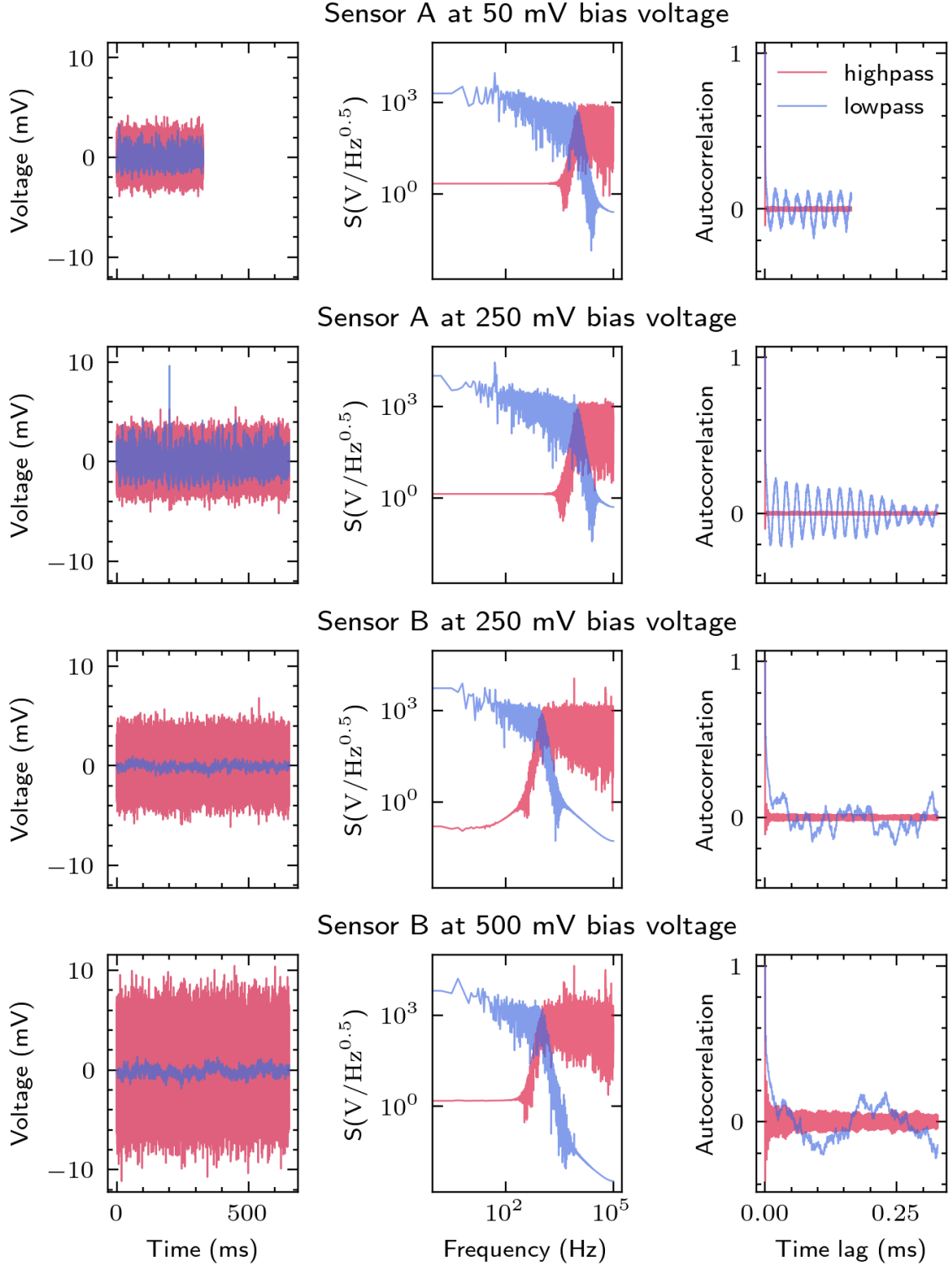


Figure 31: Experimentally measured noise time series and spectrum from two sensors, each with two different applied voltages. The sensors do not exhibit the VCMA effect under voltage change, but the two sensors have two different nominal perpendicular anisotropies. We can deduce from the placement of the characteristic 'corner' point, i.e. the point where the white noise starts dominating over $1/f$ noise, that the sensitivity of the sensor whose corner point is in the higher frequency is lower, thus its anisotropy is larger than the one of the second sensor. The strong oscillating autocorrelation in the first-top panels suggests a large, also strongly oscillating domain in the signal. The red colour denotes the data filtered with the Butterworth 6-th order high-pass filter, and the blue colour marks the signal after it has been filtered with the Butterworth 6-th order low-pass filter. The cut-off point for sensor A was 10 kHz, and for sensor B, 1 kHz; these values were selected so that they separate white noise and $1/f$ at the characteristic 'corner' point. Data were measured by Dr. Piotr Wiśniowski's laboratory and made accessible for analysis to the author. The first sensor time series was measured for a shorter time compared to others.

Algorithm 3: VMT 1/f noise generation

Result: η_i^{VMT} , noise amplitude for each step i .

$k \leftarrow$ number of sources

$p \leftarrow$ probability of success for $\mathcal{B}$, the Bernoulli distribution.

$N \leftarrow$ number of steps

$i \leftarrow 0$

$S^{(k)} \leftarrow$ state vector of length k

$S_i \leftarrow \mathcal{U}(0,1), i = 1 \dots k$ initialise

while $i < N$ **do**

 // $T^{(k)}$ is a vector of size k , sampled from the Bernoulli distribution

$T^{(k)} \sim \mathcal{B}(p)$

for s in $T^{(k)}$ **do**

if $s < k$ **then**

 // generate a new sample for that source

$S_s \sim \mathcal{U}(0,1)$

else

 // S_0 is the most frequently changing source

$S_0 \sim \mathcal{U}(0,1)$

end

end

$\eta_i^{\text{VMT}} \leftarrow \sum_j^k S_j$

$i \leftarrow i + 1$

end

From that form, we can see that the system consists of a series of infinite 1-delay blocks weighted by an appropriate binomial coefficient. Expanding the rising fractional, we can obtain an iterative implementation viable for algorithmic generation:

$$\begin{aligned} \sum_{k=0}^{\infty} (\alpha/2)^{(k)} &= 1 + \alpha/2 + \frac{\alpha/2(\alpha/2+1)}{2!} + \frac{\alpha/2(\alpha/2+1)(\alpha/2+2)}{3!} = \\ &= 1 + \sum_{k=1}^{\infty} w_{k-1} \frac{\alpha/2+k-1}{k} \end{aligned} \quad (92)$$

where $w_0 = 1$. This finally gives:

$$H(z) = 1 + \sum_{k=1}^{\infty} w_{k-1} \frac{\alpha/2+k-1}{k} z^{-k} \quad (93)$$

Further optimisation occurs by observing that consecutive terms diminish

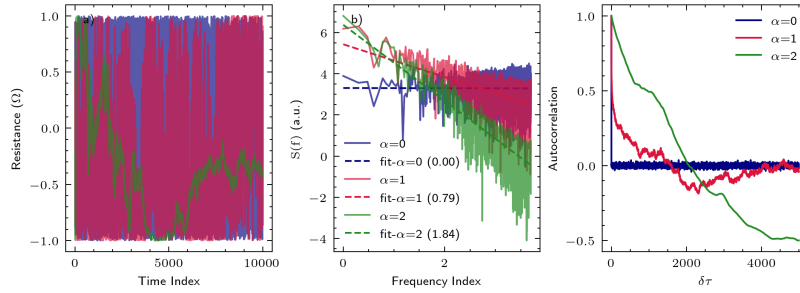


Figure 32: Three values of α corresponding to white ($\alpha = 0$), pink ($\alpha = 1$) and brown ($\alpha = 2$) noise spectra. Panel (a) shows an artificial magnetoresistance computed based on the samples drawn from a given noise distribution (not simulated). (b) The result of computing an FFT on that magnetoresistance time series. The fits, although imperfect, illustrate the increasing α parameter. (c) autocorrelation of the time signal for each of the noise types. Generated based on the Kasdin algorithm.

rapidly (for $\alpha/2 \leq 1$), and thus we can truncate the series to $k = N$, with an error term of $\mathcal{O}(N+1)$. It is worth noting in (93), when we have $\alpha = 2$, the weight term $w_k = 1, \forall k$. In the next step, we compute the FFT of the vector H^N and a vector of samples of normal distribution $\mathcal{N}(0, \sigma)$. After that, the two resultant complex vectors are multiplied and run through IFFT. Finally, we return the real part of the signal. In practice, batching might be required in some cases because, at low frequencies, we require long simulation times, often of the order of μs . This causes large buffer sizes and, more importantly, increases the size of the array based on which we compute the FFT, which, in case it grows too large, makes the computation infeasible. However, such an optimisation may lead to small continuity errors occurring at the buffer boundaries and to the destruction of the longer-scale correlation.

From now on, we will prefer the Kasdin algorithm for noise generation, as it offers greater flexibility. Fig.32 presents the spectra for three values corresponding to white, pink, and brown noise. One crucial feature of $1/f^\alpha$ noise is that it becomes increasingly more correlated in the time domain as α increases. Panel c) of Fig.32 shows the smallest autocorrelation values for white noise and the largest for brown noise, which is consistent with the

¹⁵⁷ Carpena and Coronado, “On the Autocorrelation Function of $1/f$ Noises”.

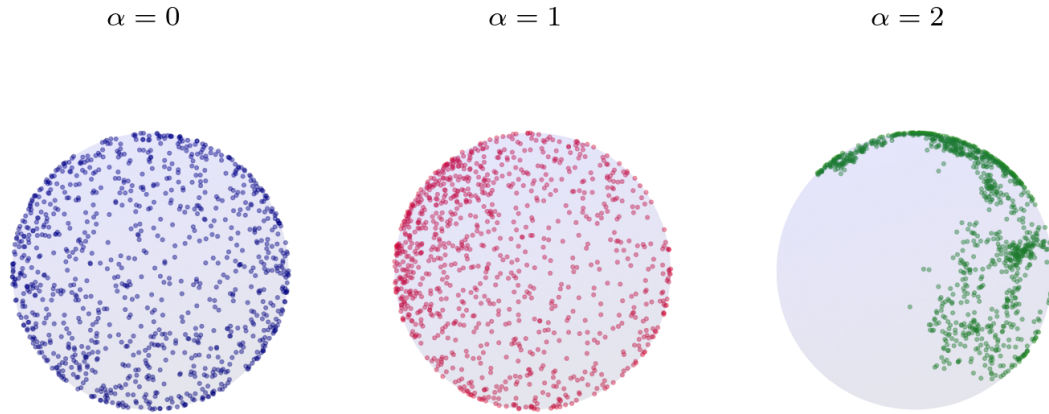


Figure 33: The noise vectors samples for different values of α demonstrating different correlation scales for $\alpha = 0, 1, 2$. The increase in correlation as α grows corresponds to the tendency of the samples to localise in a particular region of the sphere.

theoretical expectation¹⁵⁷. A similar picture emerges from Fig.33 where the dots on the sphere represent the vector samples drawn from a single buffer of the noise generated by the Kasdin algorithm, again for three different values of α . In subsequent macrospion simulations, this vector will be inserted in place of $\Delta\mathbf{W}$ at each step. In the package, the vector has each component sampled from the $1/f^\alpha$ distribution and then normalised. The user can then

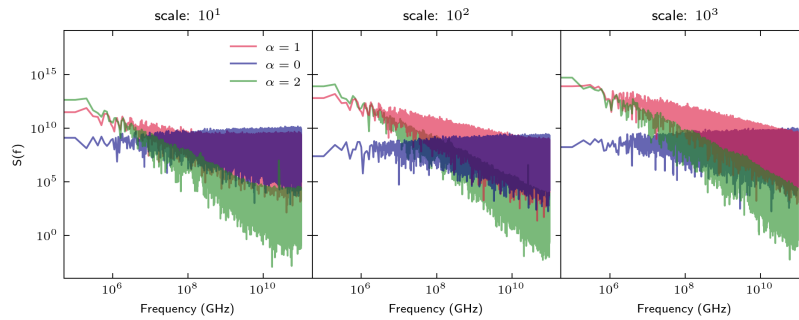


Figure 34: Effect of the $1/f^\alpha$ scaling on a sample MTJ with strong perpendicular anisotropy. Although white noise appears to be unaffected, the precise frequency at which other types of noise are overcome with white noise changes depending on the scale. Note that even though the simulation ran for a $10\ \mu\text{s}$, the low frequency part of the spectrum still received a low number of samples.

