Atomistic spin dynamics
Micromagnetics

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Few questions awaiting answers

- **What is a physical system?**
- **What is a model** (in physics)?
- **What is expected from a model?**
- **What are the means to validate a model?**
- **What is the strategy for building a model?**

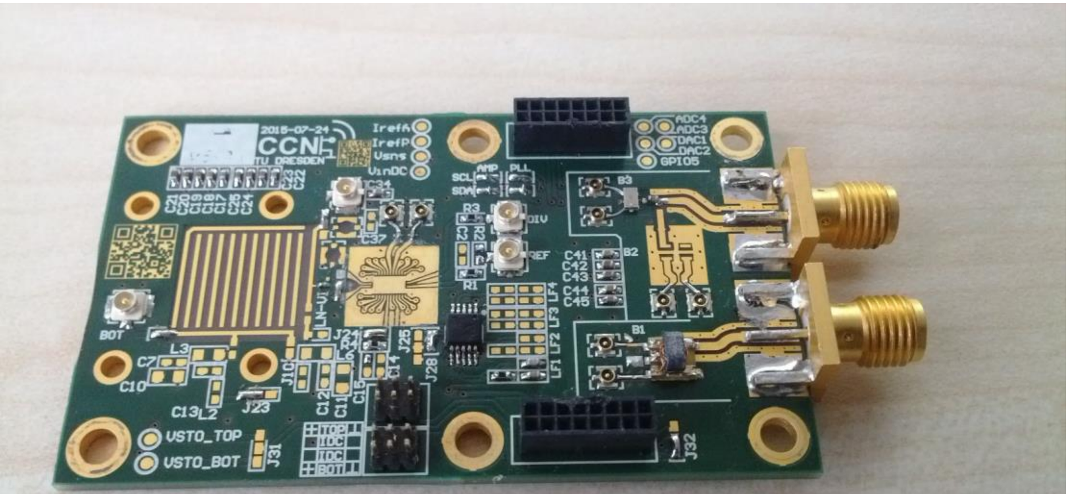
Modelling - research and debate

- **What is a physical system?**

The systems under investigation are complex:

- more than one constituent in the system
- the constituents cannot be considered as independent

Experimental characterization is challenging



PCB board with spin torque oscillators
Mosaic EU Grant

Modelling - research and debate

- **What is a model** (in physics)?

  Describe as faithfully as possible the system under investigation
  Define the physical quantities of interest
  An idealized version of a system, simple enough so that
  it can be solved but no too simple to preserve essential physics

Reality ☺

Model 1

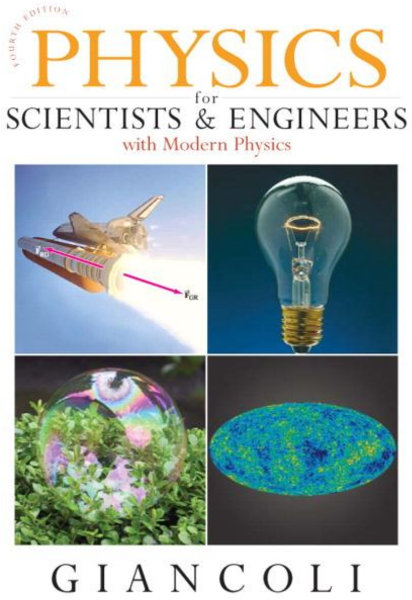
Model 2

…..

Modelling - research and debate

- **What is expected from a model?**

  Analysis of the solution leads to increased understanding of a phenomenon or process, which can lead to radical improvements and knowledge progress.



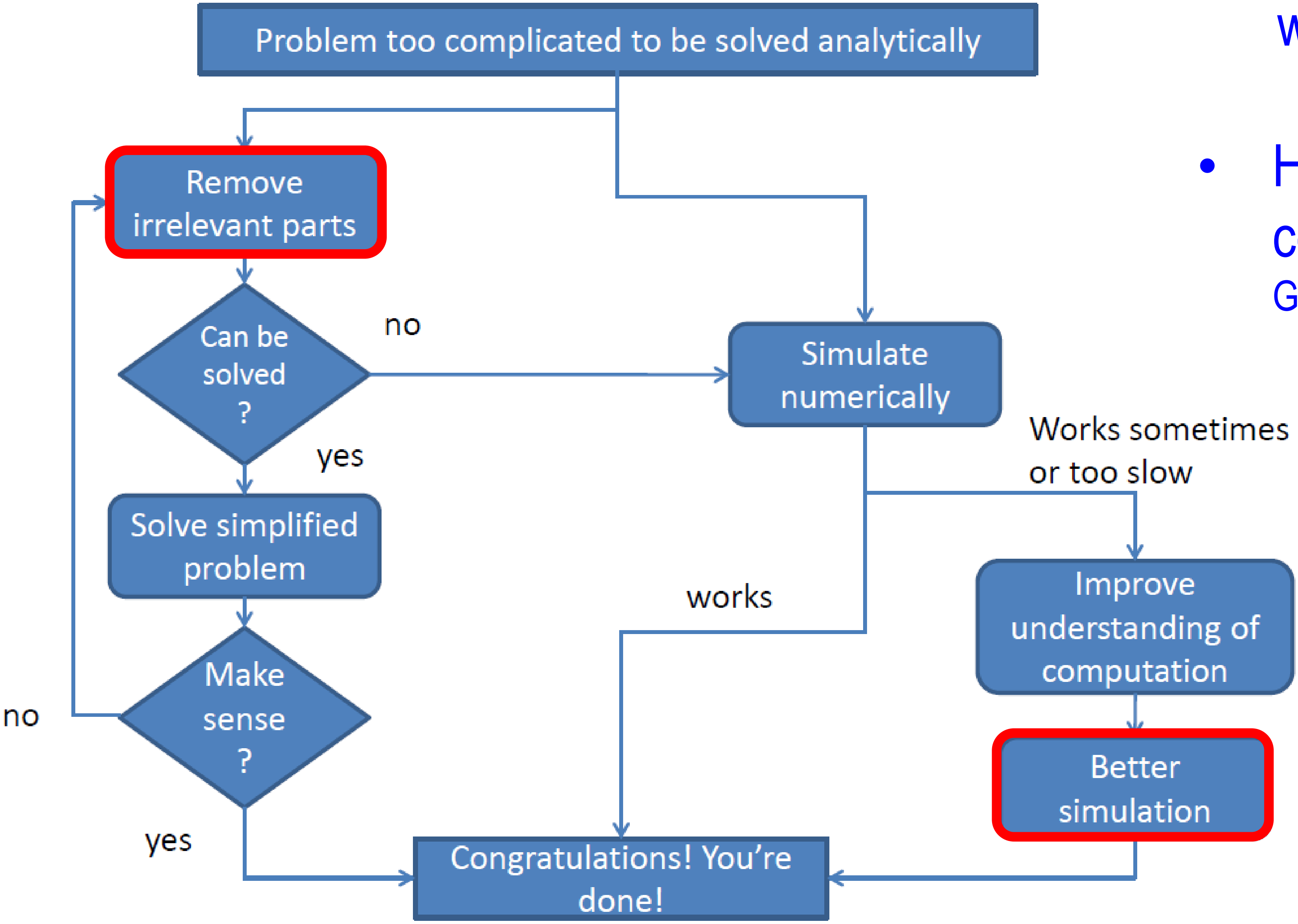
- **What are the means to validate a model?**

  Comparison with experiments and other models (it makes sense ☺)

- **What is the strategy for building a model?**

  Solve the appropriate equations, either analytically or numerically.
  $\rightarrow$ this allows to calculate the physical quantities of interest.

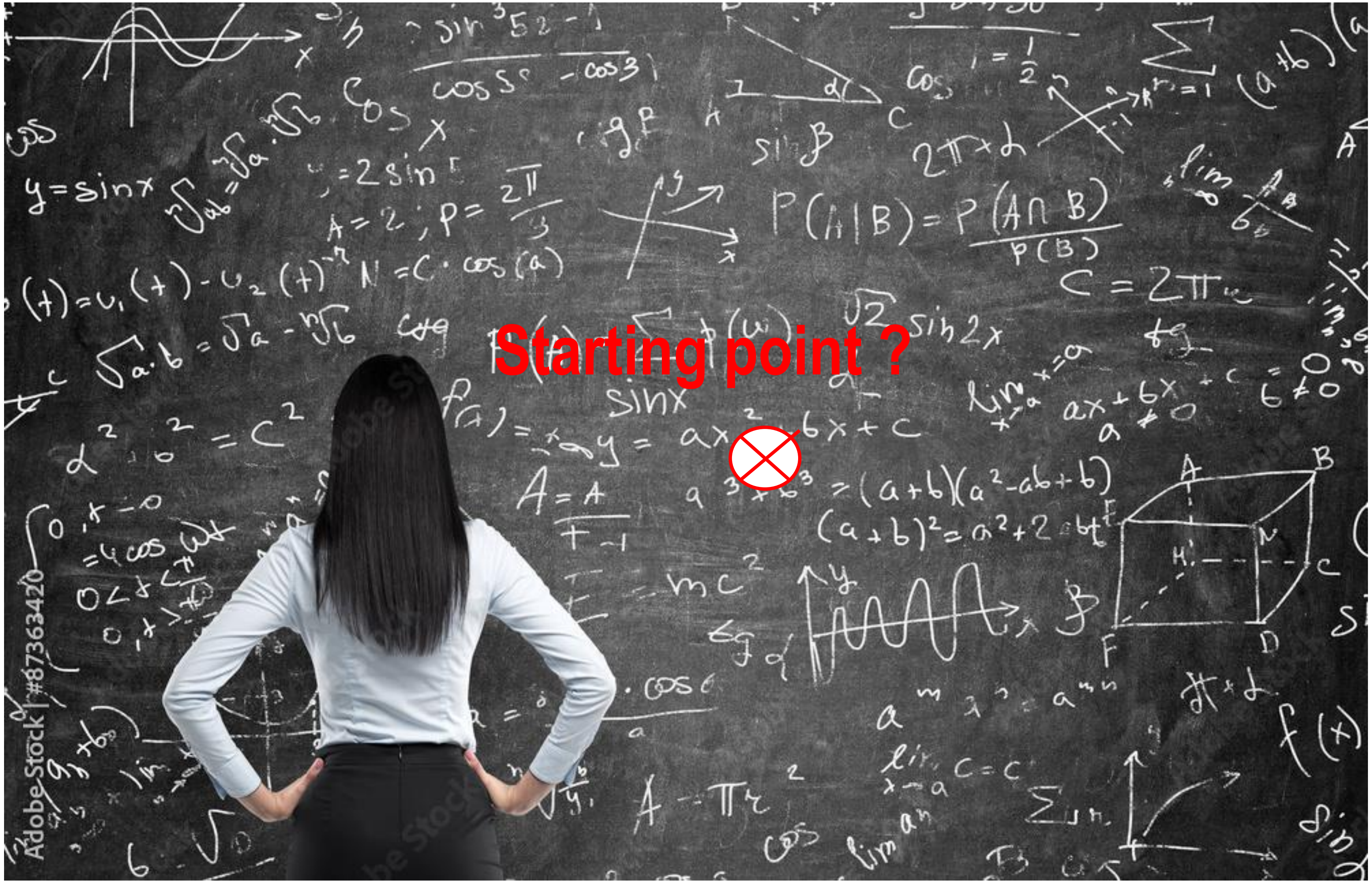
What is the strategy for building a model?



- Step by step, iteratively with rigor and critical thinking
- Hard but most of the time collective work - literature, GNU General Public License, github, <u>openscience</u>

Outline

- **Atomistic spin dynamics**
  - Formalism
  - Illustrations : alloy GdFe, Fe nanodot, AOS [Tb/Co] multilayers
- **Micromagnetism**
  - Formalism
  - Macrospin limit
  - Illustrations
- **Micromagnetism and spin related phenomena**
  - Formalism
  - Illustrations
- **Conclusions**


Starting point ?

Hierarchy of models in magnetism: space & time

few primitive cells — **ab-initio calculation**

K, J, μ

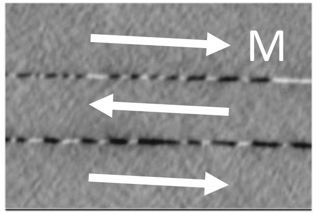
few nm^3 — **atomistic models**

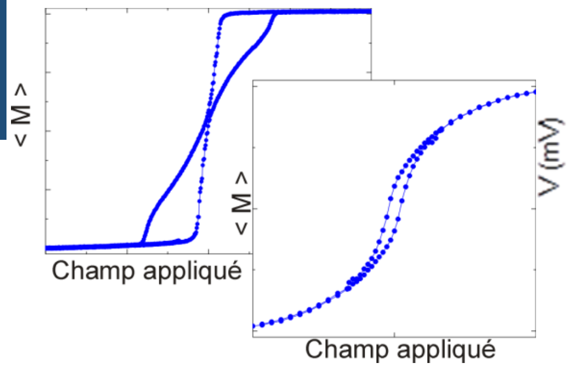
$K(T), A_{ex}(T)$
$M_s(T)$

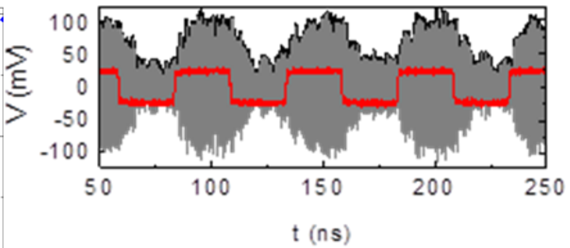
< µm — **micromagnetic models**

Experiments

RX, TEM, AFM - crystalline structure, composition topography, defects, µstructure
MFM, MOKE, NV - magnetic domain structure
VSM, SQUID, XMCD - hysteresis loops $M(H_{app})$, $M(V_{app})$
TR-MOKE: real time signals
Real time resistance measurements
many other techniques







ultra-fast — *fast* — *rare events (slow)*

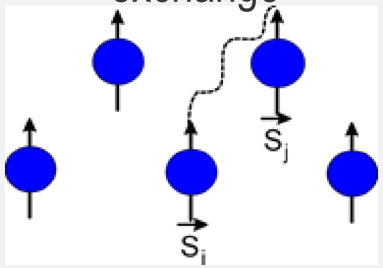
fs — *ps* — *ns* — *µs* — *h* — *year* — *time scale*

atomistic LLG — *µmicromagnetic LLG* — *kinetic Monte Carlo, minimum energy path, statistical approaches,…*

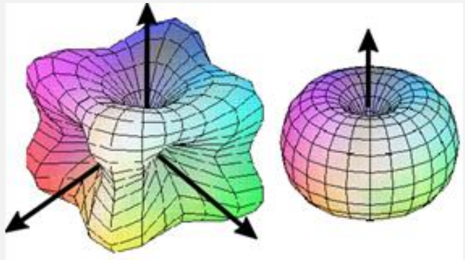
Main “ingredients” in magnetism & spintronics