define the scaling factor, k , which needs to be determined experimentally. The effect of scaling is shown in Fig.34, where we simulate an example MTJ with a strong perpendicular anisotropy for $10\ \mu\text{s}$. In addition, we also see a potential effect of noise aliasing on a lower scale, where the typical slope of the noise is disturbed at higher frequencies.¹⁵⁸

We can now investigate a couple of basic behaviours that arise from the presence of different kinds of noise. First, we return to the theoretical exer-

¹⁵⁸ Kirchner, “Aliasing in $1/f^\alpha$ noise spectra”.

cise from the beginning of this subsection and attempt to reproduce it with LLGS-simulated curves. The setup is nearly identical to the mathematical model, but the purely theoretical assumptions are made more physical. As before, we only assume thermal (white) noise generated in the system, for that we use samples drawn from normal distribution according to thermal equation. The same can be repeated by drawing the Kasdin algorithm; however, the domain methodology allows us only to replicate $\alpha \sim 1$, because the correlation length in the simulation is one, as memory persists only from a previous step. For the sample MTJ, we set $M_s = 1.5$ T, effective perpendicular anisotropy, and measure the response to noise along the z axis. Following our earlier findings, we sample the N domains (here, 1000), with the anisotropy constant of each drawn from a Gamma distribution. The final spectrum is computed with respect to the normalised volume, i.e., each domain's contribution to the spectrum $\mathcal{S}(\omega)$ is proportional to its size and its size is proportional directly to the anisotropy:

$$\mathcal{S}(\omega) = \sum_i^N w_i \mathcal{S}_i(\omega) \quad (94)$$

where $\mathcal{S}_i(\omega)$ is the spectrum of the particular domain, and w_i is the weight corresponding to the volume. In that way, we reprise the earlier conclusion that we can somewhat reproduce the $1/f$ noise characteristics using only white noise and the assumption that there are a lot of small domains of relatively small anisotropies and few domains with much larger anisotropy.

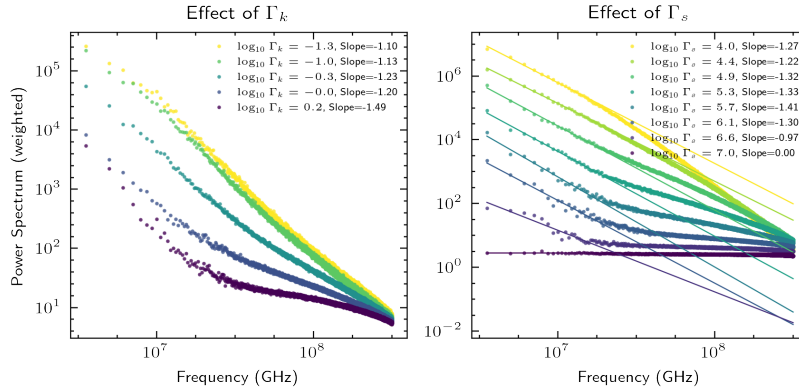


Figure 35: Effect of the scale and k parameter of the Γ function on the $1/f$ spectra produced by synthetic aggregation of multi-domain ($N = 1000$) white noise responses.

Fig.35 shows the sample spectrum in a range of Γ distribution parameters. It shows how the distribution of domains and therefore their anisotropies affects the corner noise, but not as much the effective slope of the $1/f$ distribution and that the slope does not vary with neither Γ_k nor Γ_s . However, the behaviour observed mimics the noise of $1/f$ and gives some strength to the argument that the noise of $1/f$ could be understood as a composite of white noise, gated by a varying response from different domains. In conclu-

sion, from our simulations, the key components for the reproduction of the approximate $1/f$ noise are:

1. Magnetic memory, which in simulation is ensured as the magnetisation from time t is carried over to the next step, $t + 1$ and then modified. This memory functions as a correlation component.
2. Randomly sampled thermal sample generators; the domain acts as such generators, given that T is set sufficiently high to overcome stiffness due to effective anisotropy.

The choices of distributions over the anisotropies we tested were the normal distribution, the gamma distribution, and the uniform distribution. We note that, as before, the Γ distribution is not critical to the reproduction of the linear slope, nor is the weighting by domain size, and those conditions were chosen for a closer physical reproduction of magnetic domain structures.

In the second example, we inspect two examples based on a plain MTJ oscillator with a perpendicular anisotropy, excited by a constant current density bias j_b . In Fig.36 we present such an MTJ with 0.15 kJ/m^3 anisotropy constant and in Fig.37 an equivalent MTJ but with a larger anisotropy of 150 kJ/m^3 . The scale of the noise, though slightly exaggerated to make a point, was kept constant for both runs. As expected, increasing the anisotropy improves the resistance to noise, which is clear both in the time domain and in the frequency domain. Inspecting the magnetoresistance shows a range of aharmonic contributions for the white noise, and less so for the $\alpha = 1$. Noise $1/f^2$ appears to induce a more regular disturbance, which is a particular hazard for devices that operate as frequency detectors. When $\alpha = 2$ we can observe that an additional frequency peak emerges in a frequency bin below the main resonance frequency, and so in a significant magnitude. The ratio of that peak to the main resonance peak A_0/A_{noise} is subject to particular realisation, which means that it fluctuates heavily due to the stochastic nature of the noise. Despite a large standard deviation across all realisations, there is a slight tendency for the A_0/A_{noise} ratio to increase along with an increase in the perpendicular anisotropy constant. These results seem to be in line with similar experimental findings showing that MTJs with larger perpendicular anisotropy are more robust to $1/f$ noise.¹⁵⁹

Finally, for completeness, Fig.38 is analogous to Fig.28, this time reproduced with $1/f$ noise instead of pure thermal noise. The characteristics of peak deterioration are different from the thermal noise for both $\alpha = 1$ and $\alpha = 2$, and $1/f$ noise seems to have a strong impact, even at a lower amplitude parameter k . Furthermore, the correlation component of the noise affects the ability of two MTJs to synchronise, but in asymmetric and the symmetric excitation cases.

¹⁵⁹ Wisniowski, Dabek, et al., “Effect of CoFeB electrode compositions on low frequency magnetic noise in tunneling magnetoresistance sensors”.

$$j_b = 3 \times 10^{10} \text{ A/m}^2, K = 0.15 \text{ kJ/m}^3$$

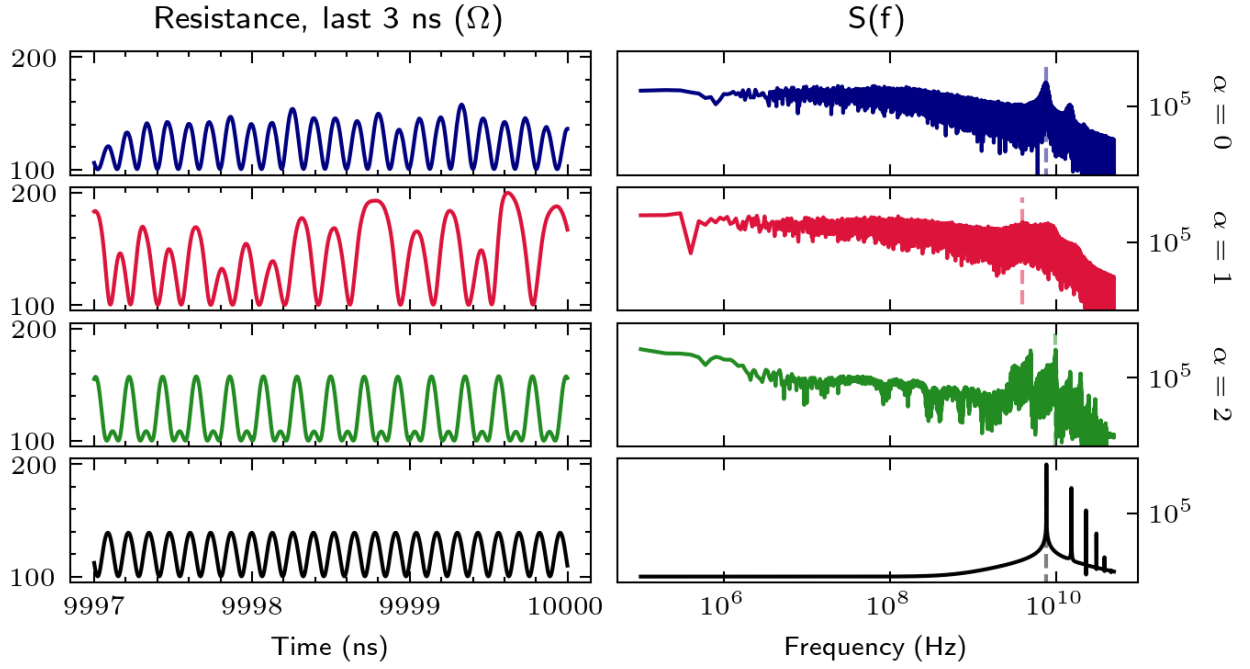


Figure 36: The spectrum for smaller anisotropy constant of 0.15 kJ/m^3 .

$$j_b = 3 \times 10^{10} \text{ A/m}^2, K = 150.0 \text{ kJ/m}^3$$

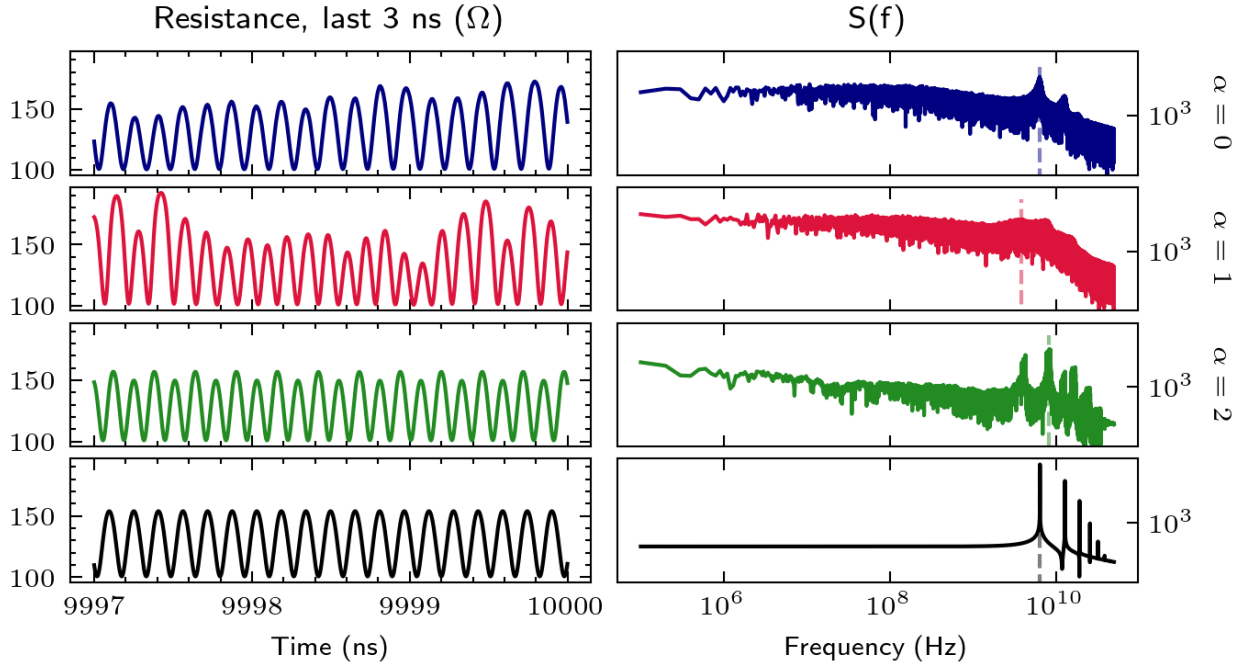


Figure 37: The spectrum for the MTJ with a larger anisotropy of 150 kJ/m^3 , 100 times larger than in Fig. 36. Compared to lower anisotropy, the peaks at $\alpha = 2$ are much more separated and thinner. In the case of $\alpha = 1$, the noise still covers the oscillation peaks.