Typical interactions

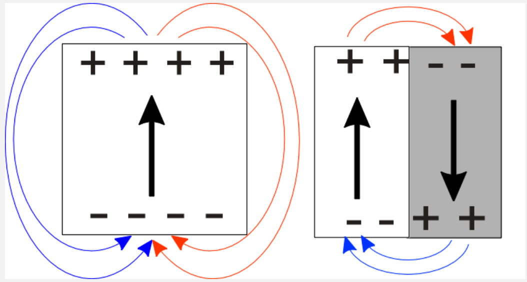
exchange



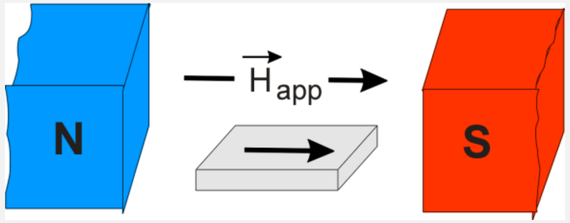
magnetocrystalline anisotropy



magnetostatic

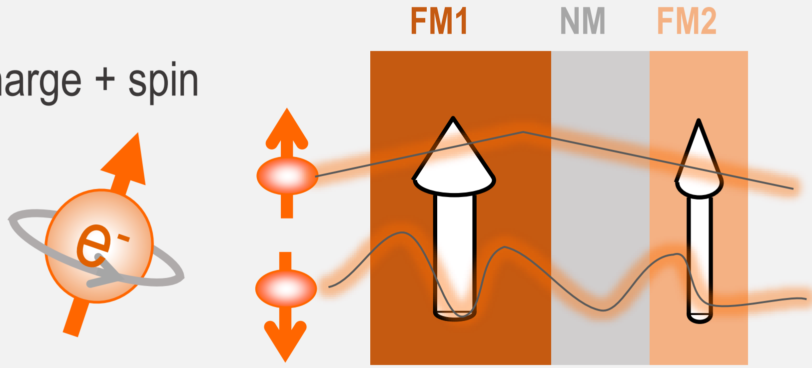


Zeeman



Special role of the spin

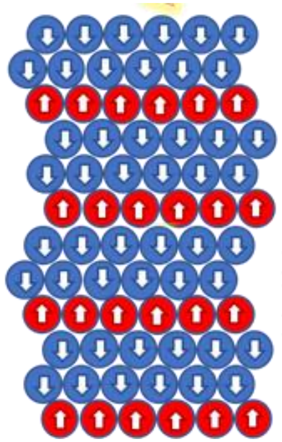
charge + spin



Spin dependent transport

Atomistic spin dynamics

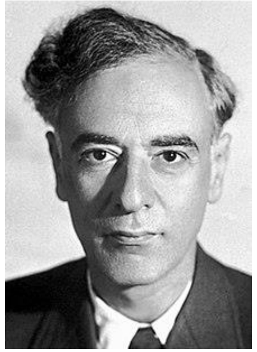
Formalism : atomistic spin model is a discrete description of magnetism (each atom possess a localized magnetic moment or spin); the time evolution of a single atomic spin given by the phenomenological Landau-Lifshitz-Gilbert equation



$$\frac{d\boldsymbol{S}_i}{dt} = -\frac{\gamma_i}{(1+\lambda_i^2)}\left[\boldsymbol{S}_i \times \boldsymbol{B}_i + \lambda_i \boldsymbol{S}_i \times (\boldsymbol{S}_i \times \boldsymbol{B}_i)\right]$$

📖 Landau LD, Lifshitz EM (1935) *Theory of the dispersion of magnetic permeability in ferromagnetic bodies.* Phys Z Sowietunion 8:153

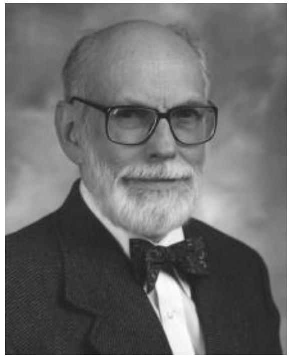
📖 Gilbert TL (1955) *A Lagrangian formulation of the gyromagnetic equation of the magnetic field.* Phys Rev 100:1243. https://doi.org/10.1103/PhysRevB.100.1235



Lev D. **Landau**

Evgeny M. **Lifshitz**

Department of Theoretical Physics National Scientific Center - Kharkiv



Thomas L. **Gilbert**

Argonne National Laboratory

Atomistic spin dynamics

$$\frac{d\boldsymbol{S_i}}{dt} = -\frac{\gamma_i}{(1+\lambda_i^2)}\left[\boldsymbol{S_i} \times \boldsymbol{B_i} + \lambda_i \boldsymbol{S_i} \times (\boldsymbol{S_i} \times \boldsymbol{B_i})\right]$$

precession term *relaxation term*

$$\boldsymbol{B_i} = -\frac{1}{\mu_i}\frac{\partial \widehat{\mathcal{H}}}{\partial \boldsymbol{S_i}} + \boldsymbol{\zeta_i}$$

γ_i - gyromagnetic ratio

λ_i - Gilbert damping is a coupling of the spin to the electronic system and lattice (loss of energy)

Hamiltonian: $$\widehat{\mathcal{H}} = -\sum_{i<j} J_{ij}\boldsymbol{S_i} \cdot \boldsymbol{S_j} - \sum_i k_u\,(\boldsymbol{S_i} \cdot \boldsymbol{u_K})^2 - \sum_i \mu_i \boldsymbol{S_i} \cdot \boldsymbol{B_{app}} + \cdots$$

exchange term *anisotropy term* *Zeeman term* *dipolar*
magnetostriction
...

Thermal field: $$\langle \boldsymbol{\zeta_i} \rangle = 0,\ \langle \zeta_{i\eta}(0)\zeta_{j\theta}(t) \rangle = 2\delta_{ij}\delta_{\eta\theta}\delta(t)\frac{\lambda_i k_B T_e \mu_i}{\gamma_i}$$

- correctly simulate the static and dynamic proprieties of ferrimagnetic and antiferromagnetic materials as alloys of transition metals (TM) and rare – earth elements (RE)

Atomistic spin dynamics : link with first principle computation

ab-initio calculation ⟷ **atomistic models**

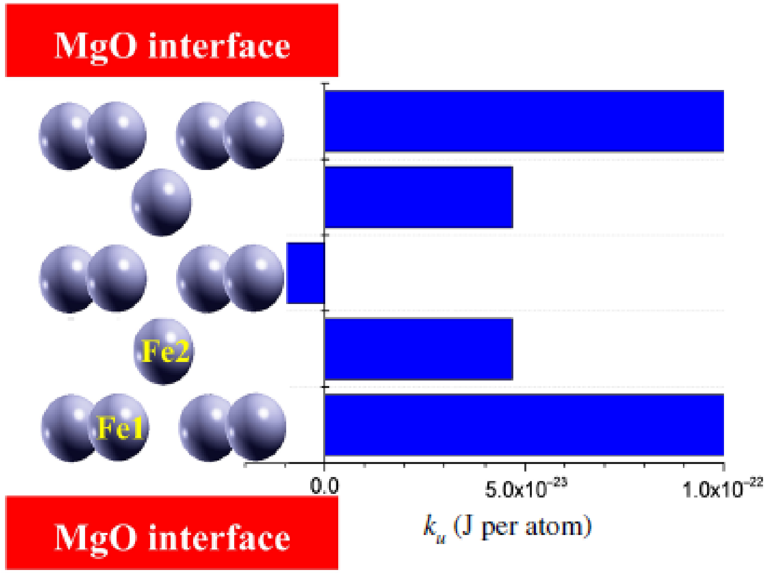
Sanyal's lecture

- Spin moments per layer
  - μ_s (Fe1)= 2.76 μ_B
  - μ_s (Fe2)= 2.49 μ_B
  - μ_s(Fe_bulk) = 2.2 μ_B
- Layer-resolved K_s and μ_s in **Fe/MgO** structures

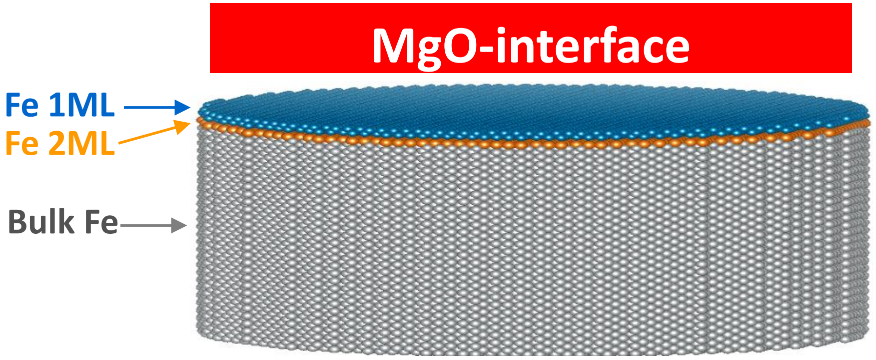
T= 0 K

- Temperature dependence of K_s and M_s
- K_s scaling with M_s
- Curie temperature T_c
- Temperature dependence of dead layer thickness

$$\hat{\mathcal{H}} = -\sum_{i<j} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \sum_i k_u\,(\boldsymbol{S}_i \cdot \boldsymbol{u}_K)^2$$



https://www.vasp.at

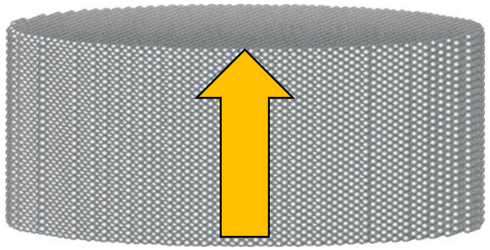


VAMPIRE
vampire.york.ac.uk

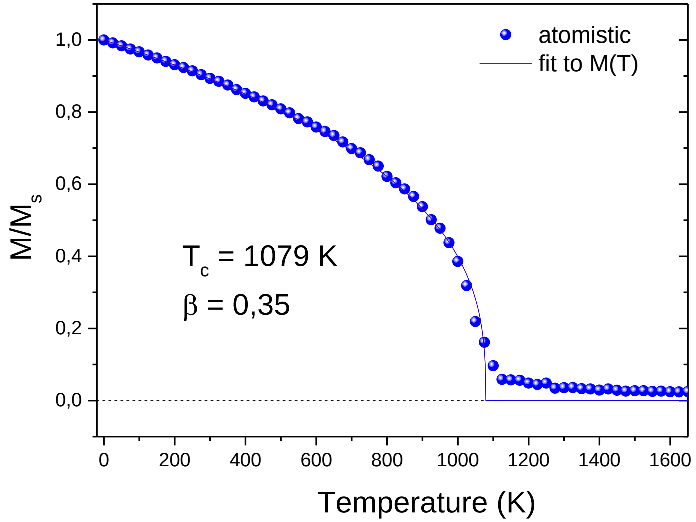
📖 *Ibrahim et al . Phys. Rev. B (2022)*

Atomistic spin dynamics

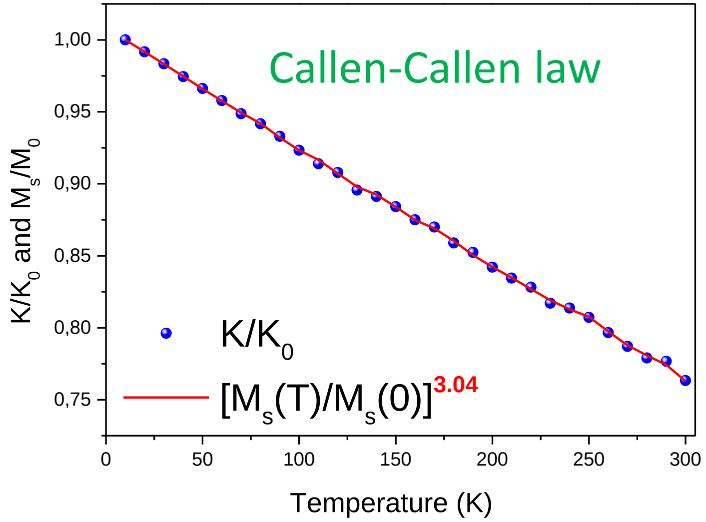
- **Bulk Fe bcc structure**



$$\frac{M_s(T)}{M_s(0)} = \left[1 - \frac{T}{T_c}\right]^{0.35}$$

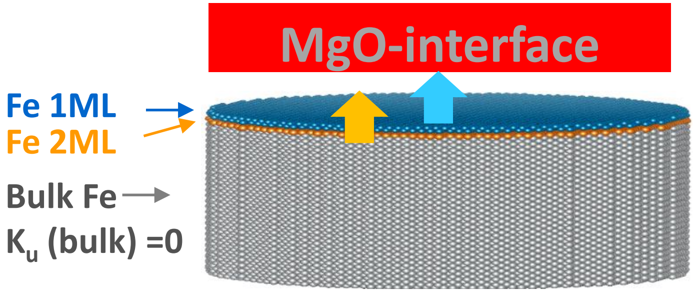


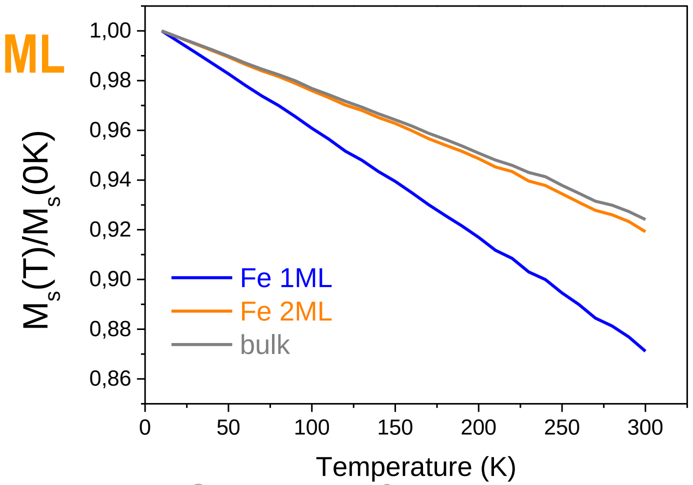
$$\frac{K_s(T)}{K_s(0)} = \left[\frac{M_s(T)}{M_s(0)}\right]^{3.04}$$

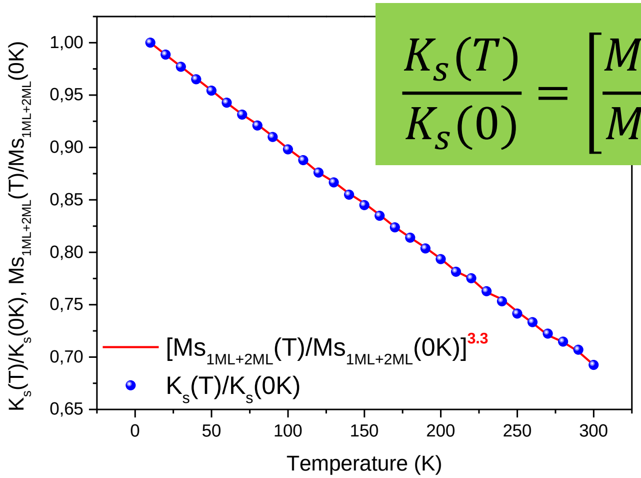


- Uniform uniaxial anis: K_u = 1.0e-24 J/atom
- Exchange constant: J = 7.05e-21 J/link
- μ_s= 2.2 μ_B

- **Model: introduce K_s for Fe 1ML & Fe 2ML**







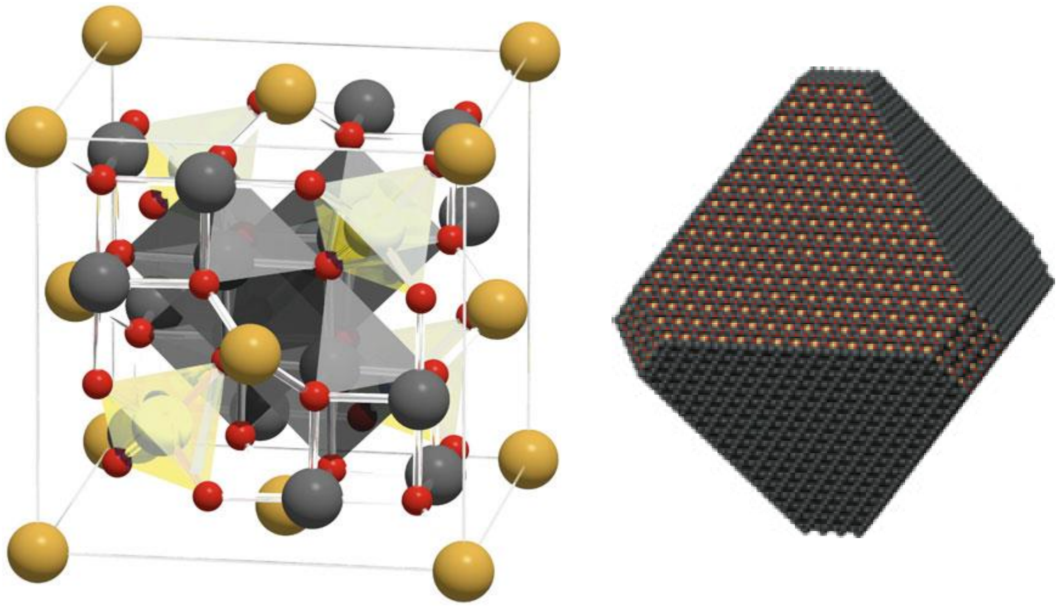
$$\frac{K_s(T)}{K_s(0)} = \left[\frac{M_s(T)}{M_s(0)}\right]^{3.3}$$

- M_s of Fe 1ML decreases more rapidly
- M_s of Fe 2ML behaves as Fe bulk

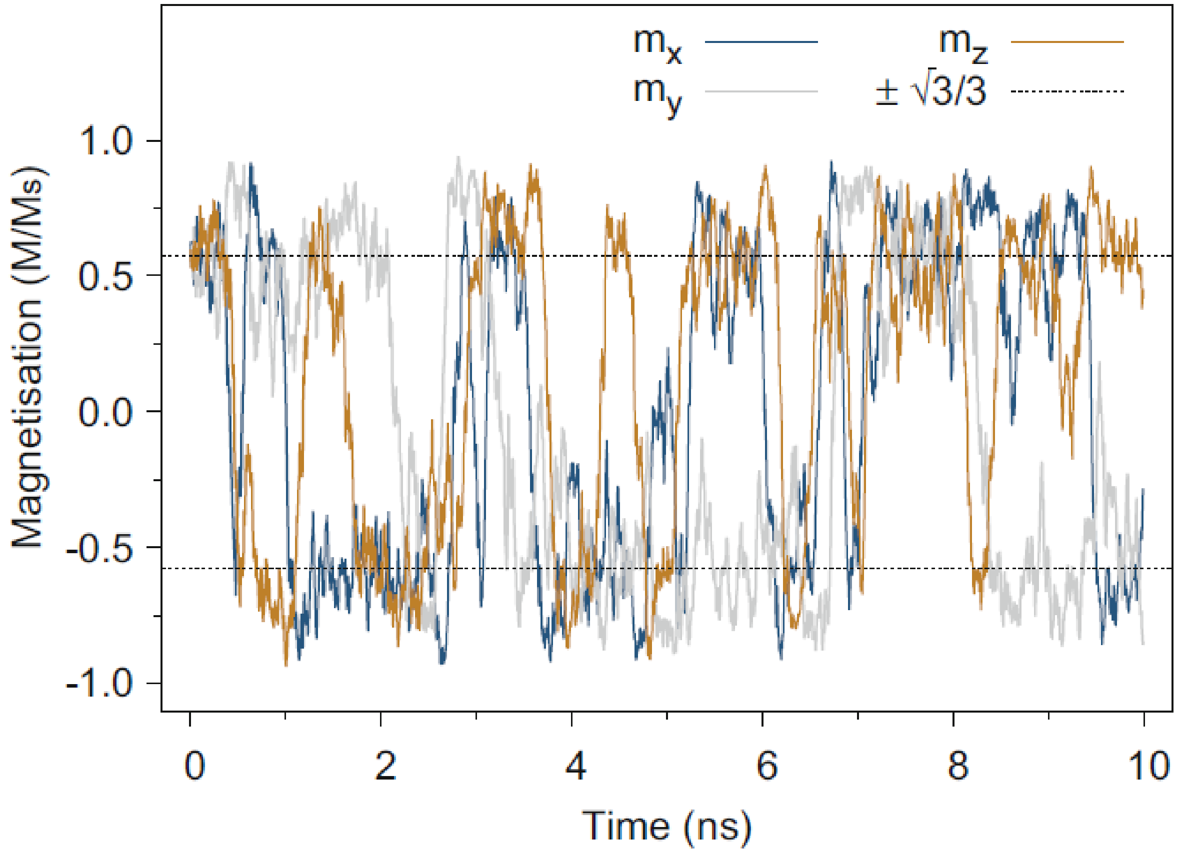
Ibrahim et al . Phys. Rev. B (2022)

Atomistic spin dynamics : finite size Fe_3O_4 nanoparticle

12 nm octahedral single crystal magnetite Fe_3O_4 nanoparticle



magnetization dynamics at 300K



✓ **Fluctuations of different magnetization components between 8 minima along [111] crystal directions due to the cubic magnetcrystalline anisotropy**

📖 *R.F.L Evans Springer (2018)*

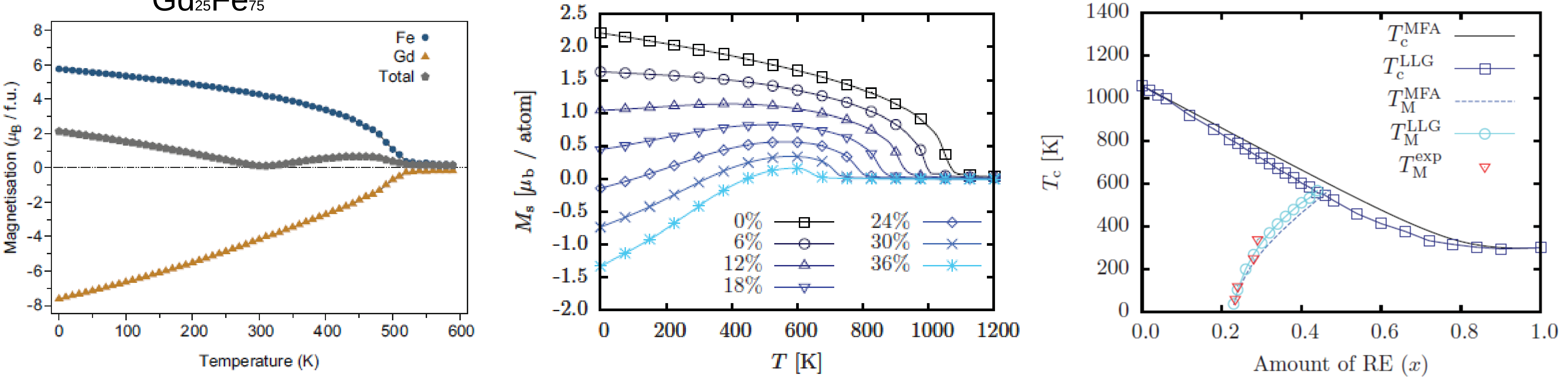
Atomistic spin dynamics : bulk ferrimagnets

Static proprieties of amorphous GdFe Alloys
→ media of magnetic hard disks

62 500 spins & periodic boundary conditions (fcc)

https://vampire.york.ac.uk/

$Gd_{25}Fe_{75}$ Gd_xFe_{100-x}

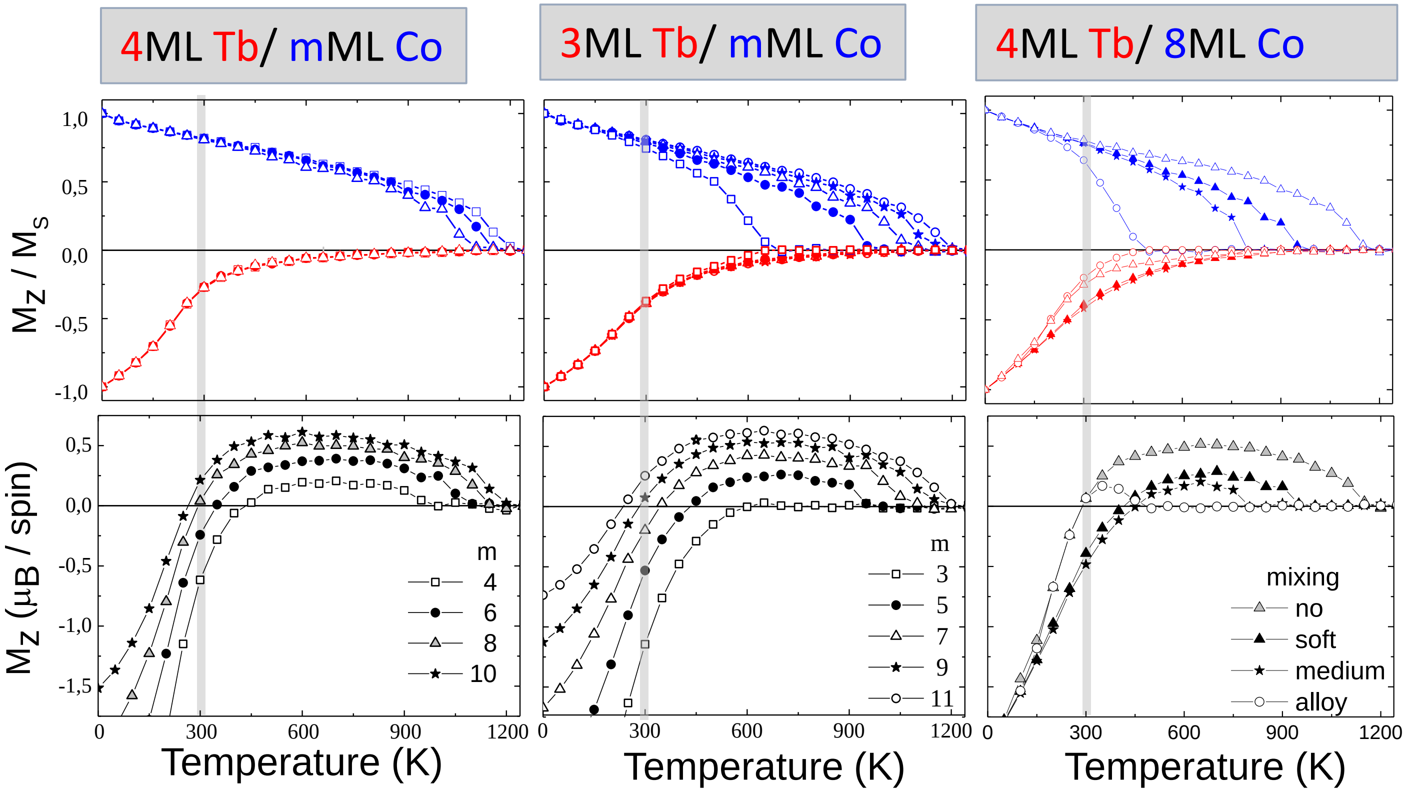


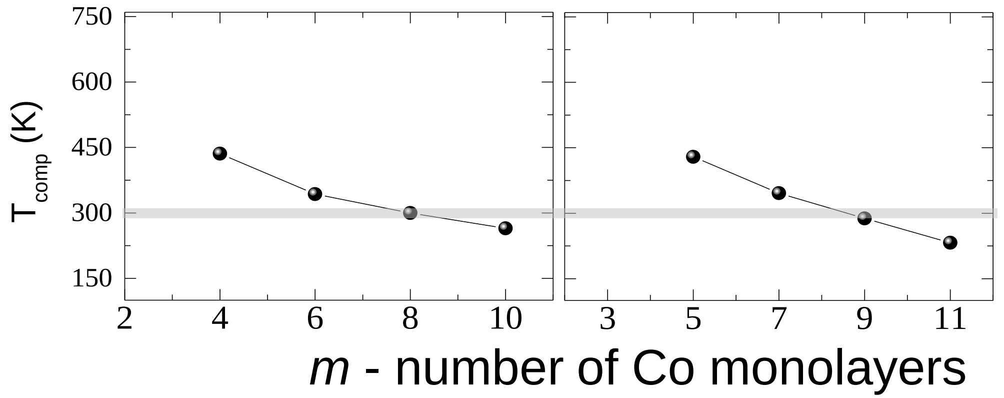
✓ **The model allows to reproduce experimental observations**
→ **validation of the model calibration**

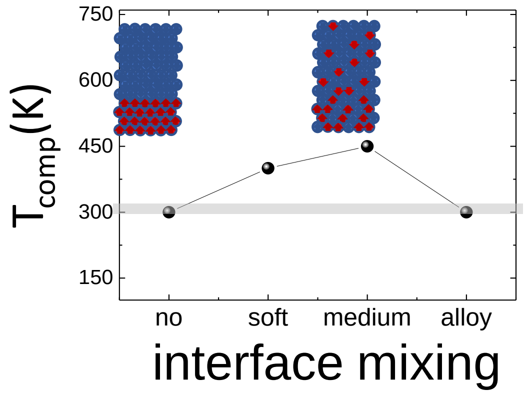
📖 *Ostler et al . Phys. Rev. B (2011)*

Atomistic spin dynamics- static properties [Tb/Co] layers

Ultrafast reversal in Tb/Co multilayers → storage layer in magnetic RAM







✓ **The model allows to finely tune composition, the structure and to explore many possible combination → prediction and prospection**

Atomistic spin dynamics & 2 Temperature model

LLG & 2 temperature model

$$\frac{d\boldsymbol{S}_i}{dt} = -\frac{\gamma_i}{(1+\lambda_i^2)}[\boldsymbol{S}_i \times \boldsymbol{B}_i + \lambda_i \boldsymbol{S}_i \times (\boldsymbol{S}_i \times \boldsymbol{B}_i)]$$

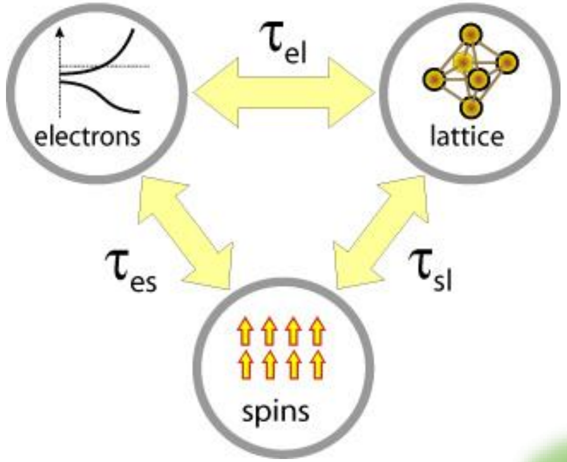
$$\boldsymbol{B}_i = -\frac{1}{\mu_i}\frac{\partial \widehat{\mathcal{H}}}{\partial \boldsymbol{S}_i} + \boldsymbol{\zeta}_i$$

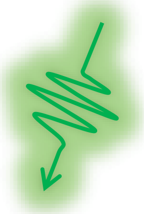
$$\langle \boldsymbol{\zeta}_i \rangle = 0, \ \langle \zeta_{i\eta}(0)\zeta_{j\theta}(t)\rangle = 2\delta_{ij}\delta_{\eta\theta}\delta(t)\frac{\lambda_i k_B T_e \mu_i}{\gamma_i}$$