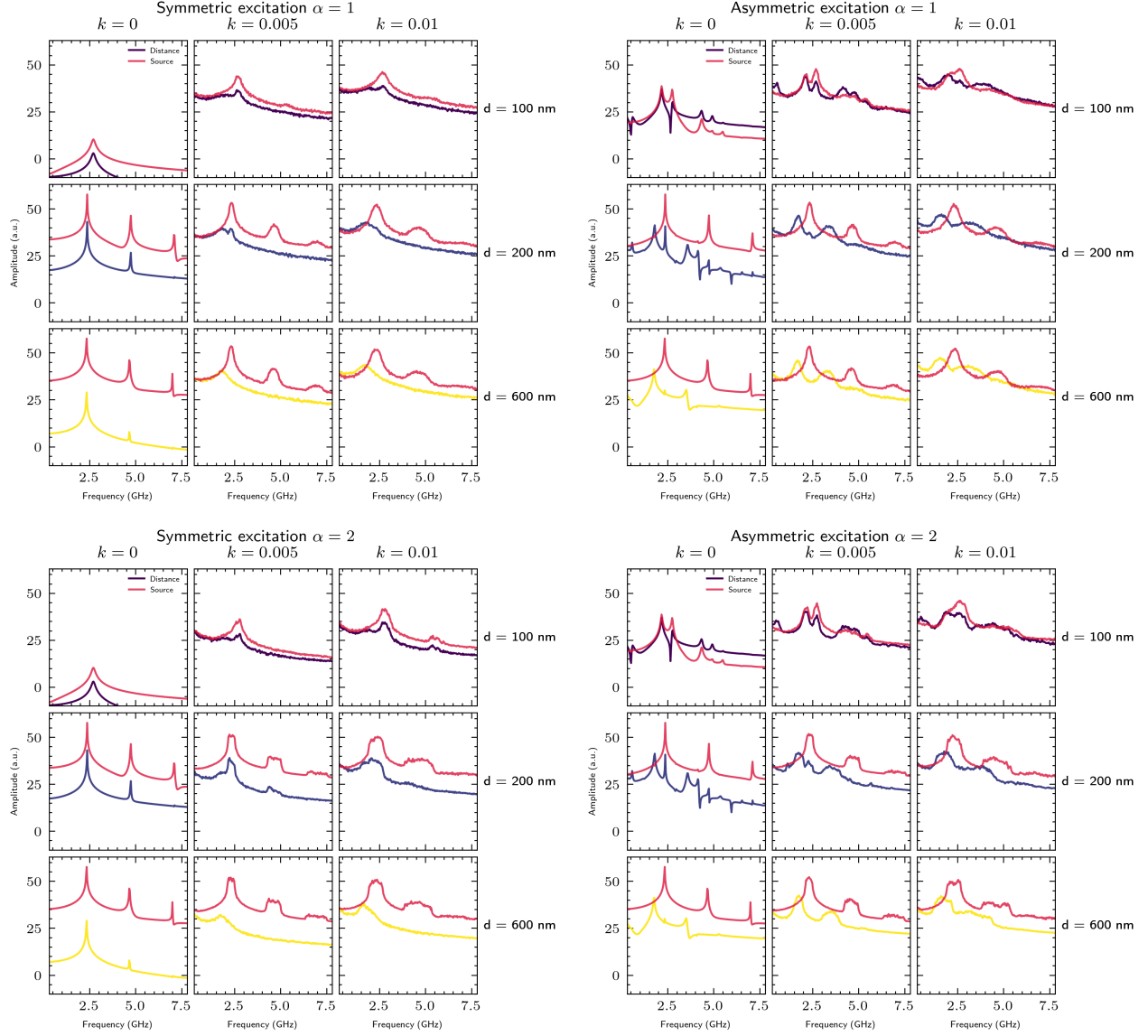


Figure 38: Dipole interaction over $\alpha = 1$ (top row) and $\alpha = 2$ (bottom row) $1/f^{\text{ff}}$ noise. Below 50 nm the system becomes too stiff to be excited. $\alpha = 2$ show faster peak deterioration than $\alpha = 1$, both with distance and with noise amplitude. However, for symmetric excitation, the synchronisation peak seems to be retained in $\alpha = 2$, but it disappears when $\alpha = 1$. k is the $1/f^{\text{ff}}$ noise scaling factor.

Chapter summary

In this chapter, we discussed selected applications of the MTJs. Electrical coupling, though difficult to achieve, presents a promising direction for different computing applications. Adequate modelling of $1/f$ noise can improve sensor design that retains its robustness in the high-sensitivity regime or can cleverly balance the trade-off between field noise, range, and sensitivity. Our simulations demonstrate how an ensemble of thermally activated domains can lead to primitive $1/f$ characteristics. Furthermore, similarly to the experimental findings, the simulated effect of $1/f$ noise on the resulting spectra diminishes with increasing perpendicular anisotropy or with increasing junction size. As a closing word to this chapter, we touch on potential areas of improvement. First, while we can create complex simulations of electrically coupled junctions, we still have little understanding of the relationship between the quantity of theoretical coupling χ and its experimental realisation. Resolving this could lead to less frustration in attempting to fabricate MTJs that synchronise at near frequencies easily – and the difficulty of achieving this has been noted in detail in¹⁶⁰. Second, we would like to have a more definitive answer to the origin of $1/f$ noise. In [Modelling correlated noise](#) we propose, using a mathematical toy model, several hypotheses that reproduce the experimental behaviour, yet the real answer will probably reveal itself in the process of observing the sensor noise under optical magnetic imaging over long acquisition times. This is again not a trivial experimental setup and remains to be implemented. Finally, a numerical issue is: How can we simulate micromagnetically $1/f$ noise in a reasonable time, in terms of computational efficiency. The simple toy model we presented at the beginning of the [Modelling correlated noise](#) is a reflection of a micromagnetic world, but it needs to be sufficiently distilled so that a full-scale simulation with LLGS dynamics would be possible.

¹⁶⁰ Rzeszut, Mojsiejuk, et al., “Towards mutual synchronization of serially connected Spin Torque Oscillators based on magnetic tunnel junctions”.

Dynamic control of devices

The meteoric rise of machine learning methods in recent years has had a profound impact on the perception of what an optimal way to approach a given problem should be. In previous chapters, an example of automatic parameter fitting was demonstrated, which eliminated the need for manual tweaking; here, we present a compelling case for a related technique: the dynamic control of various types of spintronic devices.

After a brief theoretical introduction to reinforcement learning, we propose a control problem based on a spintronic oscillator as an example. This serves as a motivating example for the reinforcement learning (RL) methods that are subsequently employed to solve it. Finally, other spintronic applications of RL are discussed.

Introduction to reinforcement learning

Recent model-free reinforcement learning algorithms fall into two broad categories: policy optimisation methods and Q-learning, with some methods combining the two. Policy, typically denoted as $\pi_\theta(a|s)$ ¹⁶¹, is a set of rules that dictates the actions of the agent in a given environment. The algorithms that perform policy optimisation explicitly represent the policy and learn an optimal policy via direct updates. In addition, the actions the agent performs are sampled from some policy; that is, $a_t \sim \pi_\theta(\cdot|s_t)$. On the other hand, Q-learning methods rely on learning a function approximator for the action-value function, $Q_\phi(s, a)$. In Q-learning, the optimal policy is not learnt directly, but through optimisation of the Q_ϕ function. The actions can be selected by following a greedy policy:

$$\pi_{\text{greedy}}(s) \in \arg \max_a Q_\phi(s, a) \quad \text{s.t.} \quad a_t = \pi_{\text{greedy}}(s_t) \quad (95)$$

There is a further distinction between on-policy and off-policy learners. On-policy algorithms use the data collected while acting with the policy to update the very same policy. Conversely, off-policy methods learn from past examples through replay, meaning they update the policy based on past experiences collected when the actions were selected using a different (a past version of) policy. Typically, off-policy algorithms are more sample-efficient because the same collected sample can be reused to improve many

¹⁶¹ $\pi_\theta(a|s)$ represents the probability of selecting an action given that the agent has observed a state s . θ denotes policy parameters.

future versions of the policy (experience replay). This comes at the cost of stability, as the examples collected in earlier versions of the policy may not reliably guide the policy gradient updates into stable optima. Sample efficiency becomes critical when the environment is costly. Simulations are quick to run, but on-device experiments are much slower, and therefore off-policy learning is important.

In this chapter, we limit ourselves to three algorithms that yielded the best results for the environments considered in our work: Soft Actor-Critic (SAC)¹⁶², Twin Delayed Deep Deterministic Policy Gradient (TD3)¹⁶³ and Proximal Policy Optimisation (PPO)¹⁶⁴. The first two are off-policy actor-critic methods that combine off-policy temporal-difference (TD) learning¹⁶⁵ of Q_ϕ with policy optimisation employing the actor network (learning $\pi_\theta(a|s)$) and two critic networks estimating $Q_\phi(s, a)$ ¹⁶⁶. Fig.39 schematically illustrates the architecture of the actor-critic pair, specifically its SAC flavour. The reasoning behind using two critic networks instead of one is that in the past iterations of actor-critic methods, the critic network had a tendency to overestimate the Q -value. Thus, in the twin-critic version, the minimum of the two is taken for the gradient update step. After the agent has been trained, only the actor part is deployed. Discarding the critic is possible only because the state-action value is not used directly when selecting actions, only for the policy improvement step during learning. Such an approach, combined with the simulated pretraining, was effectively demonstrated in many real-world applications from the physics domain, for example, recently in the magnetic control of a tokamak plasma during the fusion process¹⁶⁷.

SAC combines techniques from algorithms such as Trust Region Policy Optimisation (TRPO)¹⁶⁸ and PPO, characterised by stochastic on-policy learning, stability, and low sample efficiency, with methods such as the Deep Deterministic Policy Gradient (DDPG)¹⁶⁹ or TD3 characterised by a deterministic policy, relative instability, and the use of a replay (experience) buffer, which leads to good sample efficiency. Here, stability means that the convergence of the algorithm is not overly sensitive to the choice of hyperparameters. SAC also introduced a soft learning objective that maximises both the reward and the entropy:

$$\pi_\theta^* = \operatorname{argmax}_{\pi_\theta} \sum_t \mathbb{E}_{(s_t, a_t) \sim \pi_\theta} [\gamma^t (r(s_t, a_t) + \alpha \mathcal{H}(\pi_\theta(\cdot|s_t)))] \quad (96)$$

where γ is the discount factor, and $\mathcal{H}(\pi_\theta(\cdot|s_t))$ represents the policy entropy, α determines its weight. In practice, this objective is rewritten in terms of an optimisation constraint on the lower bound of the entropy, some $\mathcal{H}_0$. Intuitively, the entropy term should not converge to 0, as that would mean a fully deterministic policy, yet the goal of the SAC is to balance the stochasticity of the policy while maximising the reward. Since the original release of the SAC, the maximal entropy target has been used to augment other algorithms as well. This stochasticity is evident in Fig.39, the actor predicts $\mu_\theta, \sigma_\theta$ that parametrise a Gaussian $\mathcal{N}(\mu_\theta, \sigma_\theta)$ from which the actions are drawn. $\tanh$

¹⁶² Haarnoja, A. Zhou, et al., *Soft Actor-Critic*.

¹⁶³ Fujimoto, Hoof, and Meger, *Addressing Function Approximation Error in Actor-Critic Methods*.

¹⁶⁴ Schulman, Wolski, et al., *Proximal Policy Optimization Algorithms*.

¹⁶⁵ R. S. Sutton and Barto, *Reinforcement learning*.

¹⁶⁶ Here, we separately denote actor and critic parameters as θ and ϕ respectively.

¹⁶⁷ Degraeve, Felici, et al., “Magnetic control of tokamak plasmas through deep reinforcement learning”.

¹⁶⁸ Schulman, Levine, et al., *Trust Region Policy Optimization*.

¹⁶⁹ Lillicrap, Hunt, et al., *Continuous control with deep reinforcement learning*.

squashing is then applied to bound the action values.