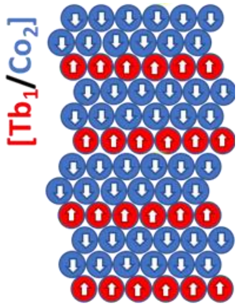
$$\begin{cases} C_e \dfrac{dT_e(t)}{dt} = -G[T_e(t) - T_{ph}(t)] + P(t) \\ C_{ph} \dfrac{dT_{ph}(t)}{dt} = G[T_e(t) - T_{ph}(t)] \end{cases}$$

$$P(t) = \frac{F}{t_{FM}\tau_L} \cdot e^{\left[-\frac{(t-t_0)^2}{\tau_L^2}\right]}$$

laser heating







✓ **Multiphysics coupling : spin dynamics and heat equations**

→ **ASD Spintec solver**

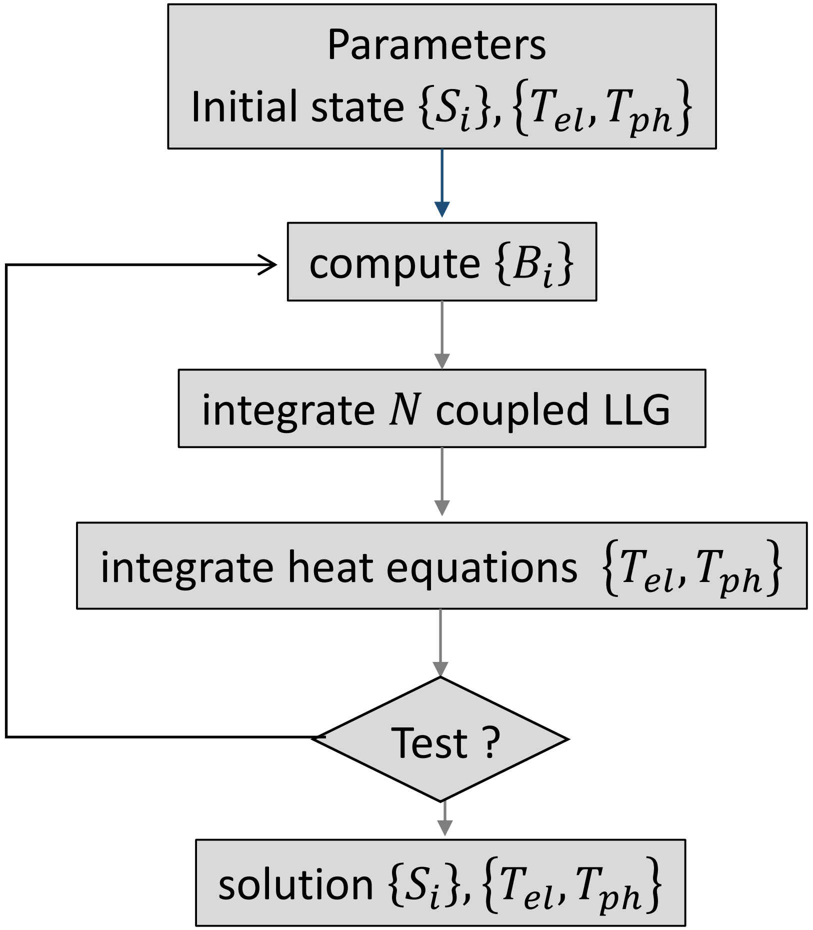
📖 *L. Aviles-Felix et al., Sci. Rep. (2021)*
📖 *R. Moreno et al. Phys Rev B (2017)*

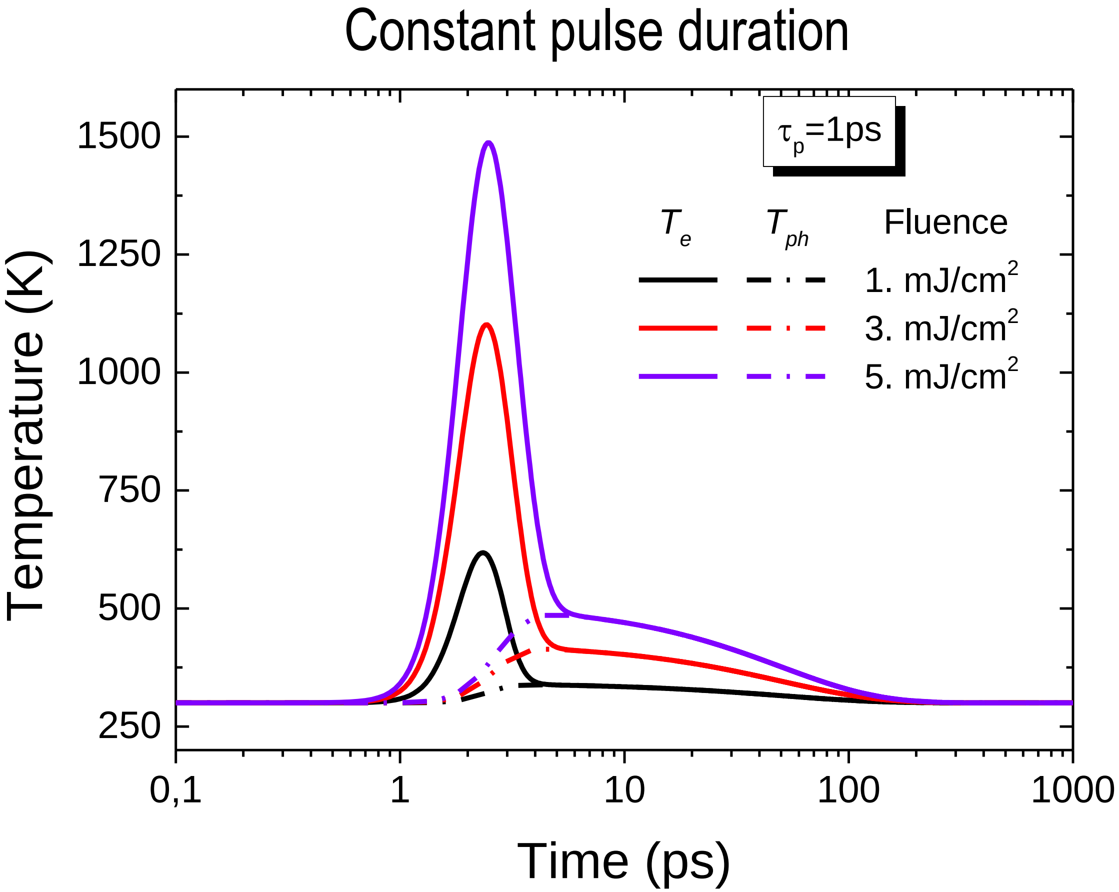
Atomistic spin dynamics : AOS of MTJ based on [Tb/Co] layers

Spindynamics (LLG)

SpinSwift (LLB)

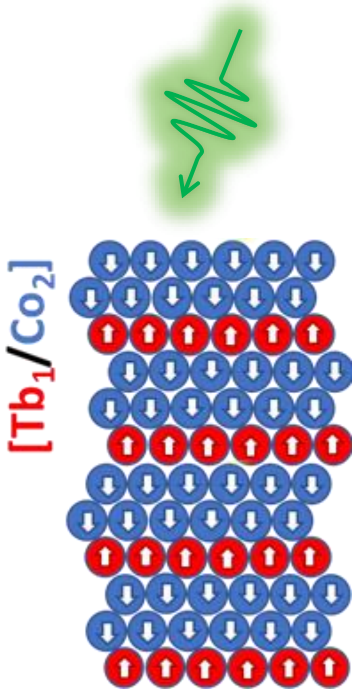
- ✓ More than 50 x 50 X 50 exchange coupled spins
- ✓ Heun's integration scheme (predictor corrector scheme)
- ✓ Parallelization of the solver (CPU , GPU releases)

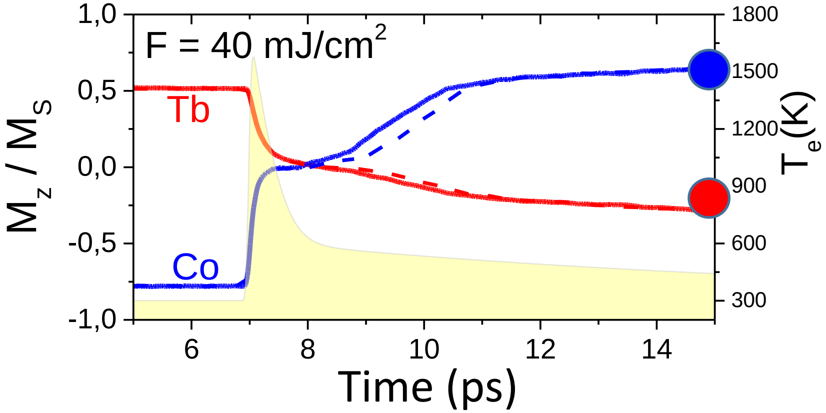


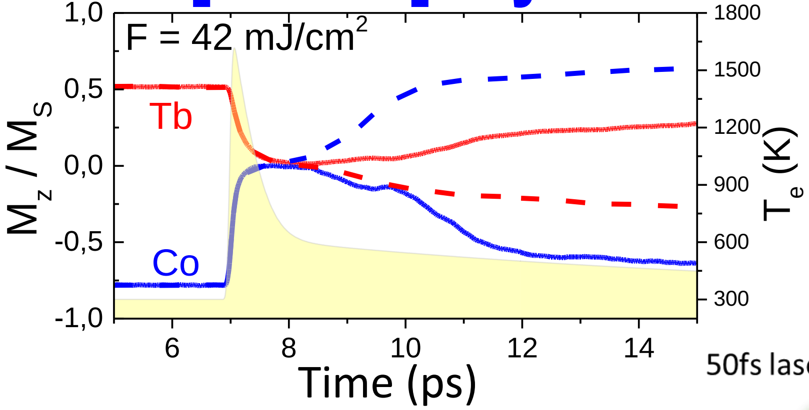


Atomistic spin dynamics : AOS of MTJ based on [Tb/Co] layers

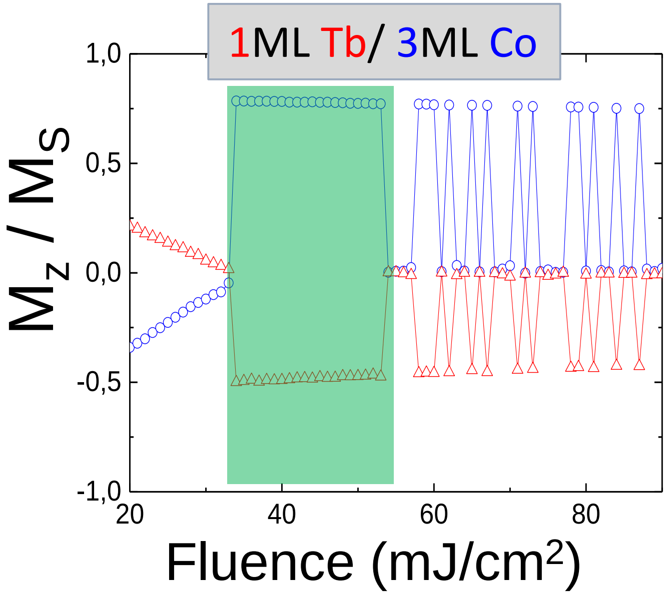
50fs laser pulse

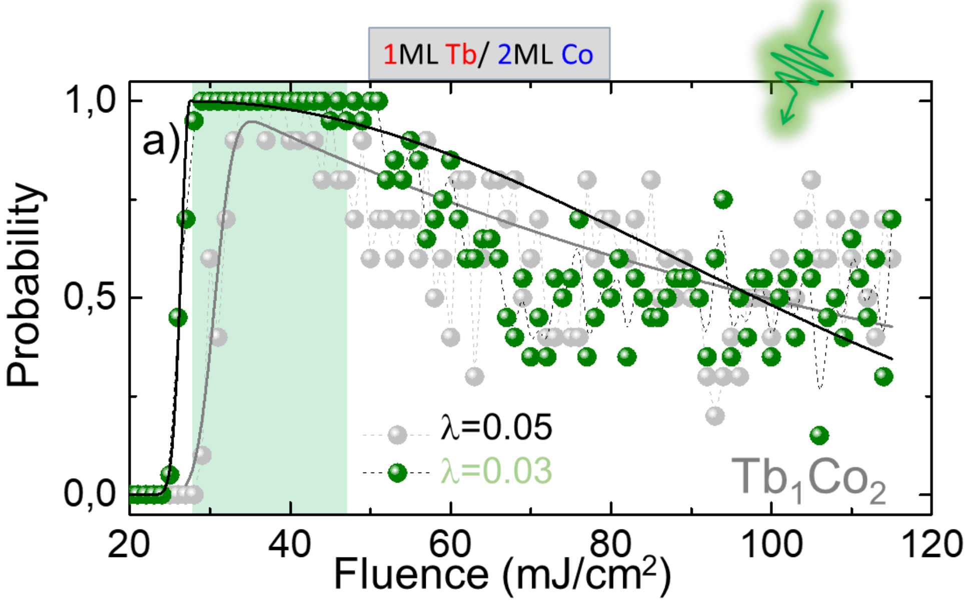






50fs laser pulse



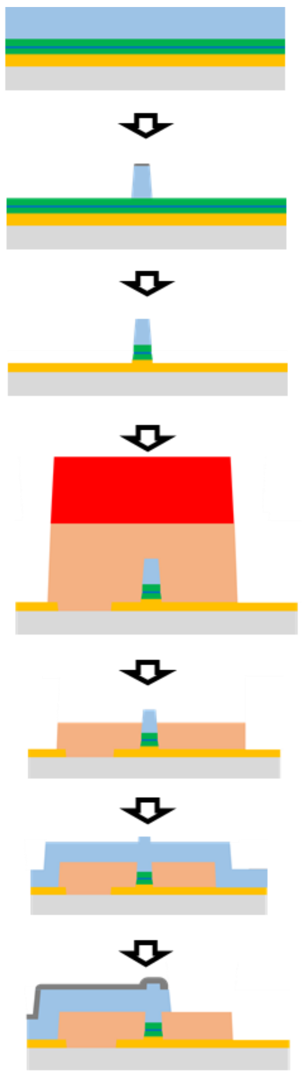


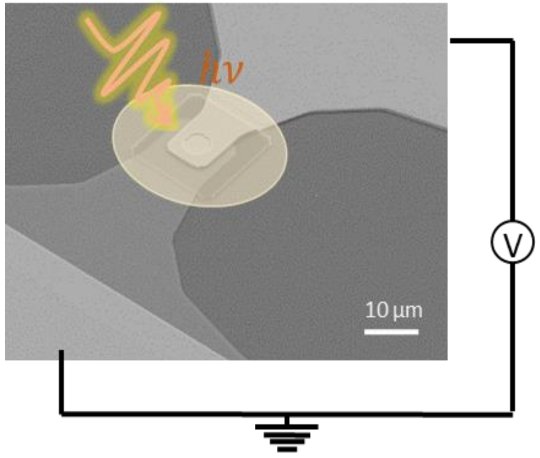
- ✓ **Mechanism of reversal : transient ferromagnetic state linked to the difference of demagnetizing time of Tb and Co.**

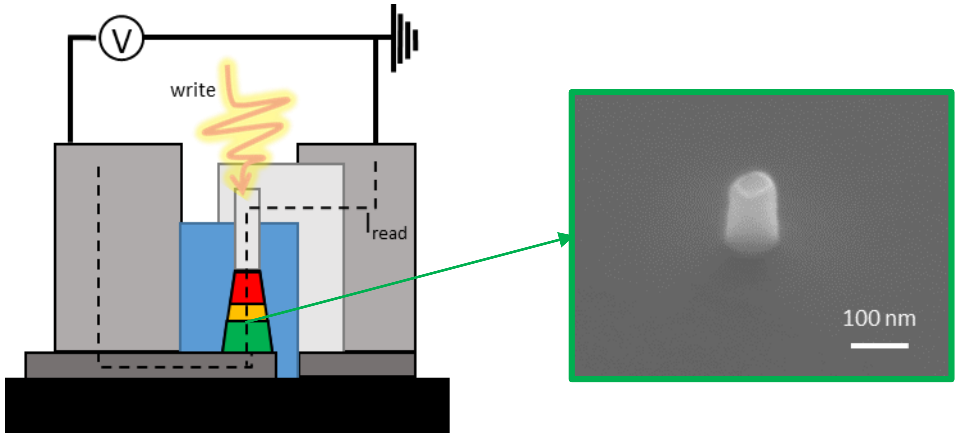
- ✓ **Key role of the material parameters (e.g. damping)**
- ✓ **Extracted diagrams to be compared with experiments**

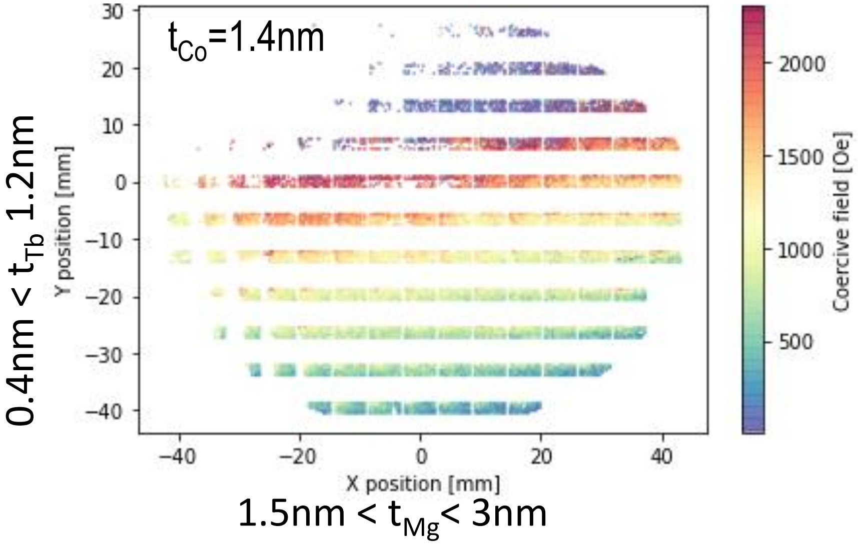
Atomistic spin dynamics : AOS of MTJ based on [Tb/Co] layers

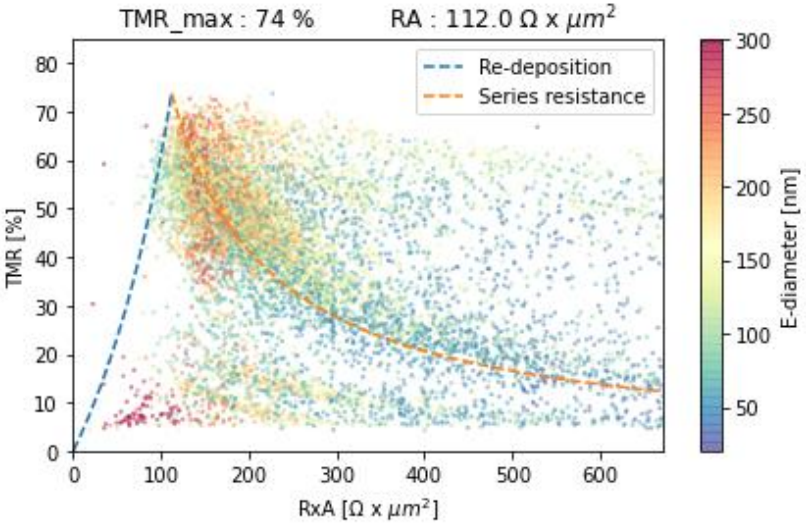
- **TCE deposition**
- E-beam litho mask
- Cr deposition
- Lift-off
- **TCE dry etching**
- **Stack IBE etching**
- Pt electrode lithography
- Pt electrode dry etching
- Resist removal
- Accuflo deposition
- Accuflo etching mask lithography
- Accuflo dy etching
- Accuflo reduction by dry etching
- **TCE deposition**
- **Top electrode lithography**
- **Cr Deposition**
- **Lift-off**
- **TCE dry etching**







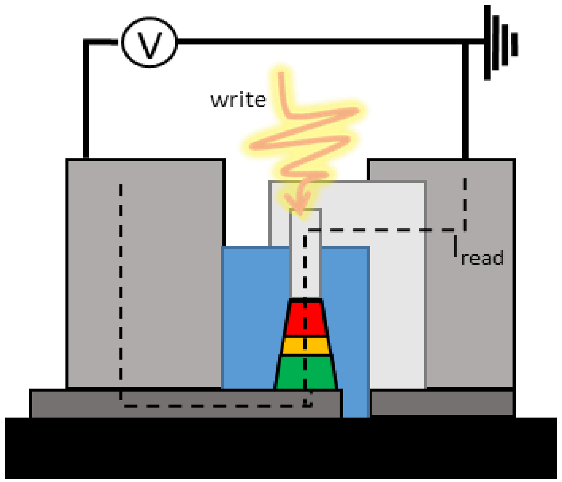




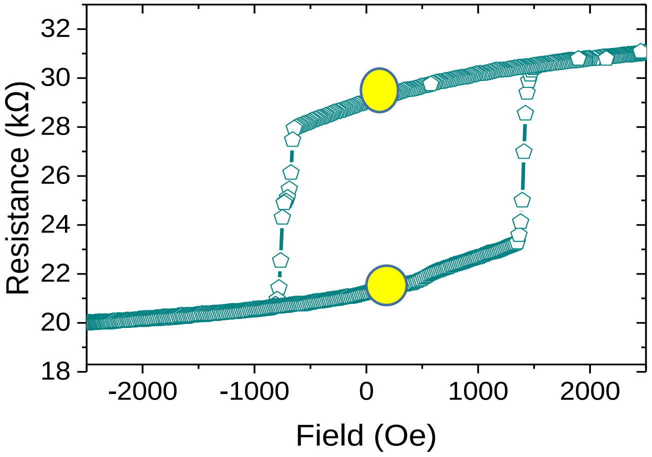
A. Olivier et al., Nanotechnology (2020)

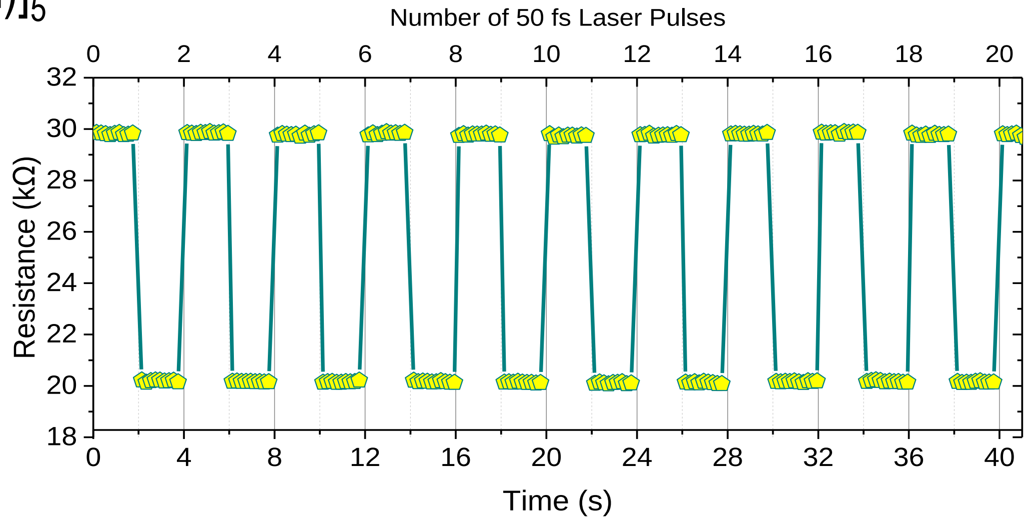
David Salomoni's PhD

Atomistic spin dynamics : AOS of MTJ based on [Tb/Co] layers



FeCoB1.3nm/ [Tb(0.6nm)/Co(1.4nm)]$_5$

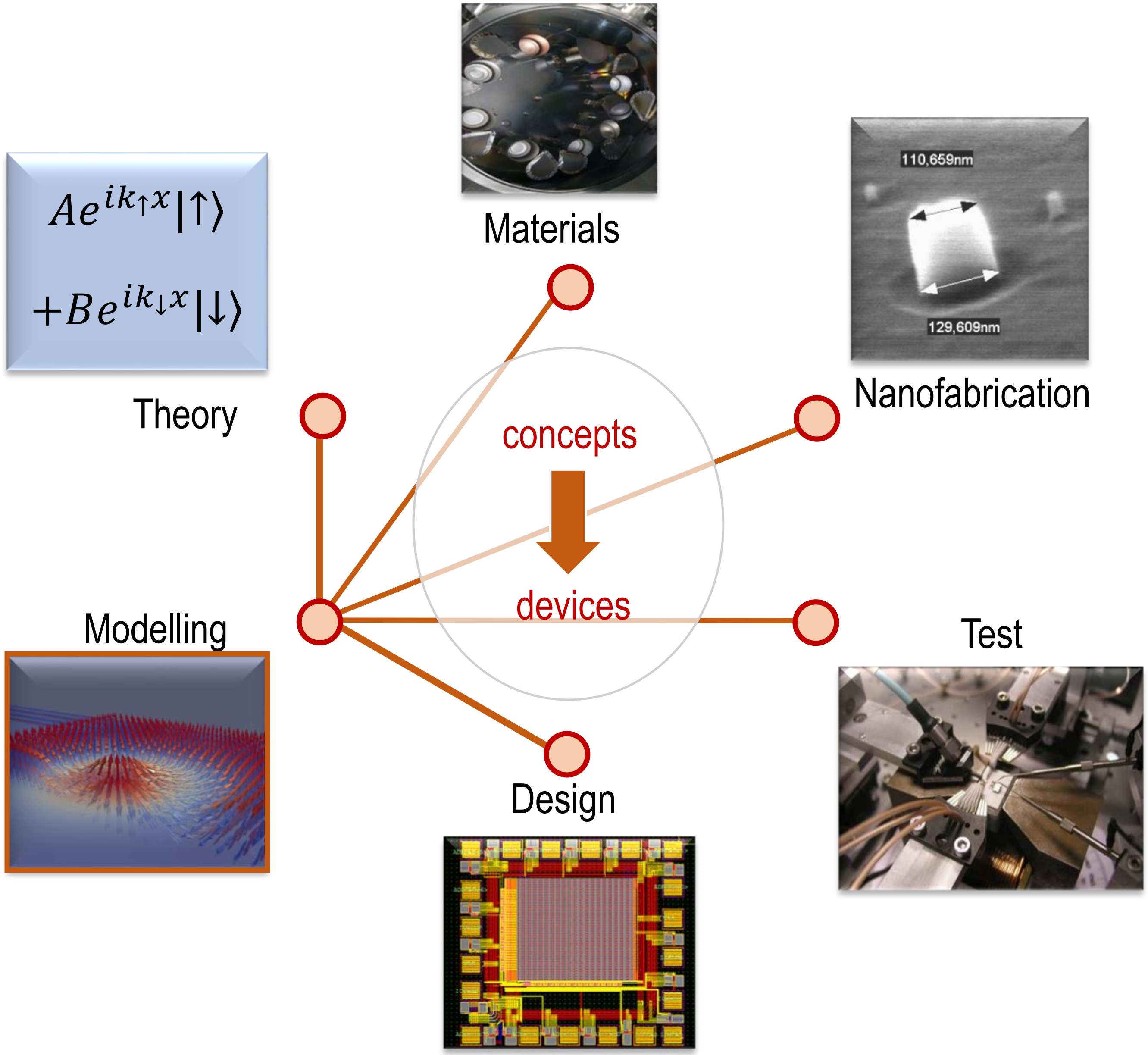




✓ **Reproducible helicity independent AOS with single shot:**

- **MTJ 100nm large with a TMR of 50%**
- **field free**
- **50fs laser pulses, 5.5 mJ/cm^2**

David Salomoni's PhD



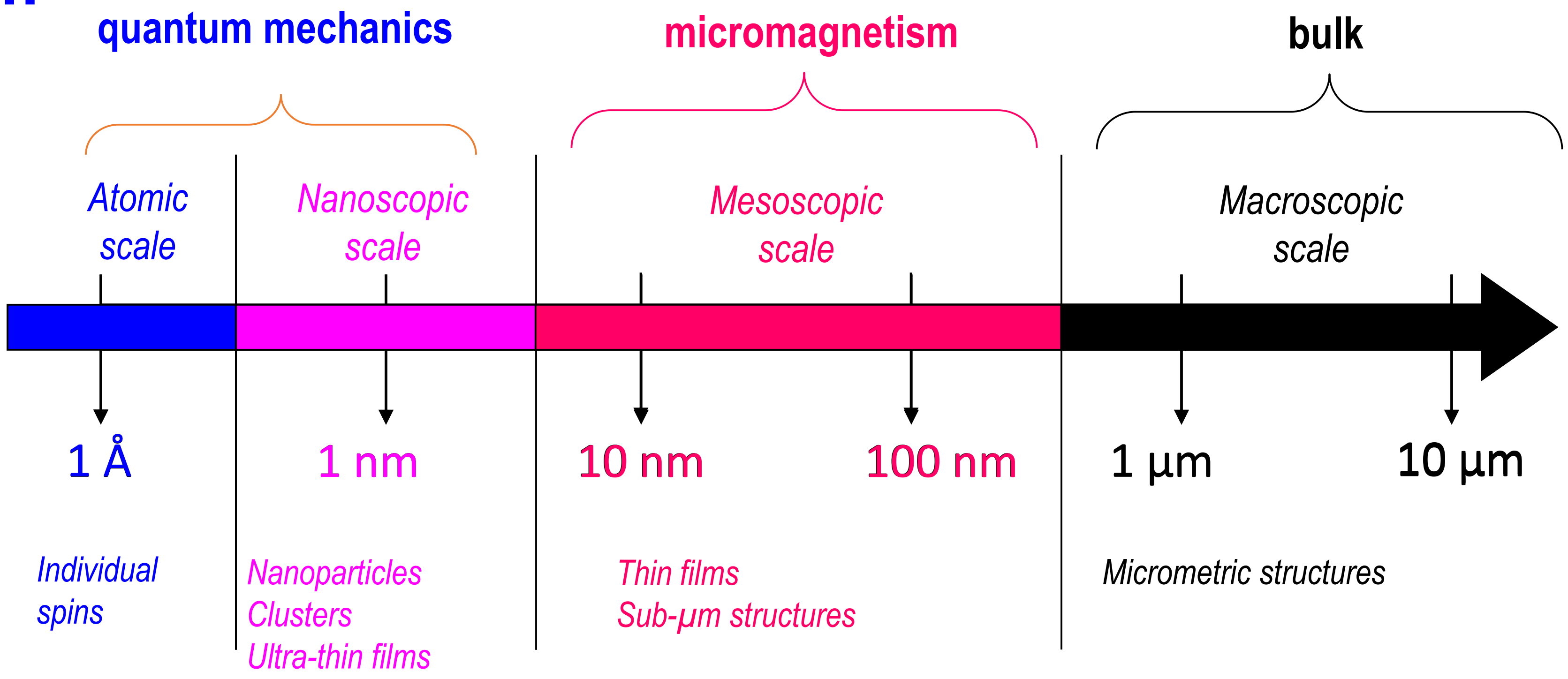
Importance of continuous exchanges between experiments and theory/modelling:

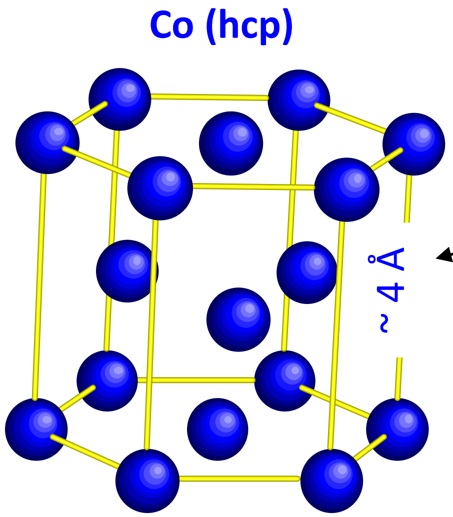
- ✓ **Validation**
- ✓ **Calibration**
- ✓ **Accurate /reliable prediction**
- ✓ **Feed / challenge the models**