On the other hand, PPO is an on-policy optimisation algorithm, which maximises a surrogate objective function. This surrogate function indicates how much the performance objective will change as a consequence of the update. In the **PPO-CLIP** variant, the algorithm attempts to limit the amount that each policy update drifts away from the old policy, improving stability and convergence. The policy update rule is given by:

$$\theta_{k+1} = \operatorname{argmax}_{\theta} \frac{1}{|\mathcal{D}_k|T} \sum_{\tau \in \mathcal{D}_k} \sum_{t=0}^T \min \left(\frac{\pi_{\theta}(a_t|s_t)}{\pi_{\theta_k}(a_t|s_t)} A^{\pi_{\theta_k}}(s_t, a_t), g(\epsilon, A^{\pi_{\theta_k}}(s_t, a_t)) \right) \quad (97)$$

where θ_{k+1} denotes the policy parameters in step $k+1$, $\mathcal{D}_k$ is a set of trajectories τ obtained from running π_{θ_k} (old policy) in the environment, T is the duration of a particular trajectory, g is defined as¹⁷⁰:

$$g(\epsilon, A) = \begin{cases} (1 + \epsilon)A & \text{if } A \geq 0, \\ (1 - \epsilon)A & \text{if } A < 0. \end{cases} \quad (98)$$

Finally, the advantage function A is defined as:

$$A^{\pi}(s, a) = Q^{\pi}(s, a) - V^{\pi}(s) \quad (99)$$

with the value function $V^{\pi}(s) = \mathbb{E}_{\tau \sim \pi} [R(\tau)|s_0 = s]$, the state-action value function $Q^{\pi}(s, a) = \mathbb{E}_{\tau \sim \pi} [R(\tau)|s_0 = s, a_0 = a]$ and $R(\tau) = \sum_{t=t_0}^{\infty} \gamma^t r(s_t, a_t)$ is the discounted return of the trajectory. The advantage function measures whether the action taken is better than the policy's default behaviour.

For all experiments in this chapter, we benefit from the implementations of the baseline algorithms provided in the Stable Baselines 3 repository¹⁷¹. The reader is also referred to¹⁷² for pseudocode on practical implementation of the policy and Q -function updates for all algorithms discussed in this section.

¹⁷⁰ Schulman, Moritz, et al., *High-Dimensional Continuous Control Using Generalized Advantage Estimation*.

¹⁷¹ Raffin, Hill, et al., “Stable-Baselines3: Reliable Reinforcement Learning Implementations”.

¹⁷² Achiam, *Spinning Up documentation*.

Spintronic oscillator environment

Introduction to the problem

Suppose that we are faced with the relatively simple problem of tuning an oscillator to some desired frequency f^* . To arrive at this frequency, we can adjust two control parameters: the first regulates the DC current, and the other modifies the external magnetic field. For a human, the procedure could probably look like this: the user first observes a frequency f , in some initial configuration of the current and field gauge. Then they pick one of the inputs and adjust it, resulting in a new frequency reading denoted as f' . If the resulting change, that is, $\Delta f = f' - f$ is positive and brings the system closer to the target frequency f^* , such that the error $\epsilon = |f^* - f|$ decreases, then they would try turning the same gauge in the same direction again. In any other case, they would either change the turning direction of the same gauge

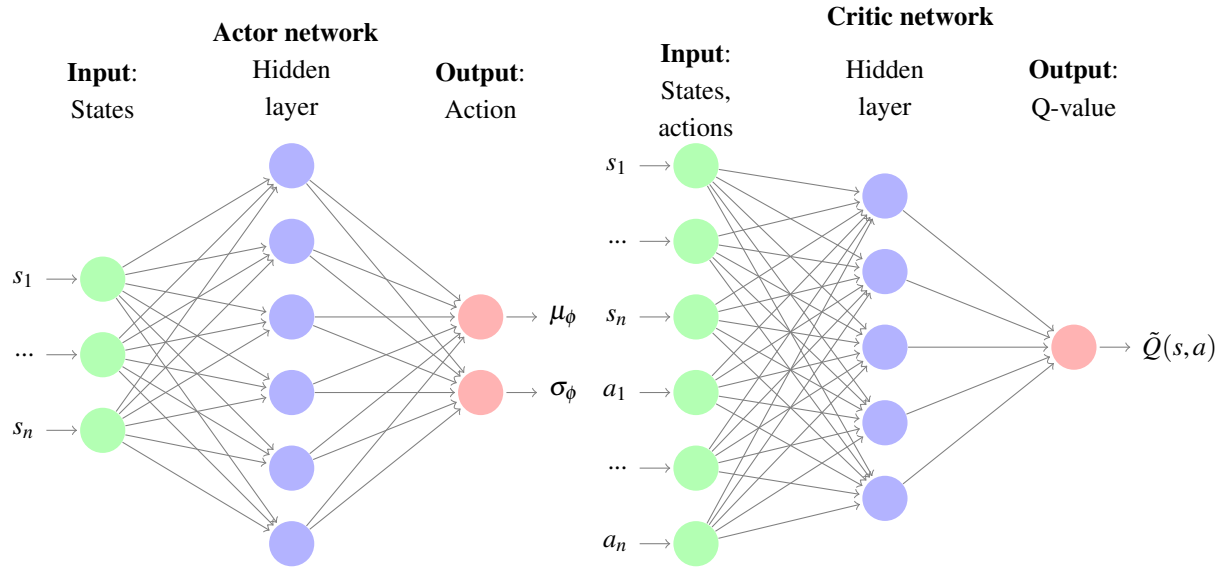


Figure 39: Actor and critic network generic architecture. TD3 introduced two critic networks to reduce the overestimation bias. In SAC the actor networks returns μ_ϕ and σ_ϕ , the mean and the standard deviation vectors representing the action vector which are then squished with either tanh or RELU. Both tanh and RELU are activation functions and the latter stands for *Rectified Linear Unit*.

or pick another gauge to test. The act of turning up or down the same gauge is called *exploitation* and the action of changing a gauge, or a direction of regulation introduces an element of *exploration*, where the user anticipates that changing the method of adjustment could lead to quicker or more precise convergence. A human agent may only require a few attempts to get a good grasp of the dependence $\frac{df}{dj}$ or $\frac{df}{dh}$, that is, the change in frequency with respect to the current or field. Content with an easy success, we may decide this is a non-problem, but in real life setup, there are just a few modifications that make the problem extremely difficult and prohibitively time-consuming for the human user. Firstly, we should observe that the dependence of frequency on current and/or on the field is often a nonlinear one, wherein one range of currents/fields yields distinctly different behaviour from some other range. Second, if the task is to be repeated for different types of oscillator, or even for oscillators of the same type that differ as a result of the fabrication process, we quickly find that there is a latent dependency on the intrinsic oscillator parameters that makes it difficult to carry over the process of tuning one oscillator to another. Finally, tying back to the issue of optimal control, we may wish to complete the task in the shortest possible manner, i.e. have an optimal procedure for going from initial state to synchronised state. In conclusion, the control problem for the simplest oscillators becomes nontrivial if we constrain the time and allow the intrinsic parameters to vary more or less freely. Conservative solutions from control theory toolboxes such as PID controllers¹⁷³ or LQRs¹⁷⁴ can help in a limited way, but fail in cases where the environment conditions change spuriously, as would be the case

¹⁷³ Proportional Integral Derivative

¹⁷⁴ Linear Quadratic Regulator

with varying parameters of the oscillator. However, such a problem turns out to be well-posed for a reinforcement learning setup, especially the one where the agent learns to be more adaptive to the environment. Reinforcement learning, although known for a relatively long time – a popular textbook by Sutton and Barto originally published in 1998¹⁷⁵ – lives through its renaissance, benefiting from tremendous progress made in effective training and design of deep learning models. In fact, those algorithms are known for integrating the aforementioned *exploration* and *exploitation* concepts into their learning mechanism.

¹⁷⁵ R. S. Sutton and Barto, *Reinforcement learning*.

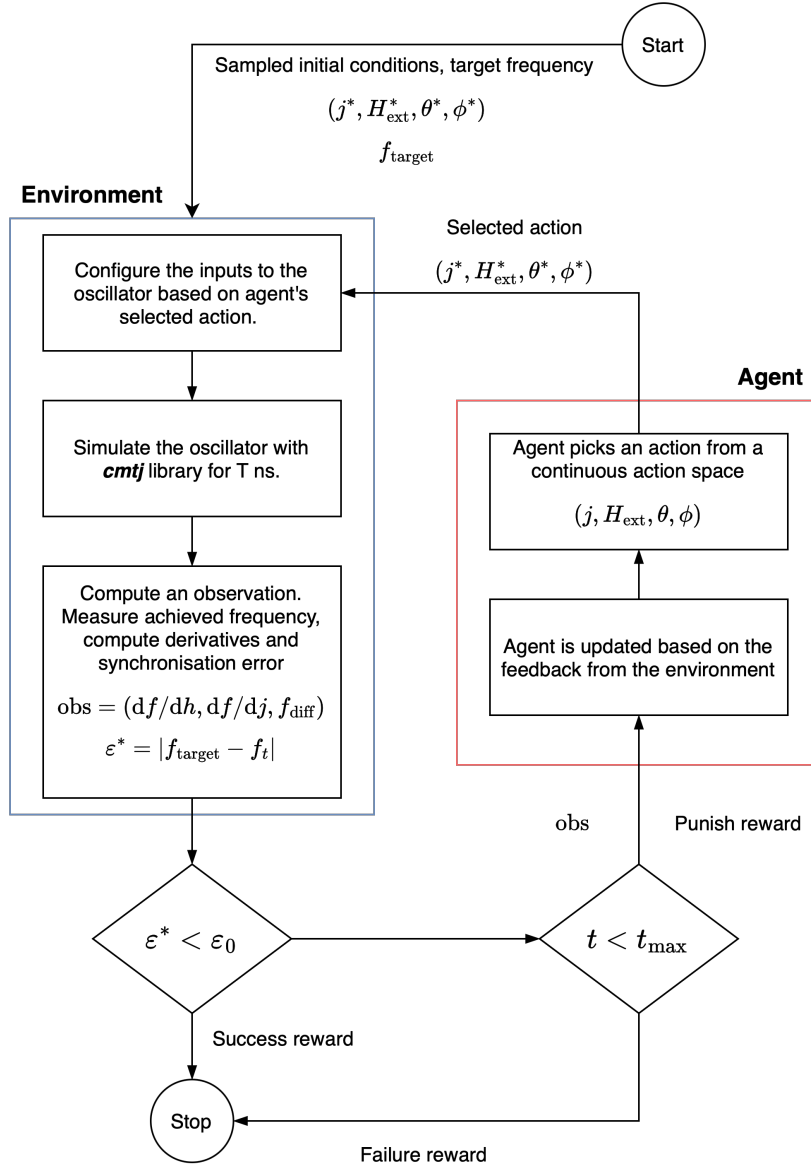


Figure 40: A schematic of a training and decision loop representing agent and environment design parts.

Implementation details

The work [Pub. 3: Reinforcement learning for spintronic oscillator application](#) outlines the implementation details for the RL-controlled environment of a spintronic oscillator. A simplified training loop schematic illustrating the setup is shown in Fig.40. The RL controller attempts to manipulate the input current and the applied external field such that the STO oscillates with a target frequency. The target frequency, starting control values, and magnetic parameters (K_u and M_s) are randomly assigned at each step, so the RL agent must be able to complete the task under varying conditions and in a fixed number of steps. The reward system has been engineered to ensure fast, but smooth synchronisation, and higher Q-factor of oscillations. The reader is referred to [Pub. 3: Reinforcement learning for spintronic oscillator application](#) for more details on the implementation of the environment design, the reward shaping, and the parameter used. Expanding on the *Reward shaping* section of that work, we stress that the design of the reward system is critical to learning behaviour and the convergence trajectory of the reinforcement learning agent. The primary objective of the agent is to reach a synchronised state, defined by a maximum synchronisation error ϵ^* (the difference between the desired and current frequency). Upon reaching this threshold, the agent receives a large success reward. At the same time, we want the agent to achieve the synchronisation as quickly as possible; therefore, we define a relatively small penalty applied at each step taken that does not result in synchronisation. If this signal is shaped, that is, is directly proportional to the synchronisation error ϵ^* , then the convergence to a good success rate is faster, and the mean path to synchronisation is shorter, as shown in Fig.41. The simulation is limited to 100 steps to ensure computational efficiency, enough to achieve synchronisation from any initial state. This truncation also helps formalise the terminal condition of the episode, although it does not affect the underlying Markovian nature of the environment.

Each time an additional reward component is introduced, the challenge of properly adjusting the reward weights ζ resurfaces. Unfortunately, resolving this issue requires trial-and-error experimentation. As the complexity of the reward system grows, the task of tuning becomes increasingly tedious. For example, if excessive weight is given to the error-shaping component relative to the action magnitude control term, the agent may learn to disregard the latter entirely. Similarly, assigning too large a weight to the Q-factor reward function overshadows the primary objective of achieving synchronisation, leading to much lower success rates. Furthermore, the time horizon over which the rewards are evaluated has a significant influence on the agent's behaviour. Consider a two-component reward system, with the reward for achieving the synchronised state ($\mathcal{R}_{\text{synch}}$) and the punishment relative to the synchronisation error ϵ^* ($\mathcal{R}_{\delta f}$). Suppose that the agent reaches a state s_1 where it receives a small penalty $\mathcal{R}_{\delta f} = 0.1$. The agent can choose to stay

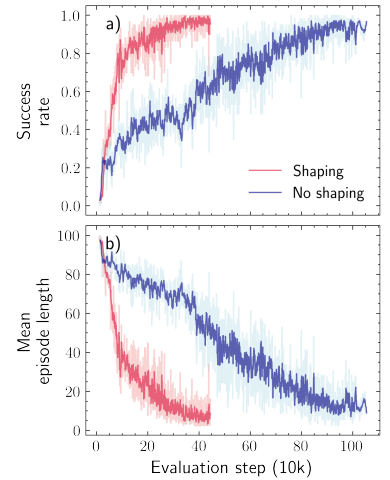


Figure 41: Impact of shaping on the success rate convergence speed and mean number of steps required for synchronisation. Making a part of the reward proportional to the synchronisation error ϵ^* (red) significantly improves the speed of training over a reward system where there is only a reward for achieving synchronisation (blue). The graph presents results averaged over 4 runs per each reward system.

in this state s_1 , for the remainder of the simulation, over 10 steps, which yields an expected return proportional to a discounted sum of $\mathcal{R}_{\delta f}$ over these steps. If some trajectories from s_1 to some other state s_2 produce a temporarily larger $\mathcal{R}_{\delta f}$, but ultimately achieve synchronisation, it is essential that the final reward for achieving the synchronised state does not vanish over the discounted sum in the expected reward. Otherwise, the agent may prefer suboptimal but locally rewarding behaviour. In other words, the magnitude of $\hat{\mathcal{R}}_{\text{synch}}$ must be sufficiently large compared to $\mathcal{R}_{\delta f}$ and the expected number required for synchronisation, to ensure that its signal is not lost in the cumulative return estimate.

Impulse shaping

CIMS is another strong application use case for RL. Ender et al. focused on reducing SOT-MRAM failure rates, employing reinforcement learning to adjust the time and amplitude of the two current impulses necessary for a single memory write operation¹⁷⁶. In that work, the authors assumed a step of variable duration and amplitude, but in this section we explore the possibility of learning the impulse shape itself. Two switching configurations are considered, as shown in Fig.42, one using the STT mechanism (a) and the other using the SOT mechanism (b).

The impulse shaping simulation is composed of many meta-steps, where each meta-step itself consists of multiple LLG simulation steps. Depending on the configuration, we adjust the meta-step simulation size and the number of LLG steps inside, but we keep the integration parameters constant. The agent can only set the controls at the meta-step level, and their values are considered constant for the duration of that meta-step. To improve sensitivity to change and decrease learning time while increasing the final success rate, the current is controlled through its exponent $j_t = \text{sgn}(a_t^j) 10^{\max(a_t^j + j^0, j^{\max})}$ A/m² where sgn is the signum function, j^0 is the offset of the exponent and $j^{\max}$ is the absolute maximum bound on the exponent. a_t^j corresponds to the unnormalised current density component of the controller action. This setup comes at the cost of some precision control and the lowest exponent should be treated as an effective zero signal. The observation space includes a z component of magnetisation, m_z , averaged over several last simulation steps of the meta-step, and its change over the duration of the meta-step, $\partial_t m_z$ and j . During our experiments, increasing the observation space with the remaining components did not significantly impact the learning process. Each episode has two stages: the control stage where the control input affects the simulation and the evaluation stage where the controller is disconnected. The evaluation stage only considers the alignment reward, and its role is to ensure that the magnetisation remains in a stable target state.

The baseline reward system is simple and focuses on rewarding the persis-

¹⁷⁶ Ender, De Orio, et al., “Improving failure rates in pulsed SOT-MRAM switching by reinforcement learning”; Ender, Lacerda De Orio, et al., “Reinforcement learning to reduce failures in SOT-MRAM switching”.

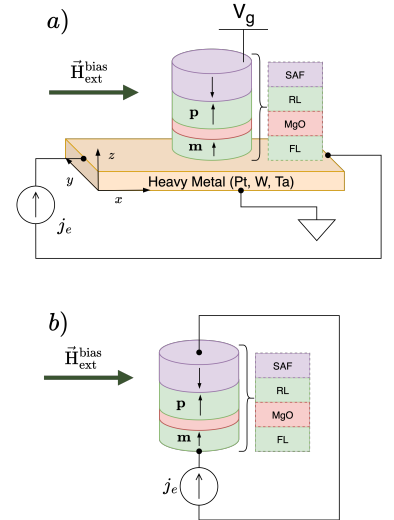


Figure 42: Proposed setups for RL impulse control in CIMS. (a) SOT configuration with optional VCMA control, (b) STT configuration. A small external applied magnetic field is needed to break the symmetry in this geometry.

tent and accurate alignment of the m_z component with the target state m_z^* :

$$\mathcal{R}_t = \zeta_{\text{energy},j} |a_t^j|^2 + \zeta_{\text{align}} |m_z^* - m_{z,t}|^2 + \hat{\mathcal{R}}_{\text{term}}. \quad (100)$$

where ζ denote weights of each reward component (they can be negative), and $\hat{\mathcal{R}}_{\text{term}}$ is a terminal reward which is awarded during the evaluation stage, after completing k control meta-steps. $\hat{\mathcal{R}}_{\text{term}}$ is positive if the magnetisation remains stable in the target state and becomes negative if the target has not been achieved within a small error $\varepsilon = 0.05$.

To conduct the simulation for a given meta-step, we use the standard LLGS equation, depending on the configuration: STT (7), or SOT (10). In STT configuration, the following parameters are fixed $\lambda = 0.69, P = 1.0$, in SOT we set $\theta_{\text{SH}} = 0.35$, utilising the following torque scaling of the damping-like torque ($H_{\text{FL}} = 0$ in the experiments)¹⁷⁷:

$$H_{\text{DL},t} = \frac{\hbar \theta_{\text{SH}} j_t}{2e M_s t_{\text{FM}}} \quad (101)$$

where t_{FM} is the thickness of the free FM layer. In both configurations, $\alpha = 0.035$, $t_{\text{FM}} \sim (1, 1.5) \text{ nm}$, $M_s \sim [(1 - \vartheta) M_s^0, (1 + \vartheta) M_s^0]$, $K_u \sim [(1 - \vartheta) K_u^0, (1 + \vartheta) K_u^0]$ ¹⁷⁸ where ϑ is the dispersion, usually between 2% and 15%, $M_s^0 = 0.95 \text{ T}$, $K_u^0 = 0.95 \text{ MJ m}^{-3}$.

Fig.43 illustrates a set of trajectories obtained from sample models trained in each of the configurations. In SOT switching, the agent clearly prefers to induce short-term current bursts and attempts to align them adequately to quickly maximise the $|m_z^* - m_z|$ component.

In our simulations, we observed that both the meta-step duration, operational current range, and parameter dispersion strongly affect the models ability to learn successful switching control. The dispersion of the parameters, that is, the thickness ranges, M_s and K_u , has a strong impact on both the final success rate and the learnt amplitude of the impulse. Since the model has no access to the underlying magnetic and dimensional parameters of the device during the control stage, the only cue that it can use is the response of the magnetisation at a given current impulse. As the model is punished for superfluous application of current, it does not have a 'probing' stage where it would attempt to triage the device parameters. Instead, the model opts for global optimisation (i.e. across various device realisation) of the current impulse, which yields maximal average success rate, and thus mostly chooses to operate with timed-short impulses of large amplitude and, if necessary, delivers secondary impulse of lesser amplitude to correct the trajectory. The latter strategy is highlighted in Fig.44, and we note that this approach to switching is learnt at random by selected models. Intuitively, the expectation could be that the model learns some sort of oscillatory pattern to improve switching rates and efficiency, but that requires a setup where the model has an option to probe or judge the parameters – this could either happen by a delivery of an additional observation entry or, through, as mentioned before,

¹⁷⁷ K.-S. Lee, S.-W. Lee, et al., "Threshold current for switching of a perpendicular magnetic layer induced by spin Hall effect".

¹⁷⁸ Here, the values were uniformly sampled from a given interval.

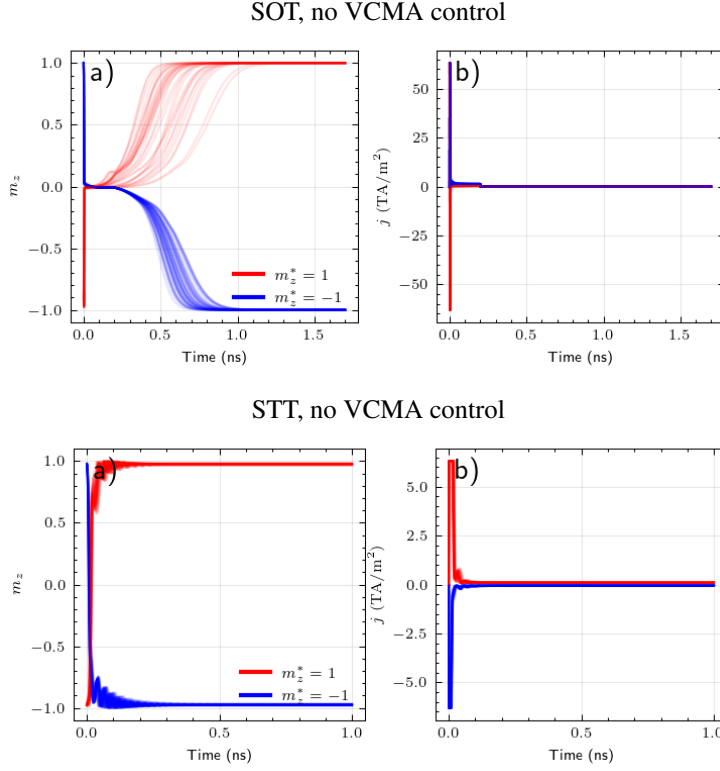


Figure 43: Overall comparison 100 assembled trajectories of the SOT and STT configurations. Magnetisation state over the switching period is shown in (a) and the corresponding current densities in (b). In the SOT configuration, the controller opts for two-stage current impulse to speed up magnetisation alignment with the target state. In the STT configuration, the model learns a single impulse, but of more shaped structure. Note that the current scales and time scales are different in each configuration. $\vartheta = 0.1$

a ‘probing’ stage preceding the control stage. Furthermore, as we mentioned, the duration of a metastep and the controller current density range also play an important role in the learning process. From an energy perspective, for successful switching, enough energy must be supplied to the system, not only exceeding the critical current, but also the minimal duration of the impulse. If the number of meta-steps is large, but they are short, the complexity of the problem for the model increases, and it is only aggravated by the increase in the controllable range of the current. Suppose a theoretical current threshold of 80% of the maximum range $j_c = 0.8j_{\max}$, a minimum pulse duration of 0.2 ns. Given a metastep of 1 ps, the model needs to learn to more or less consecutively apply the current at least above threshold for 200 steps in a row. The number of possible combinations becomes enormous if we additionally take into account the variation in magnetic parameters. In conclusion, we find that for the STT configuration, a meta-step duration of 0.8 ps, and a current exponent $x \in (10, 12.9)$ yield repeatable learnable models. In the SOT setup, the polarisation vector is set along the y direction, which necessitates that the current density drops nearly to 0 so that the magnetisation can relax to a stable state. Because of that, the relaxation seems to also take longer, which necessitates slightly longer meta-simulation steps. Therefore, we use $x \in (11, 13.8)$ and, at minimum, 0.8ps. We note that the temporal resolution is impractical in the real world, but it represents the *lower bound* of what the control algo-

rithms presented in this section can handle. For real-world application two sets of critical values must be established: (i) the controller resolution, that is, the minimal interval between successive control inputs (for example, the minimal time between a registered change in current from j_t to $j_{t+\Delta t}$), and (ii) the minimal resolution of the output quantity, in this case the resistance or voltage. Optionally, to keep the two timescales at comparable levels, one could take the maximum of (i) and (ii), and apply an estimator to the quantity with a finer resolution, for example by averaging the signal. Reward shaping

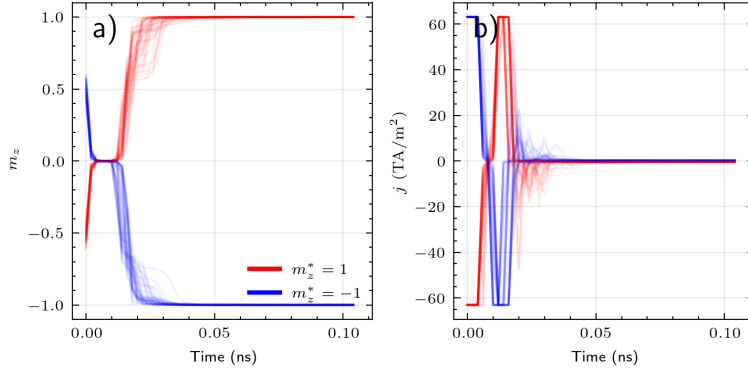


Figure 44: Sample trajectories from a controller that learnt a double impulse strategy for switching.