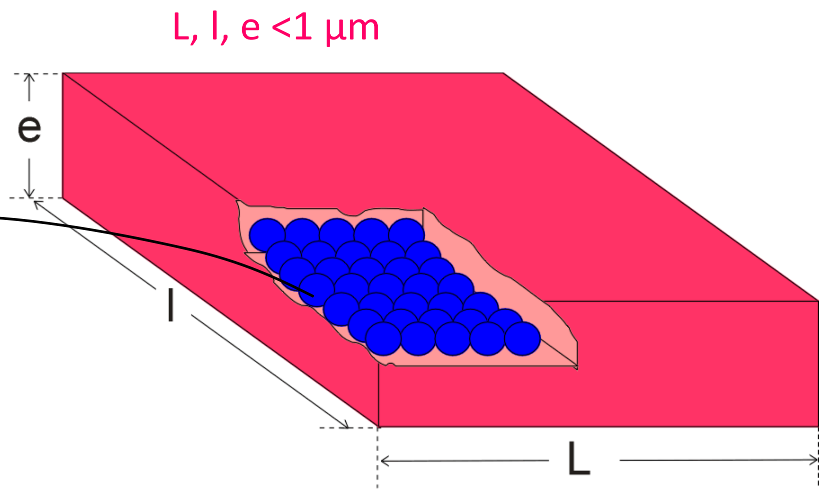
Outline

- **Atomistic spin dynamics**
  - Formalism
  - Illustrations : alloy GdFe, Fe nanodot, AOS [Tb/Co] multilayers
- **Micromagnetism**
  - Formalism
  - Macrospin limit
  - Illustrations
- **Micromagnetism and spin related phenomena**
  - Formalism
  - Illustrations
- **Conclusions**

Micromagnetism







Micromagnetism : the beginning & hypothesis

Classical theory of continuous ferromagnetic material

1963 - W. F. Brown Jr.
- 1907 P. Weiss / magnetic domains
- 1937 Landau-Lifshitz / domain walls

Continuous functions (space & time)

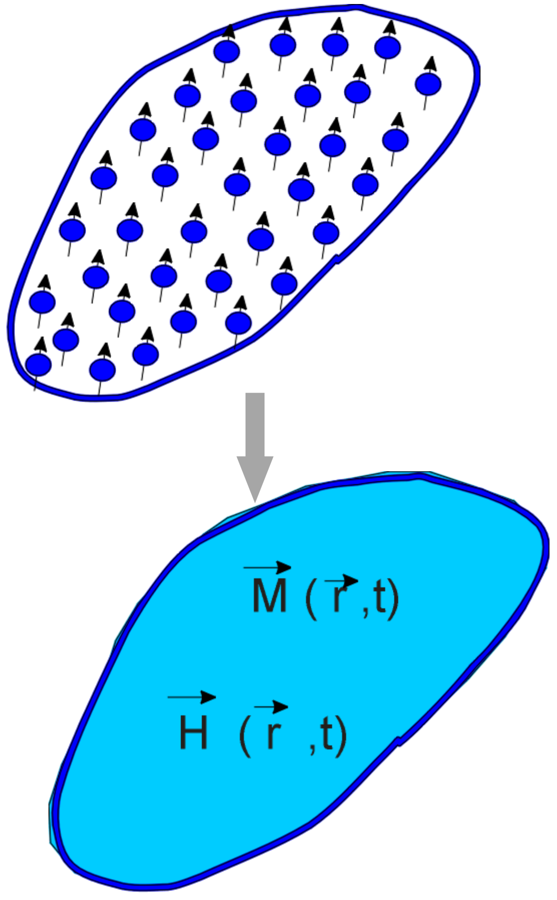
- magnetization $\boldsymbol{M}(\boldsymbol{r},t)$
- field $\boldsymbol{H}(\boldsymbol{r},t)$
- energy $E(\boldsymbol{M}(\boldsymbol{r},t))$

Magnetization – constant amplitude vector $|\boldsymbol{M}(\boldsymbol{r},t)|=M_S$

Thermal effects- temperature dependent parameters

$$M_S(T), A_{ex}(T), K_u(T)$$

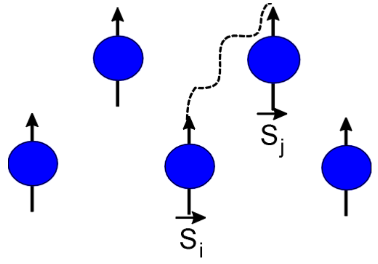
Very large number of individual spins



Continuous media

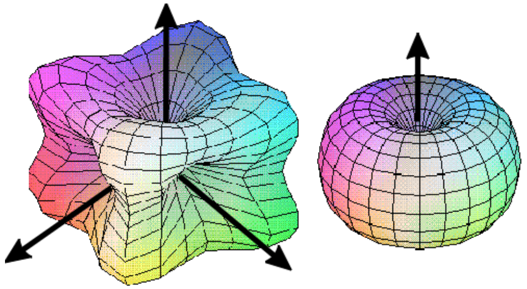
Micromagnetism: Gibb's free energy

Exchange interaction
magnetic order ($T<T_c$)
parallel alignment of spins
short range interaction but very strong



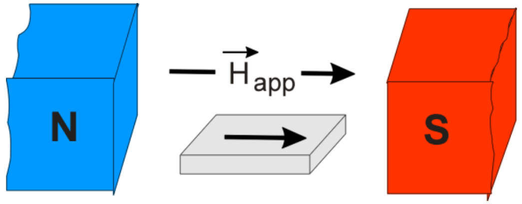
$$\int_\Omega A_{ex} \left(\nabla \boldsymbol{m}(\boldsymbol{r},t)\right)^2 dV$$

Magnetocrystalline anisotropy
easy axis and hard axis
Impact of the crystal symmetry
Local interaction



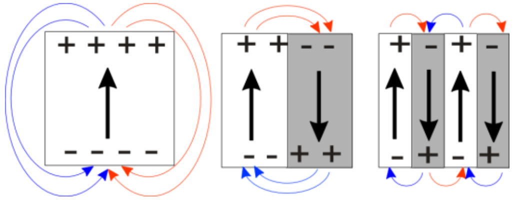
$$\int_\Omega K_u \left[1-\left(\boldsymbol{u_k}\cdot \boldsymbol{m}(\boldsymbol{r},t)\right)^2\right] dV$$

Zeeman coupling
Externally applied field
Local interaction



$$-\mu_0 M_S \int_\Omega \boldsymbol{m}(\boldsymbol{r},t)\cdot \boldsymbol{H_{app}}(\boldsymbol{r},t)\, dV$$

Magnetostatic interaction
Maxwell's equations
long range interaction



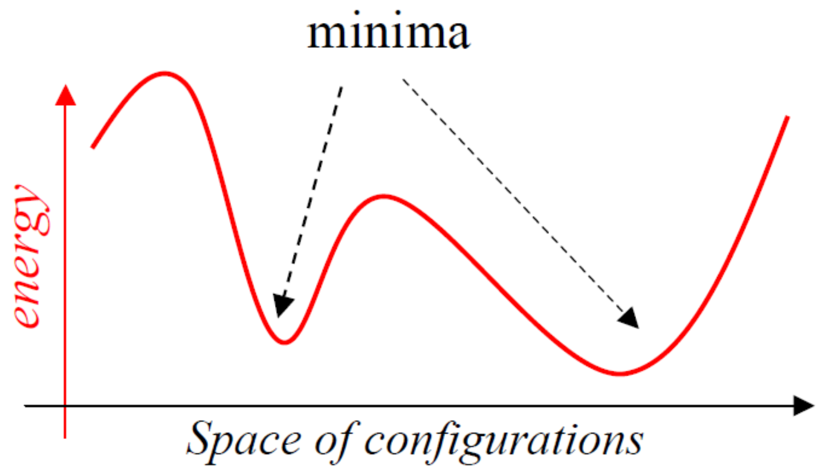
$$-\frac{1}{2}\mu_0 M_S \int_\Omega \boldsymbol{m}(\boldsymbol{r},t)\cdot \boldsymbol{H_D}(\boldsymbol{r},t)\, dV$$

Micromagnetism : magnetic stable state

Magnetization distribution:

$$\boldsymbol{M}(\boldsymbol{r},t), = M_S\boldsymbol{m}(\boldsymbol{r},t) \ \ \boldsymbol{r} \in \boldsymbol{\Omega}$$

$$|\boldsymbol{m}(\boldsymbol{r},t)|=1$$



Gibb's free energy:

$$E_{total} = \int_{\Omega} [\varepsilon_{ex} + \varepsilon_K + \varepsilon_{app} + \varepsilon_D]\, dV$$

Magnetic stable state = minimum of the Gibb's free energy functional

$$\boldsymbol{m} \rightarrow \boldsymbol{m}+\delta\boldsymbol{m}$$

$$\delta E_{total}(\boldsymbol{m}) = 0$$

$$\delta^2 E_{total}(\boldsymbol{m}) > 0$$

← variational principle

Micromagnetism : static equilibrium equations

✓ **Possible thus to find the magnetic stable states**

Brown's equations $\left(\boldsymbol{m} \times \boldsymbol{H}_{eff}\right) = \boldsymbol{0}, \forall\, \boldsymbol{r} \in \Omega$ $\qquad$ $\dfrac{\partial \boldsymbol{m}}{\partial \boldsymbol{n}} = \boldsymbol{0}, \forall \boldsymbol{r} \in S$

$$\delta E_{total} = -\mu_0 M_S \int_\Omega \left(\boldsymbol{m} \times \boldsymbol{H}_{eff}\right) \cdot \delta\boldsymbol{\theta}\, dV + 2A_{ex} \oint_S \left(\boldsymbol{m} \times \frac{\partial \boldsymbol{m}}{\partial \boldsymbol{n}}\right) \cdot \delta\boldsymbol{\theta}\, dS$$

Effective field: $\boldsymbol{H}_{eff} = -\dfrac{1}{\mu_0 M_S} \dfrac{\delta E_{total}}{\delta \boldsymbol{m}} = \boldsymbol{H}_{ex} + \boldsymbol{H}_{K} + \boldsymbol{H}_{D} + \boldsymbol{H}_{app} + C\boldsymbol{m}$

A. Hubert, R. Schafer Magnetic Domains

Micromagnetism : dynamic equation

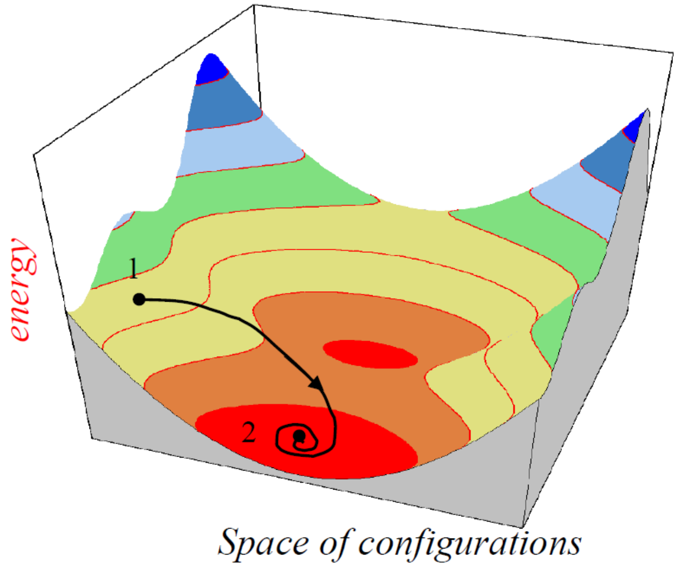
Equation de Landau-Lifshitz-Gilbert + more interactions

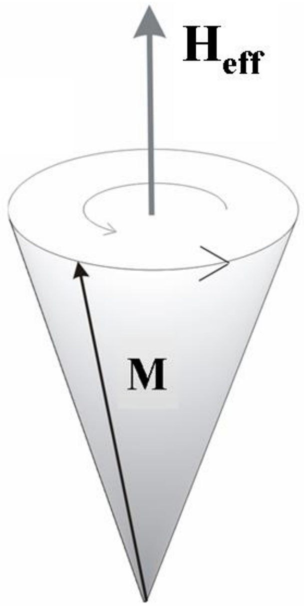
$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma_0\left(\mathbf{m}\times\mathbf{H}_{\mathbf{eff}}\right) + \boldsymbol{\alpha}\left(\mathbf{m}\times\frac{\partial \mathbf{m}}{\partial t}\right) + \left(\frac{\partial \mathbf{m}}{\partial t}\right)_{add}$$

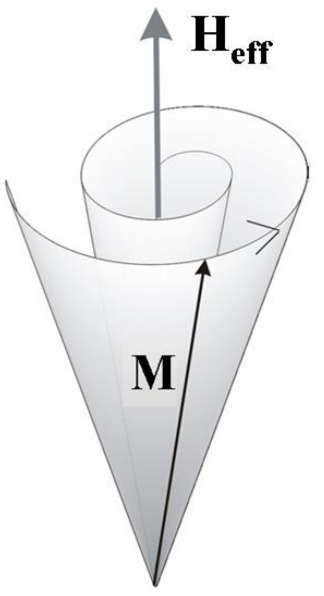
macrospin

Space & time dependence

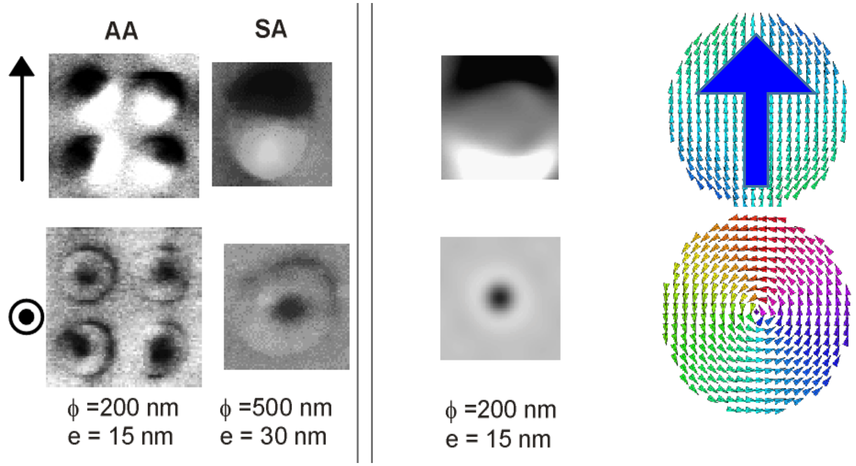
$\boldsymbol{m}(\boldsymbol{r},t), \boldsymbol{r}\in\boldsymbol{\Omega}$







Experiments *Simulation*

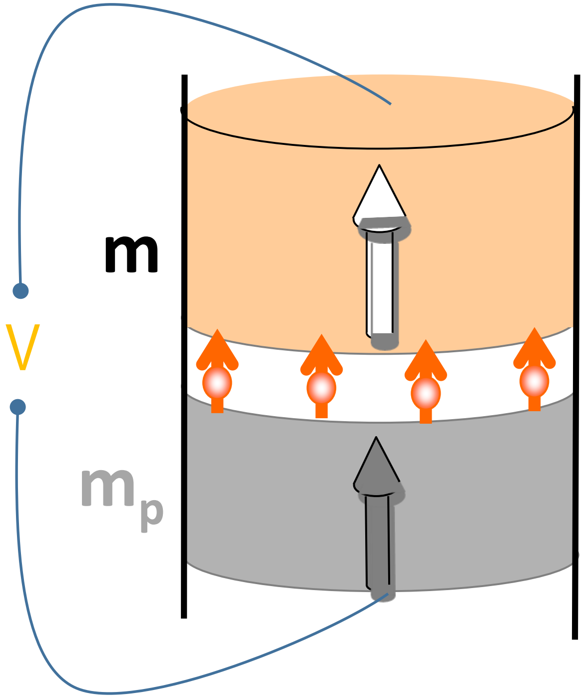


✓ **Magnetization trajectory between two magnetic states**

Macrospin: micromagnetic limit if the exchange interaction is infinite

Circular magnetic tunnel junction pillar: polarizer $\mathbf{m_p}$ / insulator (MgO) / CoFeB (**m**)

m is supposed to be uniform in each point of the CoFeB and have coherent dynamic.



$$\frac{\partial \boldsymbol{m}}{\partial t} = -\gamma_0 (\boldsymbol{m} \times \boldsymbol{H_{eff}}) + \alpha \left(\boldsymbol{m} \times \frac{\partial \boldsymbol{m}}{\partial t} \right)$$