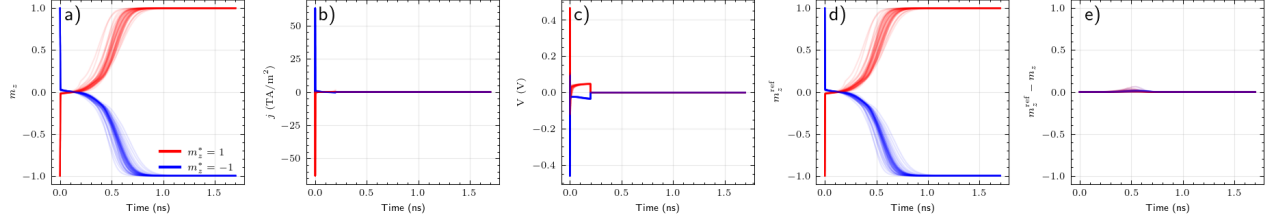
poses another challenge in this environment. Unlike the spintronic oscillator environment, the standard shaping signal, the alignment component of (100) is a weak signal during control stages due to general bistability of the system, and the terminal reward dominates. As mentioned in the previous subsection, good shaping speeds up training and can potentially improve stability. We tested two strategies that aim to increase the learning speed: directional current reward and progress reward. The former rewards the model for applying the current in the correct direction (positive or negative) given the target state. The progress reward applies a small positive reward each time the magnetisation is pushed towards the target state which depends on the change in the distance to the target:

$$\mathcal{R}_{\text{prog.}} = \zeta_{\text{prog.}} (|m_z^* - m_{z,t-1}| - |m_z^* - m_{z,t}|) \quad (102)$$

However, neither of those strategies caused any substantial increase in training speed. Instead, we continuously keep a N -element buffer of metastep errors, and if all elements fall within ϵ_0 , the evaluation period is initiated, which shortens the reward horizon, but disadvantages the model in learning to zero the current output after observing a successful switch. Contrary to what we observed in the spintronic oscillator environment, the PPO algorithm yielded a faster convergence to a good success rate and produced stable switching results. There are two potential reasons for this behaviour: one, the PPO should converge faster than SAC because of its direct policy optimisation focus in the environment where sample efficiency is not that relevant. Second, the

CIMS environment has a much narrower space of successful trajectories, and the reward landscape is rather sparse. Therefore, entropy-driven exploration of SAC and off-policy learning offer no advantage and may actually slow down the learning process.

SOT configuration with VCMA control



STT configuration with VCMA control

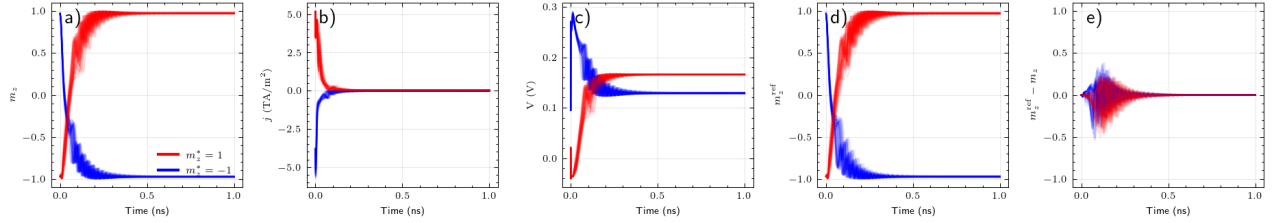


Figure 45: Overall comparison 100 assembled trajectories of the SOT and STT configurations, with additional VCMA control. The magnetisation state over the switching period is shown in (a) and the corresponding current densities in (b). $\vartheta = 0.1$ and δK is linear in V . The first column (a) presents the m_z trajectory with VCMA on, the second, (b) shows the current applied by the controller, and the third, (c), the voltage. The fourth column (d) shows the trajectory of a reference device that does not use VCMA, but was simulated under the same current trajectory as the VCMA device, and the last panel (e) shows the difference between the m_z trajectory of the reference device and the VCMA device.

Having studied the base case, we move on to the VCMA control which we will apply to both our configurations. We note that independent, simultaneous voltage and current control is not practically possible in the STT setup, yet as a means of comparison, it is included in the simulated cases. In the SOT configuration, we anticipate, based on (64), that the controller should prefer to apply the maximum possible voltage to lower the anisotropy, thus reducing the theoretical critical current. To our baseline reward from (100), we add the term linearly dependent on the voltage change that represents the current flow:

$$\mathcal{R}_t = \zeta_{\text{energy},j} |a_t^j|^2 + \zeta_{\text{energy},V} (a_{t-1}^V - a_t^V) + \zeta_{\text{align}} |m_z^* - m_{z,t}|^2 + \hat{\mathcal{R}}_{\text{term}}. \quad (103)$$

where a_t^V is the voltage action component of the controller at time t . If, instead, it is preferred to avoid large voltage values, not just change, then the term $\zeta_{\text{energy},V} (a_{t-1}^V - a_t^V)$ can be substituted with the component analogous to the current control: $\zeta_{\text{energy},V} |a_t^V|^2$. The result of learning with the VCMA control is shown in Fig.45. While for the SOT configuration there is no visible advantage to learning with V control, the STT setup slightly benefits

by reducing the current density impulse amplitude. This is probably due to the agent having difficulty in properly learning VCMA application in a timely fashion, that is, lowering the anisotropy barrier before initiating the impulse current rather than attempting both at the same time.

When comparing both the VCMA control and the baseline, the agent prefers to induce short-term current bursts, which in effect resembles the standard impulse excitation used in CIMS. The short time scale is due to the macrospin assumption, which underestimates current densities, but is not uncommon in similar modelling scenarios involving microspin approaches¹⁷⁹. Additionally, the RL agent autonomously learns to set both the voltage and the current to 0 after having observed that the target position has been attained. This behaviour is achieved by balancing the energy and the alignment reward.

¹⁷⁹ Ender, Lacerda De Orio, et al., “Reinforcement learning to reduce failures in SOT-MRAM switching”.

Chapter summary

The chapter introduces the field of reinforcement learning with specific applications to spintronic devices. Fast simulation times enabled by efficient implementation in CMTJ offer tremendous opportunities to facilitate this kind of research. The examples given so far are based on the simulation alone, but further research should focus on the on-hardware implementation of the trained agents, with potential prior fine-tuning. Designing more intelligent devices can shorten the time to market of potential spintronic devices, for example, via efficient optimisation of the input controls, which we have shown with the synchronisation example. In terms of simulation, the next step could concentrate on optimising micromagnetic models such that they too could be easily integrated into the RL training procedures; at the moment, this is computationally challenging, as such training requires thousands, if not millions, of simulations per training run. Additionally, more effort can be directed towards creating more realistic simulations by taking into account device and measurement limitations with a greater degree of fidelity. For instance, during our simulations, although we include a relatively small parameter dispersion, little to none experimental noise is assumed. Those assumptions can be addressed in the RL context as well, but require meticulous revision when discussing a specific experimental setup.

Summary and outlook

This thesis presents contributions to the large-scale modelling of multilayer spintronic devices. With a rapid increase in general-purpose computational power, we anticipate that the methods discussed in this thesis will soon become computationally feasible on personal computers also in the micro-magnetic setting. However, at present, our focus is on providing tools and techniques to help the community achieve faster device design iterations, simplify parameter fitting, and streamline the theoretical workflows required to reproduce experimental results. This goal is particularly evident in the first two contributions: Mojsiejuk, Ziętek, Grochot, et al. (“[cmtj](#)”) and Ziętek, Mojsiejuk, et al. (“[Numerical model of harmonic Hall voltage detection for spintronic devices](#)”), which open-source the simulation software and provide easy-to-use recipes for reproducing various numerical models corresponding to known experiments. The utility of these solutions was then demonstrated and elaborated in subsequent chapters, notably in [Modelling spin Hall devices](#) and [Modelling magnetic tunnel junctions](#), highlighting the explanatory capabilities of the methods when applied to numerically complex systems.

Another exciting research direction emerges from the final contribution that employs methods developed within reinforcement learning to spintronics. As outlined in the chapter [Dynamic control of devices](#), automating processes via real-time control of multiple device implementations may facilitate their industrial adoption, addressing a persistent challenge common to various scientific disciplines.

The subchapter of [Modelling magnetic tunnel junctions](#) discusses $1/f$ noise with a similar intention. Capturing the nature of this noise numerically has a broader potential, as identifying operating points with optimal signal-to-noise ratios has been an ongoing difficulty for nearly a century in classical electronics. The ability to incorporate the noise as an extra field contribution may lead to more realistic and accurate device simulations.

Appendix

Estimate of the MLS gap

To complement the simulation-based discussion on the introduction of the β parameter, we now derive a semi-analytical calculation for the bounds of the non-zero δ_{MLS} gap. In a numerical sense, the asymmetry is defined as a discrepancy between the AHE resistances between two Co-Pt interfaces that make up the structure. As per the diagram in Fig.46, we denote a state $s_{XY}^{+/-}$ as a state of m_X on the Y side of the hysteresis, because we are concerned only with the edge states (left, right) for both magnetisations. We compute the resistance (R_{XY}) of the hysteresis in the state of the left or right edge (the leftmost and rightmost value) as: $R_L^+ = s_{00}^+ + \beta s_{10}$ and $R_R^+ = s_{01}^+ + \beta s_{11}$ respectively, for the positive field (the negative field has the same, but we swap the superscript $+ \rightarrow -$).