LLG equation

$$-\gamma_0 a_{DL} V (\boldsymbol{m} \times (\boldsymbol{m} \times \boldsymbol{m_P})) + \gamma_0 a_{FL} V^2 (\boldsymbol{m} \times \boldsymbol{m_P})$$

Spin Transfer Torques

damping-like *field-like* *Slonczewski terms*

$$\boldsymbol{H_{eff}} = \begin{pmatrix} 0 \\ 0 \\ H_K m_z + M_S m_z + H_{app} \end{pmatrix}$$

the effective field includes contributions due to the anisotropy, demagnetizing and applied field

$$\boldsymbol{m_p} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

the spin current polarization is parallel with the out-of-plane direction

Macrospin: micromagnetic limit if the exchange interaction is infinite

$$(1+\alpha^2)\frac{\partial \boldsymbol{m}}{\partial t} = -\gamma_0(\boldsymbol{m}\times\boldsymbol{H_{eff}}) - \gamma_0(a_{FL}V^2 - \alpha a_{DL}V)(\boldsymbol{m}\times\boldsymbol{m_P})$$
$$-\alpha\gamma_0\left(\boldsymbol{m}\times(\boldsymbol{m}\times\boldsymbol{H_{eff}})\right) - \gamma_0(-\alpha a_{FL}V^2 + a_{DL}V)(\boldsymbol{m}\times(\boldsymbol{m}\times\boldsymbol{m_P}))$$

$$\boldsymbol{m}^2 = 1$$

Holstein –Primakoff transformation :

$$c = \frac{m_x - i m_y}{\sqrt{2(1+m_z)}}$$

$$c^* = \frac{m_x + i m_y}{\sqrt{2(1+m_z)}}$$

$$\left(\frac{\partial \boldsymbol{c}}{\partial t}\right)_{prec} = -ic[\omega_H + (\omega_D - \omega_K)(2|c|^2 - 1)]$$

$$\left(\frac{\partial \boldsymbol{c}}{\partial t}\right)_{damp} = -\alpha c(1 - |c|^2)[\omega_H + (\omega_D - \omega_K)(2|c|^2 - 1)]$$

$$\left(\frac{\partial \boldsymbol{c}}{\partial t}\right)_{FL} = i[\alpha\omega_{DL} + \omega_{FL}]c$$

$$\left(\frac{\partial \boldsymbol{c}}{\partial t}\right)_{DL} = -[\omega_{DL} - \alpha\omega_{FL}](1 - |c|^2)c$$

$$\omega_H = \frac{\gamma_0 H_{app}}{1+\alpha^2}$$

$$\omega_K = \frac{\gamma_0 H_K}{1+\alpha^2}$$

$$\omega_D = \frac{\gamma_0 M_s}{1+\alpha^2}$$

$$\omega_{DL} = \frac{\gamma_0}{1+\alpha^2}\frac{a_{DL}V}{\mu_0}$$

$$\omega_{FL} = \frac{\gamma_0}{1+\alpha^2}\frac{a_{FL}V^2}{\mu_0}$$

Timopheev et al. Phys Rev B (2017)

Macrospin: micromagnetic limit if the exchange interaction is infinite

$$\frac{\partial c}{\partial t} = -ic\left[\omega_H - (\alpha\omega_{DL} + \omega_{FL}) + (\omega_D - \omega_K)(2|c|^2 - 1)\right]$$
$$-\alpha c(1 - |c|^2)\left[\omega_H + \left(\frac{\omega_{DL}}{\alpha} - \omega_{FL}\right)(\omega_D - \omega_K)(2|c|^2 - 1)\right]$$

$$c = \sqrt{p}e^{-i\phi}$$

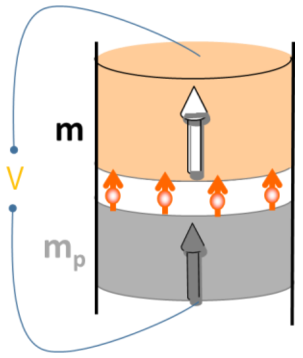
Power equation
$$\frac{\partial p}{\partial t} = -2\alpha\left[\omega_H + \left(\frac{\omega_{DL}}{\alpha} - \omega_{FL}\right) + (\omega_D - \omega_K)(2p - 1)\right](1 - p)p$$

Phase equation
$$\frac{\partial \phi}{\partial t} = -[\omega_H - (\alpha\omega_{DL} + \omega_{FL}) + (\omega_D - \omega_K)(2p - 1)]$$

$$\omega_H = \frac{\gamma_0 H_{app}}{1 + \alpha^2}$$
$$\omega_K = \frac{\gamma_0 H_K}{1 + \alpha^2}$$
$$\omega_D = \frac{\gamma_0 M_s}{1 + \alpha^2}$$
$$\omega_{DL} = \frac{\gamma_0}{1 + \alpha^2}\frac{a_{DL}V}{\mu_0}$$
$$\omega_{FL} = \frac{\gamma_0}{1 + \alpha^2}\frac{a_{FL}V^2}{\mu_0}$$

- ✓ **Stability analysis around the equilibrium state** $p_{eq} \rightarrow p_{eq} + \delta p$
- ✓ **Extraction of the critical lines, draw state diagrams**

Macrospin: micromagnetic limit if the exchange interaction is infinite



State "up" $\boldsymbol{m} = (0 \quad 0 \quad 1)$ stable if :

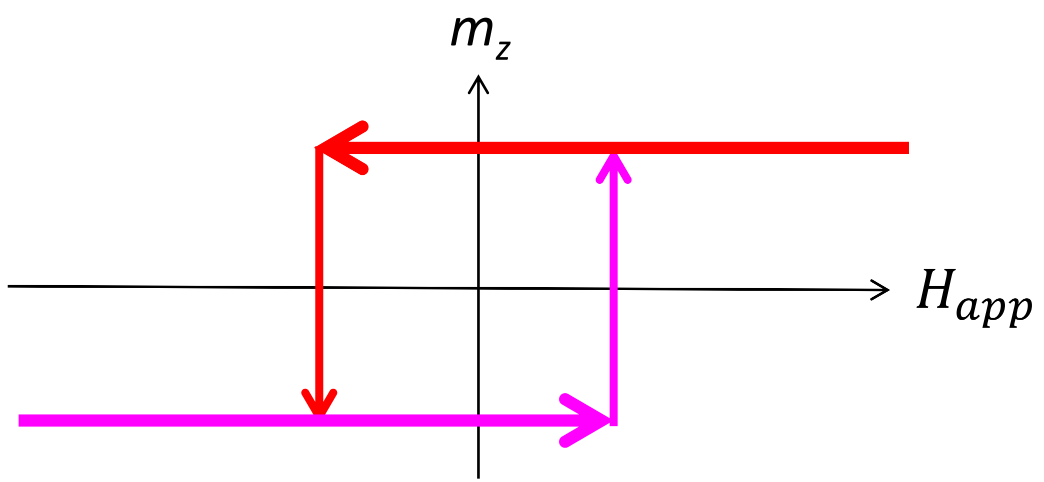
$$V = 0 \qquad H_{app} > \; -(H_K - M_s)$$

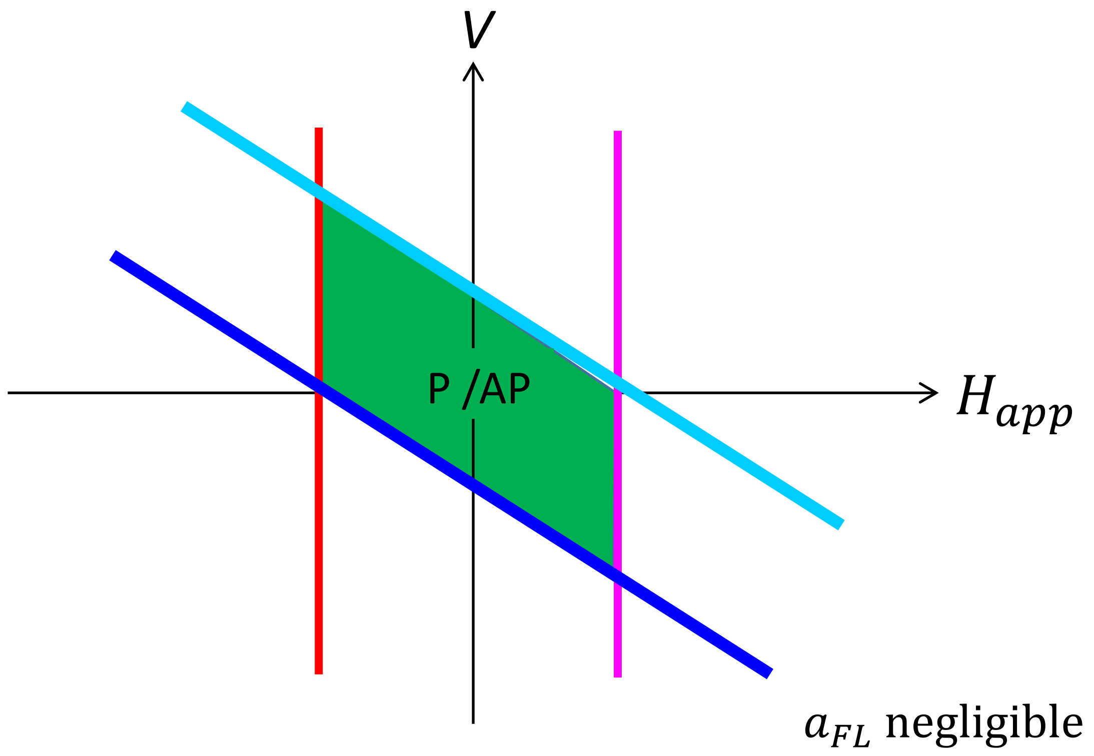
$$V \neq 0 \qquad H_{app} + \left(\frac{a_{DL}V}{\alpha\mu_0} - \frac{a_{FL}V^2}{\mu_0}\right) - (M_S - H_K) > 0$$

State "down" $\boldsymbol{m} = (0 \quad 0 \quad -1)$ stable if :

$$V = 0 \qquad H_{app} < +(H_K - M_s)$$

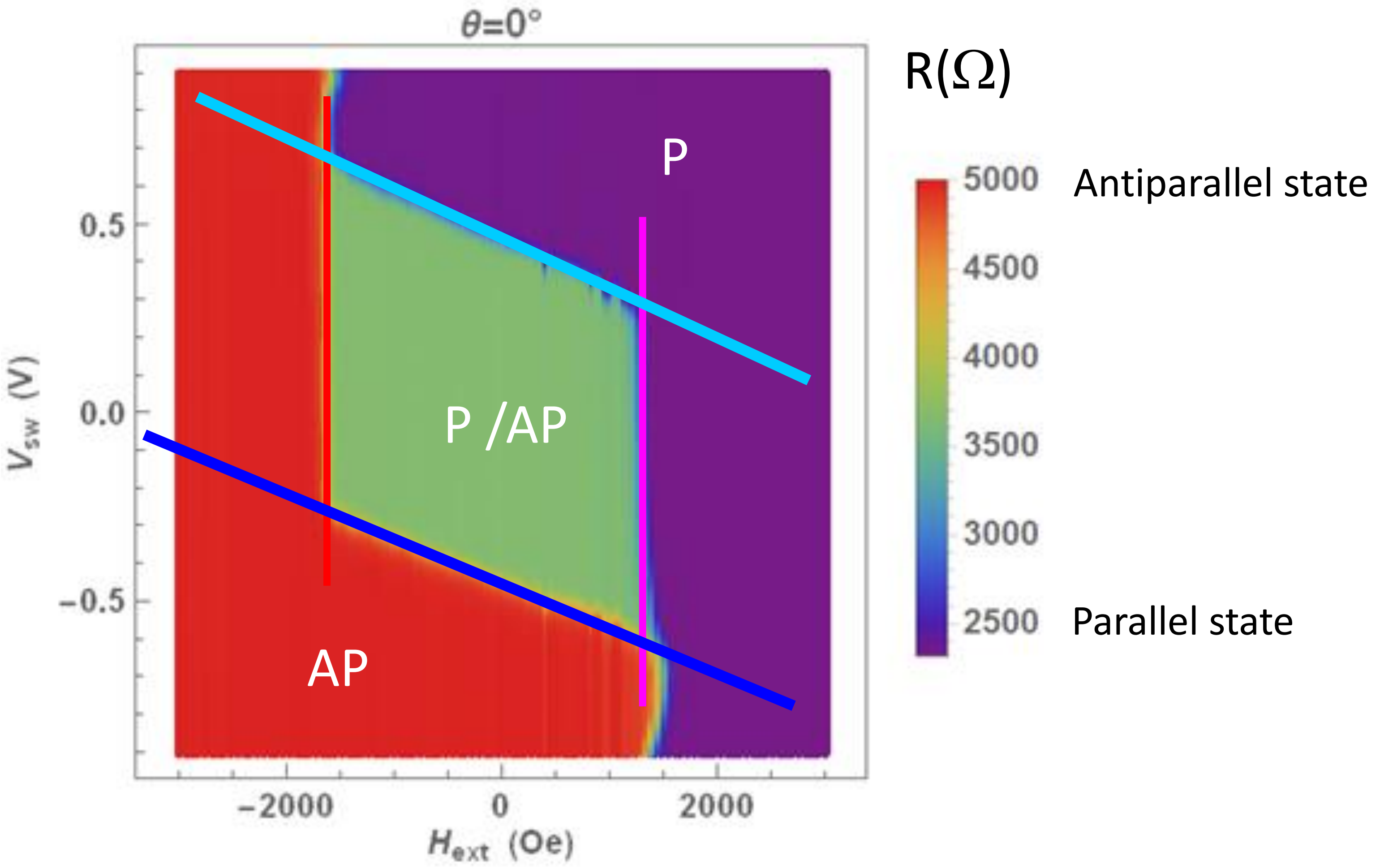
$$V \neq 0 \qquad H_{app} + \left(\frac{a_{DL}V}{\alpha\mu_0} - \frac{a_{FL}V^2}{\mu_0}\right) + (M_s - H_K) < 0$$





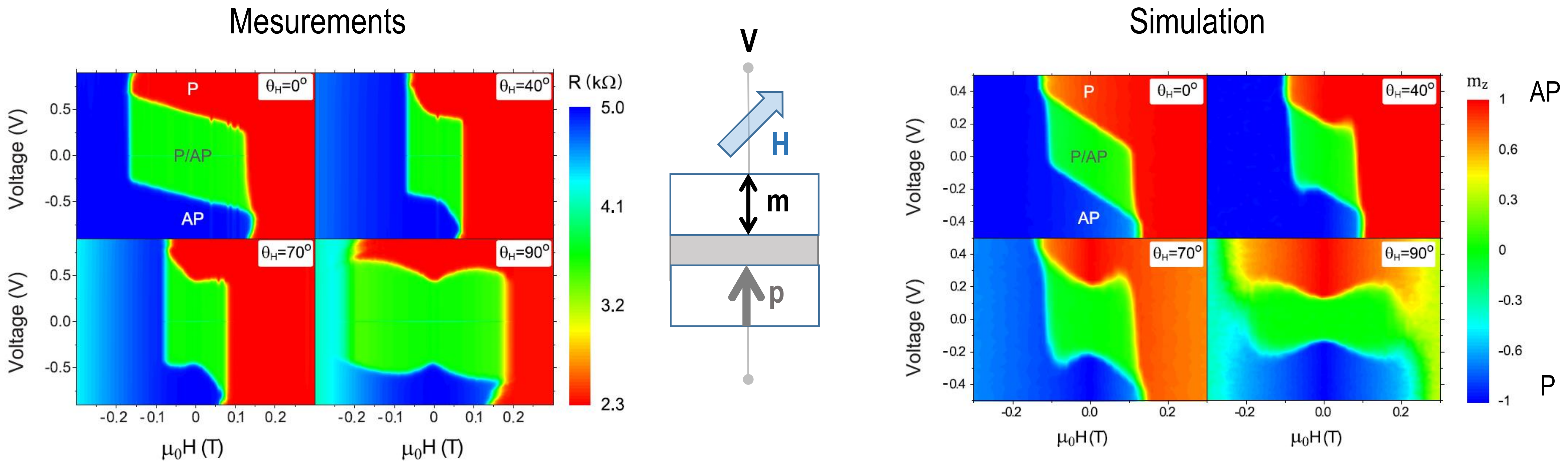
Macrospin: micromagnetic limit if the exchange interaction is infinite