For state separation δ_{MLS} , we are concerned only if the left (right) state in positive H_{ext} is above the left (right) state in negative H_{ext} . Alternatively, we are allowed to swap the inequality, saying that the state at the left (right) state at the positive field is below that at the negative field. Assume that the positive field hysteresis is to be above the negative field hysteresis:

$$\begin{aligned}
 & R_L^- < R_L^+ \wedge R_R^- < R_R^+ \\
 & \text{starting with: } R_L^- < R_L^+ \\
 & s_{00}^- + \beta s_{10}^- < s_{00}^+ + \beta s_{10}^+ \\
 & s_{00}^- - s_{00}^+ < \beta (s_{10}^+ - s_{10}^-) \\
 & \text{which produces:} \\
 & \beta > \frac{s_{00}^- - s_{00}^+}{s_{10}^+ - s_{10}^-}, \text{ if } (s_{10}^+ - s_{10}^-) > 0 \\
 & \beta < \frac{s_{00}^- - s_{00}^+}{s_{10}^+ - s_{10}^-}, \text{ if } (s_{10}^+ - s_{10}^-) < 0
 \end{aligned}$$

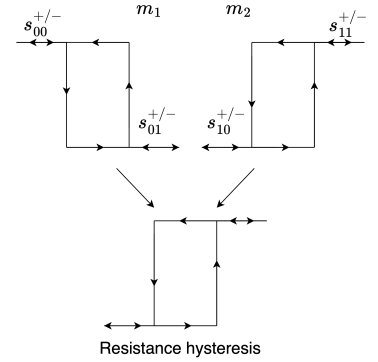


Figure 46: Diagram of switching. The top two hysteresis are magnetisation trajectory switching for each current density that composes the final resistance hysteresis. The picture is given for a specific value of H_{ext} . Arrows indicate the current sweep direction.

likewise, for $R_R^- < R_R^+$:

$$\begin{aligned}
 s_{01}^- + \beta s_{11}^- &< s_{01}^+ + \beta s_{11}^+ \\
 s_{01}^- - s_{01}^+ &< \beta(s_{11}^+ - s_{11}^-) \\
 \beta &> \frac{s_{01}^- - s_{01}^+}{s_{11}^+ - s_{11}^-}, \text{ if } (s_{11}^+ - s_{11}^-) > 0 \\
 \beta &< \frac{s_{01}^- - s_{01}^+}{s_{11}^+ - s_{11}^-}, \text{ if } (s_{11}^+ - s_{11}^-) < 0
 \end{aligned}$$

The reverse condition (i.e., where the negative-field hysteresis exceeds the positive) can be derived by inverting the inequality signs. The state separation

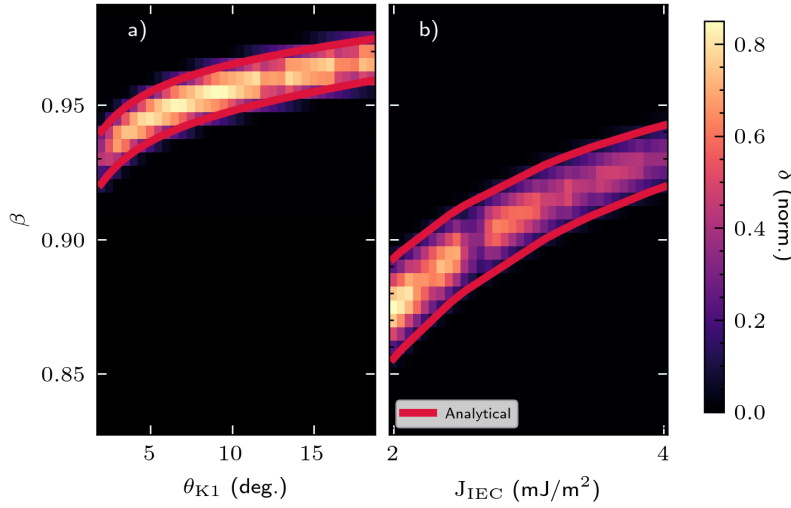


Figure 47: Solid red line follows analytical determination of β (AHE asymmetry) from conditions on $\delta_{\text{MLS}} > 0$. (a) state separation according to the anisotropy polar angle θ_{K1} and β , (b) state separation as a function of J_{IEC} and β . The δ_{MLS} is normalised respective to a maximum value. There is a clear gap size divergence from the centre of the gap interval – the gap gets smaller as it nears the red analytical line.

is thus defined as:

$$\delta_{\text{MLS}} = \min\{R_L^+ - R_L^-, R_R^+ - R_R^-\} \quad (104)$$

subject to constraint above on β . The existence of state separation will depend on the fact that β can be found such that it satisfies the condition for $R_L^- < R_L^+ \wedge R_R^- < R_R^+$. Fig.47 depicts ranges of β , θ_{K1} (a) and β , J_{IEC} (b) producing non-zero δ_{MLS} . The red line comes from the analytical calculation of δ_{MLS} given a set of $(m_{z+}^{(1)}, m_{z+}^{(2)}, m_{z-}^{(1)}, m_{z-}^{(2)})$ states, with the subscript denoting positive or negative H_{ext} .

Coupled current for the in-series configuration of STOs

In our research, we have considered two models: one as discussed in [Numerical modelling of electrical in-series coupling](#), and the other where the current strictly follows Kirchoff's current law (KCL) and is the same for both MTJs, that is,

$$j_{\text{total}} = j_0 + j_0\chi(\mathbf{m}_L \cdot \mathbf{p}_L + \mathbf{m}_R \cdot \mathbf{m}_R) \quad (105)$$

where j_0 is the baseline current and j_{total} is the current flowing in the circuit. Generally, after assuming (105), the simulation results are qualitatively the same, and for comparison, we show the reproduction of Figs.24 and 27; see Figs.48 and 49, respectively. In those figures, we only modified the value of χ so that the synchronisation regions have a size similar to that in Fig.24.

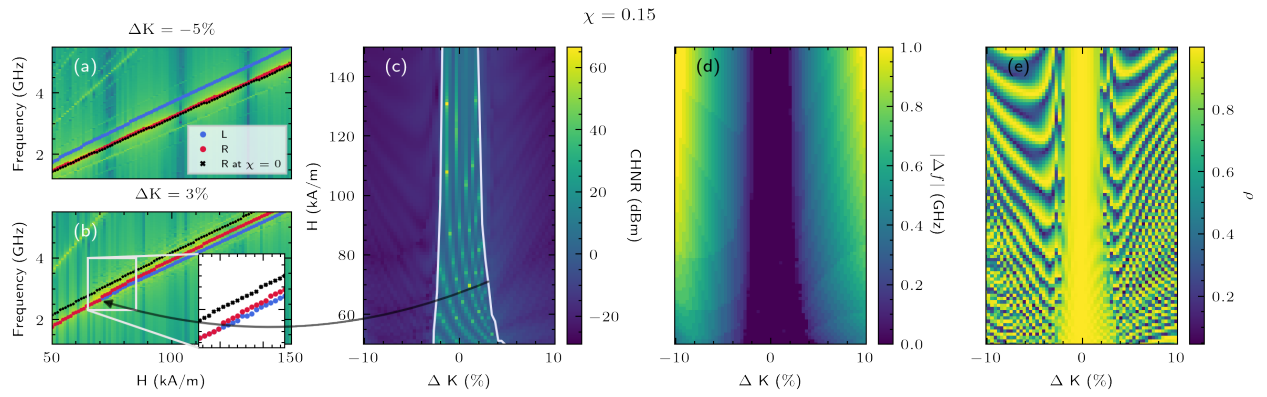


Figure 48: Reproduction of Fig.24 from the manuscript with j_{total} . The $\chi = 0.15$, a smaller value than the one in the manuscript to bring the regions to a scale similar to that in the original figure. (b) panel has also been adjusted to show the desynchronisation field at $\Delta K = 3\%$. The remaining parameters are preserved exactly as per Fig.24.

The major difference is the smaller asymmetry towards larger ΔK which is directly related to the fact that the oscillation mode of L stays fixed, and thus the order of MTJs in the in-series configuration plays a more significant role. However, in the case presented here, the asymmetry is still visible, especially if we enlarge the regions by increasing χ , and it is similarly skewed towards positive ΔK . Regardless of the specific details of the coupling mechanism, the key factor behind the proposed *desynchronisation* still lies in the asymmetry in magnetic parameters between the two coupled oscillators, a condition that remains the same in both cases discussed.

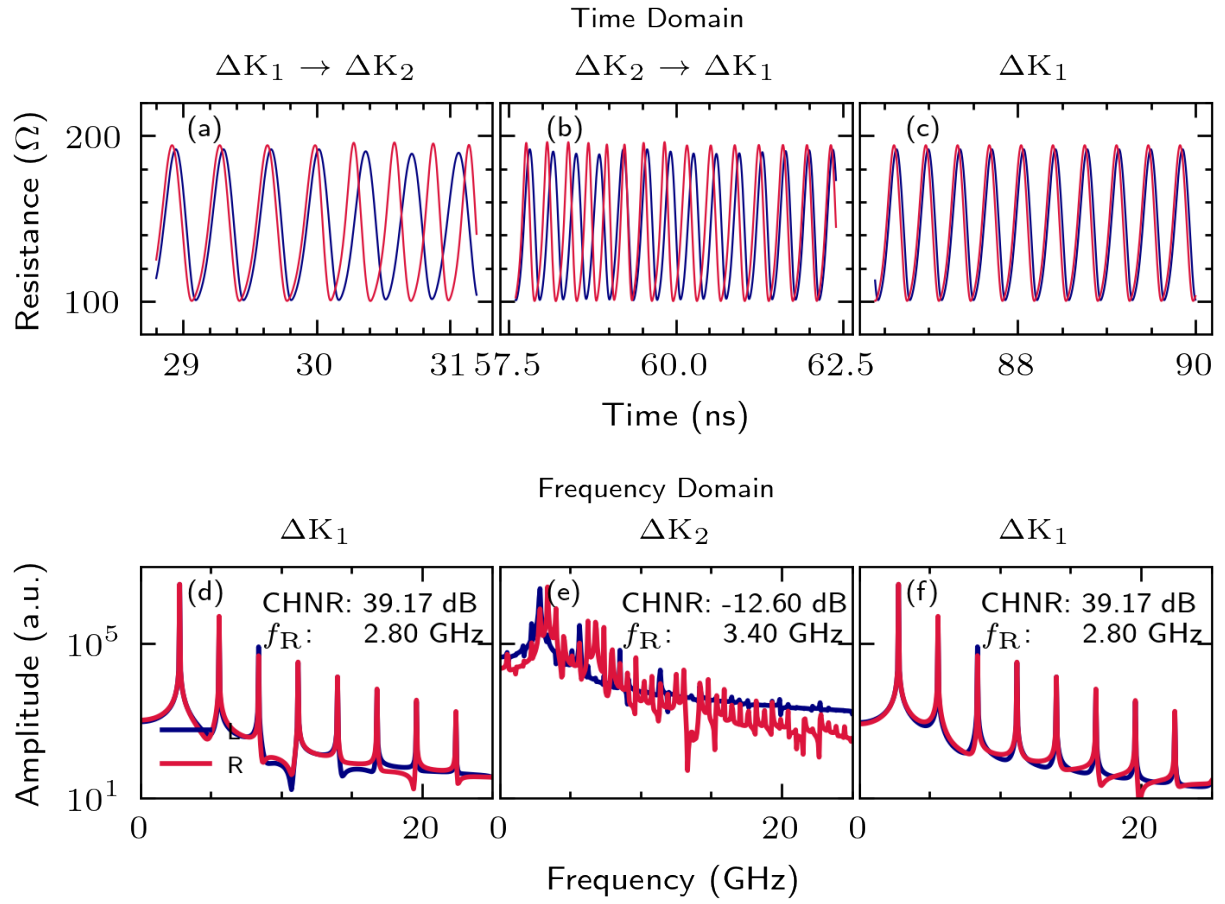


Figure 49: Reproduction of Fig.27 from the [Numerical modelling of electrical in-series coupling](#), but with strict preservation of KCL, with $j_{\text{total}} \cdot \chi = 0.1$, all the remaining parameters as in the original figure.

Additional Tools and Interfaces for CMTJ

For a description of the full range of CMTJ, together with comprehensive simulated examples, the reader is encouraged to visit the package documentation at <https://lemurpwned.github.io/cmtj/>. In this section, we briefly discuss some of the additional tooling that enhances the CMTJ library.

Web interface

Built with the Streamlit framework, the web interface enables quick and intuitive parameter fitting using standard measurement techniques such as VSD or PIMM. It offers a user-friendly interface, specifically designed for experimentalists who might have limited experience with simulation software. Users can access the application directly from the Web browser at <https://cmtj-app.streamlit.app> and run simulations without requiring software installation or dependency management. The interface allows users to adjust the number of layers and their basic magnetic and geometric parameters, change the system's excitation type, and modify field or frequency scanning parameters.

Agentic package helper

In addition to the WebUI, we also provide a large language model (LLM) agentic system that can help the user navigate the world of macrospin simulations. The code is available at <https://github.com/LemurPwned/cmtj-cursor>. Fig. 50 shows the high-level overview of the agent with four categories of nodes: standard non-LLM nodes (blue), LLM nodes (green), tool nodes (red), and data nodes (purple). As the user query enters the flow, it is first classified – the system determines whether the user asks for code or asks a general question about simulations or spintronics. If the input is classified as a question, the subquery generator node produces up to three additional questions to broaden the search scope. Then a vector search is performed on the local index of the spintronics literature. Optionally, web search results can be included, but the article search is always preferred by the response synthesis model. If the user input asks for code, the flow is transferred to a planning agent that has access to a range of tools: *code search*, *documentation search*, and *code validation*. The code search is performed on the CMTJ repository and a set of curated simulation examples. *Docstring search* is a special index that parses function signatures and class documentation. Such a search enables partial keyword matching across the parsed fields. Finally, there is a code validation and fixing loop, where the *Validate code* first compiles and runs the code and the *Fix code* attempts to fix any simple errors before handing it over to the main agent again for further processing. When the code agent completes the generation, it calls the LLM to prepare the final user-friendly response. The code generation agent with tool calling

benefits most from reasoning models, whereas the remaining LLM nodes do not require such capabilities.

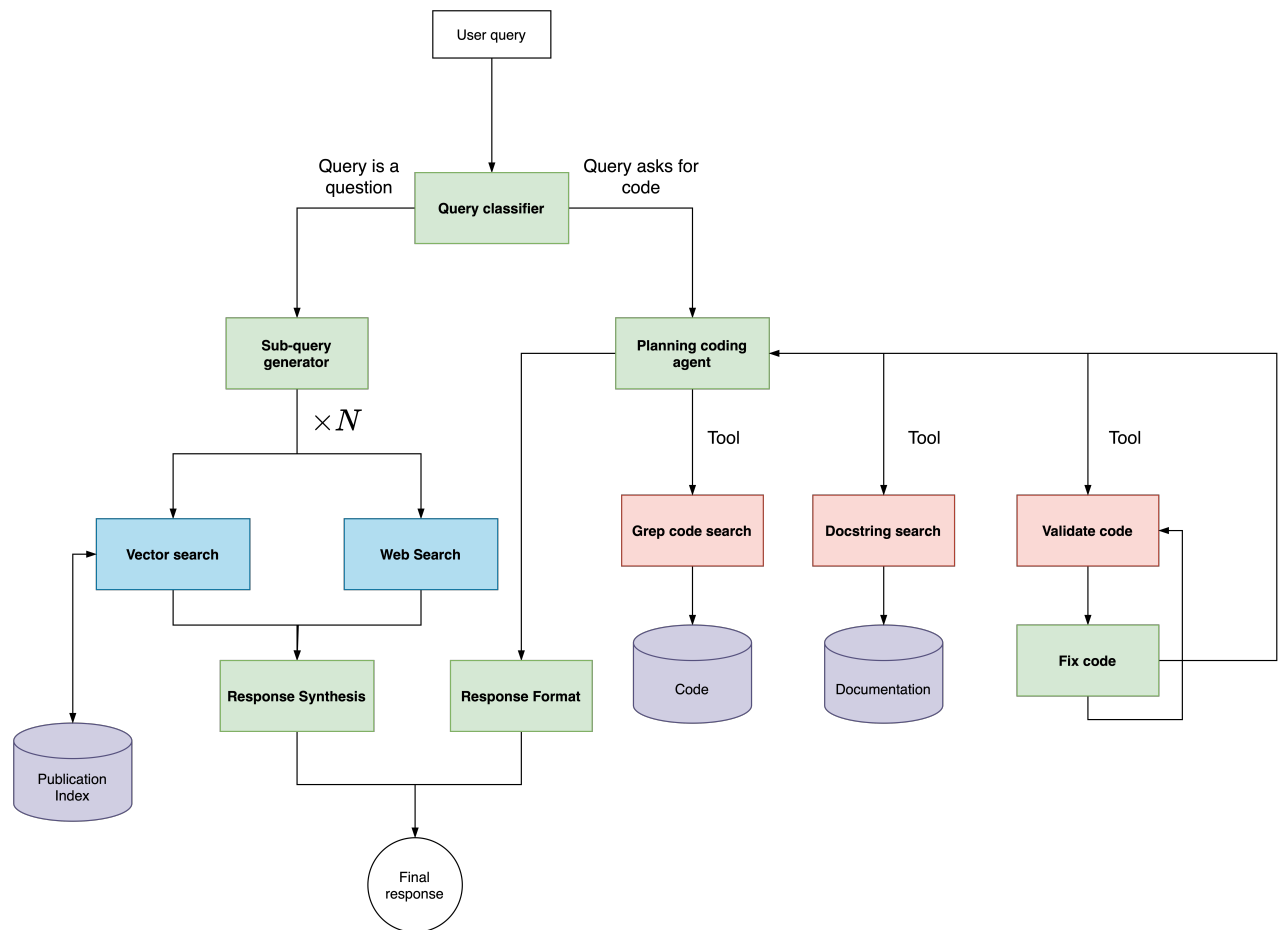


Figure 50: A layout of the LLM Q&A and code agent. Green denotes LLM nodes, blue non-LLM nodes, red denotes the *tool* nodes, and document databases are shown in purple.

Magnetization dynamics driven by displacement currents across an MTJ

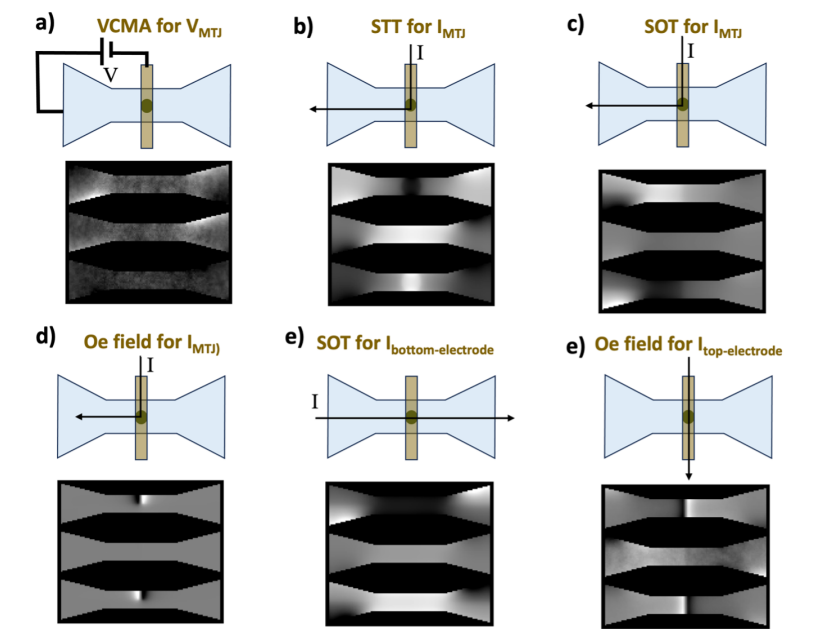


Figure 51: 'Micromagnetic simulation showing the expected magnetization dynamics in the bottom electrode if (a) voltage across MTJ leads to VCMA, (b) current through MTJ gives STT, (c) SOT generated at bottom electrode region where the current flows, (d) Oersted field generated from the top electrode region where the current flows, (e) the current is applied through only bottom electrode generates SOT at the entire bottom electrode, and (f) the current is applied only through top electrode leading opposite Oersted field along both sides of the top electrode. For each case, the top panel shows the current or voltage configuration, and bottom image consists of 3 snapshots of simulated magnetization dynamics at time=maximum, minimum and zero nodes. The black and white contrast corresponds to magnetization variation along +Z and -Z directions respectively'. Figure sourced from appendix of Safeer, C., Keatley, P. S., (Aug. 2024). "Magnetization dynamics driven by displacement currents across a magnetic tunnel junction". In: *Physical Review Applied* 22.2, p. 024019.

¹⁸⁰ Safeer, Keatley, et al., "Magnetization dynamics driven by displacement currents across a magnetic tunnel junction".

Although relevant to the topics discussed in this dissertation, we placed the description of the simulations from Safeer et al.¹⁸⁰ in the Appendix due to their micromagnetic nature. The structure described in that work consists of an MTJ pillar (CoFeB/MgO/CoFeB) placed atop a W substrate. The purpose of the simulations was to explain the origin of the magnetisation dynamics observed in the experiment. In total, six alternatives were considered: excitation via the VCMA across MTJ leads (mostly, through the top layer), the STT through the MTJ, the SOT generated in the bottom electrode (W) or top electrode (Pt), the Oersted field from the top electrode (Pt), and bottom electrode (W). All of these options are shown in the top diagrams of Fig.51. We simulated the corresponding cases with Mumax3¹⁸¹, taking the approximate magnetic parameters from the work. The particular strip geometry was replicated in the simulation using cutout geometry, we set the cell size at 2 nm, $A = 13 \text{ pJ m}^{-1}$. The following is an excerpt from the publication that describes in detail the simulations conducted to pinpoint the mechanism responsible for the magnetisation dynamics patterns observed in the experiment.

At first, we induce magnetization saturation by applying an in-plane field, $B_y = 75 \text{ mT}$. For each excitation type, we use the RF signal in the GHz range 3-9GHz (depending on what the system responds best to) and take snapshot at maximum, minimum and zero nodes as shown in Fig.51. In the VCMA

¹⁸¹ Vansteenkiste, Leliaert, et al., "The design and verification of MuMax3".

simulation, we lower the B_y field to 1 mT, and increase the anisotropy to better capture the excitation via the RF signal. In the STT and VCMA simulations (Fig. 51 a-b), we excite the system exclusively in the center, where the circular MTJ pillar meets the FM layer. Similarly, for the case (c, bottom), where the system is excited with the current flowing through the top electrode and then through the pillar, we model SOT excitation only in the left half of the geometry.

Following the results of the simulation, the conclusion was reached that the Oersted field (as shown in Fig. 51e) best replicates the experimental observation.

Sample fabrication process

For completeness sake, we include a short mention of the fabrication techniques of the spintronic devices in question. Most of the multilayer thin film samples, of which numerical fits are presented in this work, were prepared by Singulus, the Advanced Institute of Industrial Science and Technology (AIST) and the Institute Molecular Physics of the Polish Academy of Sciences. In most cases, samples were deposited using the magnetron sputtering technique on thermally oxidised silicon wafers. The samples were then patterned in the cleanrooms of the AGH Academic Centre for Materials and Nanotechnology.

The deposition method depends on the target type; most commonly, metallic layers are stacked onto an oxidised silicon wafer using magnetron sputtering. In this technique¹⁸², a gas¹⁸³ is pumped into a vacuum chamber where the target material is located in the cathode and the substrate in the anode. The magnetrons create shaping magnetic fields that, combined with a high electric field, trap electrons into circular paths close to the target. This process increases the ionisation efficiency of the gas and leads to the creation of high-density plasma regions at the cathode. Consequently, a high kinetic impact of the ions knocks out the target material particles that eventually deposit at the substrate. Quite often, as a method of streamlining the measurement process, the sample is prepared in the form of a wedge with varying thicknesses of critical elements in the stack. For instance, later sections discuss the Co/Pt/Co interfaces, where the Pt thickness is varied. This is achieved by slowly moving the wafer at a constant deceleration rate under the sputtering target and at a constant deposition rate¹⁸⁴. Other techniques such as MBE^{185,186} are also common in the MTJ fabrication process. MBE is based on the epitaxial growth of deposited vapour particles released from so-called K cells¹⁸⁷ that contain the target material. Usually, the growth rate and its quality can be monitored using the accompanying RHEED¹⁸⁸ technique. Alternatively, AFM targets such as NiO can be deposited using PLD¹⁸⁹, wherein a strong pulse-gated laser beam incident on the target causes the plasma plume to be kinetically ejected towards the substrate and film growth.

After the deposition process, micro- and nanofabrication is performed at the Academic Centre for Materials and Technology of AGH University using optical or electron lithography, ion-beam milling, and the lift-off process. The first of those steps involves coating the sample with a negative photoresist¹⁹⁰ – this usually occurs by means of a spin coating, with the photoresist uniformly spreads on the substrate as a result of a high but constant spinning rate of the sample. After the sample is annealed, the lithography mask is imprinted, for example, using an adapted SEM¹⁹¹ and then etched, often with the ion milling method¹⁹². After the etching stage, the Ti/Au contact layers are deposited and then, during the lift-off process, the positive photoresist is removed along with the redundant conducting layers atop.

¹⁸² Swann, “Magnetron sputtering”.

¹⁸³ usually a noble gas such as Argon or Xenon

¹⁸⁴ as an example, given 6 cm distance between the target and the substrate, the deposition rate of wolfram at 4 W is about 0.01 nm s^{-1}

¹⁸⁵ molecular beam epitaxy

¹⁸⁶ Singh, Bhardwaj, et al., “Fabrication of Magnetic Tunnel Junctions”.

¹⁸⁷ Knudsen cells

¹⁸⁸ reflection high energy electron diffraction

¹⁸⁹ Pulsed Laser Deposition

¹⁹⁰ a negative photoresist hardens after exposure to the UV light, making it resistant to etching. In contrast, a positive photoresist becomes easily solvable in the etching solution after it has been exposed to UV light

¹⁹¹ scanning electron microscope

¹⁹² dry etching process in which high energy ions kinetically knock off the unmasked material. Plasma is usually generated using a strong RF field

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