Experimental stability *V-H* diagrams of 80 nm diameter MTJ at room temperature



Strelkov et al. Phys Rev B (2017)

Macrospin: micromagnetic limit if the exchange interaction is infinite



✓ **The model pointed out the necessity to add a new term to the crystalline anisotropy:**

$$E_K = -K_1(\boldsymbol{u}_k \cdot \boldsymbol{m})^2 - K_2(\boldsymbol{u}_k \cdot \boldsymbol{m})^4$$

✓ **The macrospin model is simple but enables a straightforward analysis**

Strelkov et al. Phys Rev B (2017)

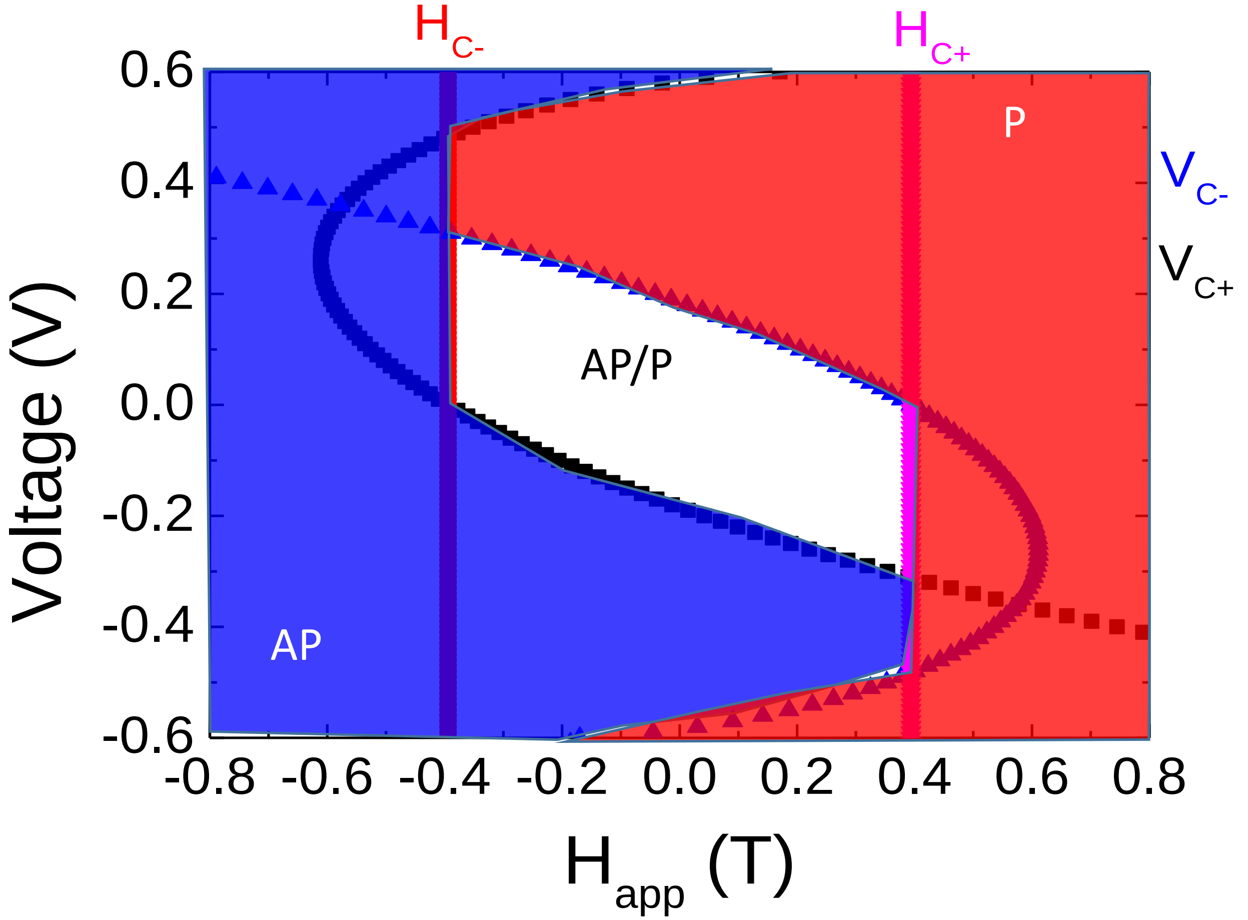
Macrospin: micromagnetic limit if the exchange interaction is infinite

Joule heating changes the temperature during the operation

$$C\frac{dT}{dt} = -Q(T - T_0) + \frac{V^2}{R}$$

$$\frac{M_s(T)}{M_{s0}} = \frac{a_{DL}(T)}{a_{DL,0}} = \left[1 - \left(\frac{T}{T_c}\right)^{1.73}\right]$$

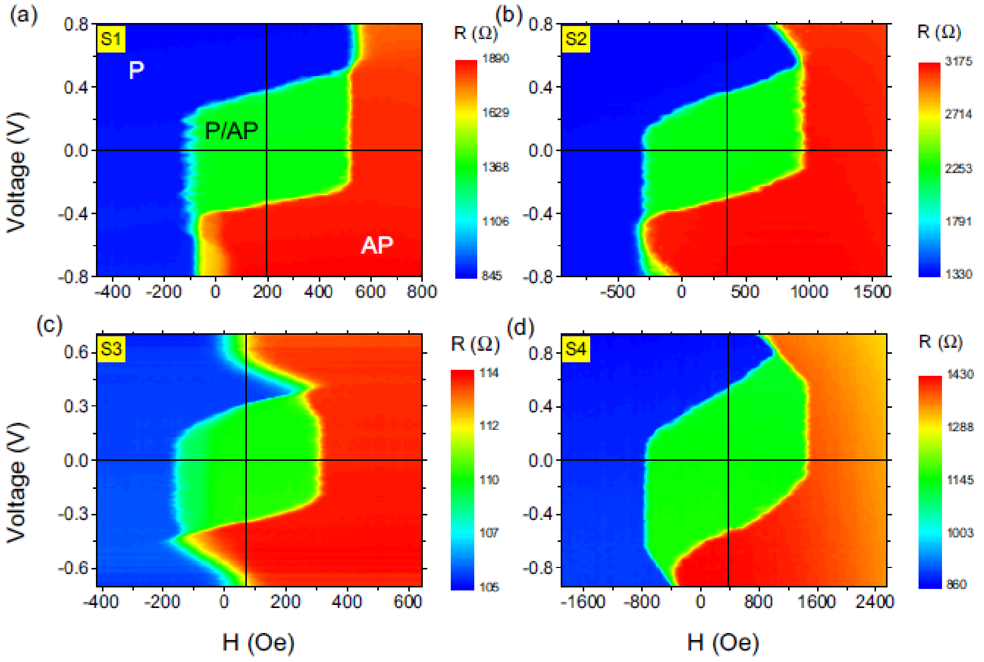
$$K_u(T) = K_0\left[\frac{M_s(T)}{M_{s0}}\right]^{\xi}$$



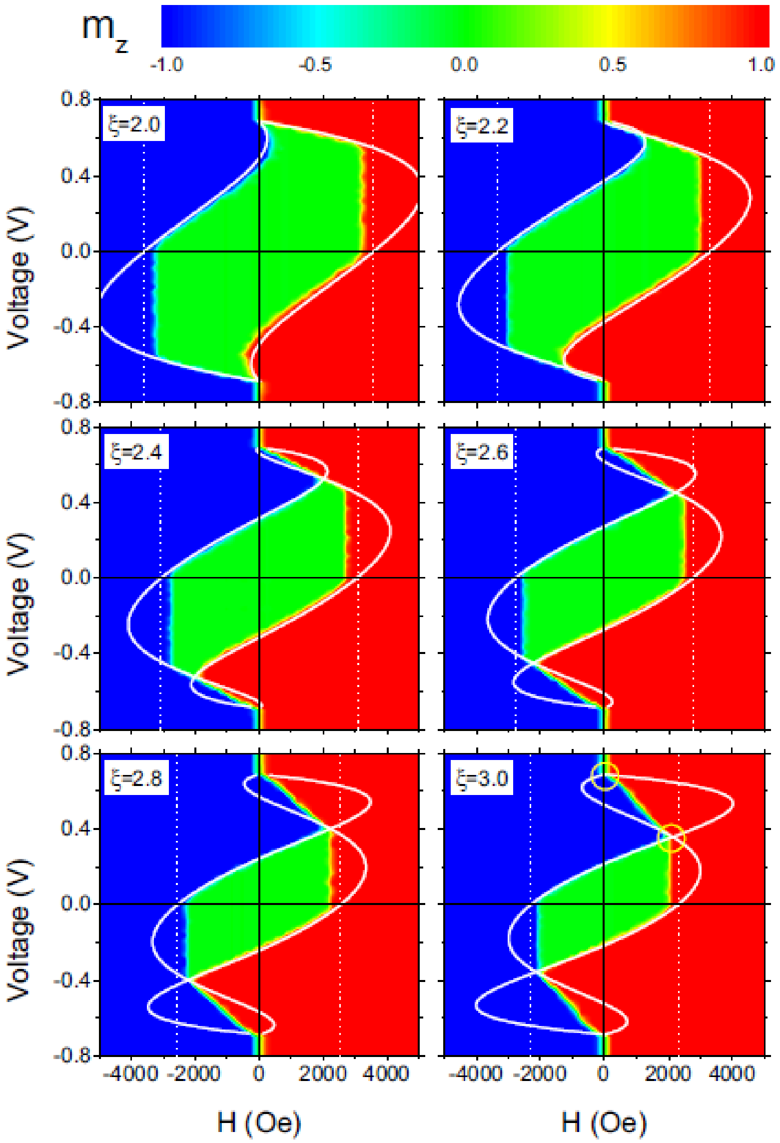
Strelkov et al. Phys Rev B (2017)

Macrospin: micromagnetic limit if the exchange interaction is infinite

Mesurements



Simulation

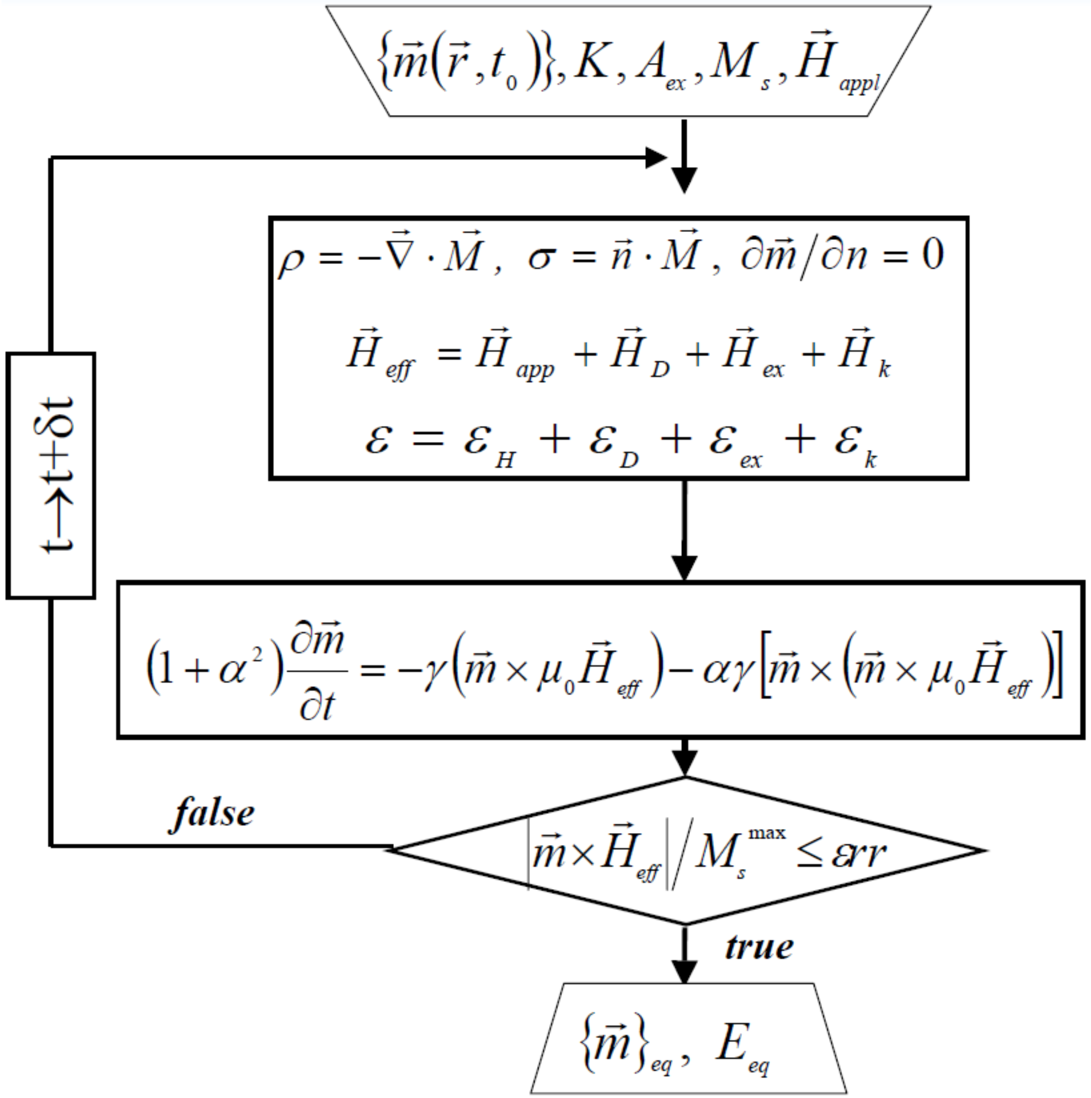


✓ **Sample dependent features**

Outline

- **Atomistic spin dynamics**
  - Formalism
  - Illustrations : alloy GdFe, Fe nanodot, AOS [Tb/Co] multilayers
- **Micromagnetism**
  - Formalism
  - Macrospin limit
  - Illustrations
- **Micromagnetism and spin related phenomena**
  - Formalism
  - Illustrations
- **Conclusions**

Micromagnetisme



- Defining the problem
  - -geometry description
  - -material parameters
  - -initial conditions (time & space)
- State characterization
  - -magnetic charges
  - -magnetostatic field
  - -fields & energy terms
- LLG time integration
  - - amplitude conservation
- Check equilibrium criteria
- Stable state- numerical solution

Micromagnetisme

OOMMF

micro3D

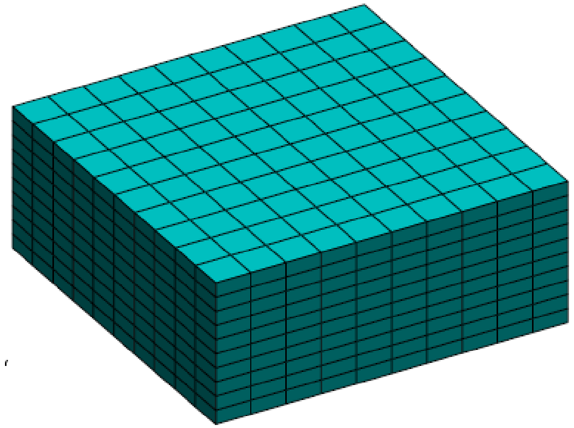
MicroMagus

mumax3

MAG TENSE

MAGNUM fd

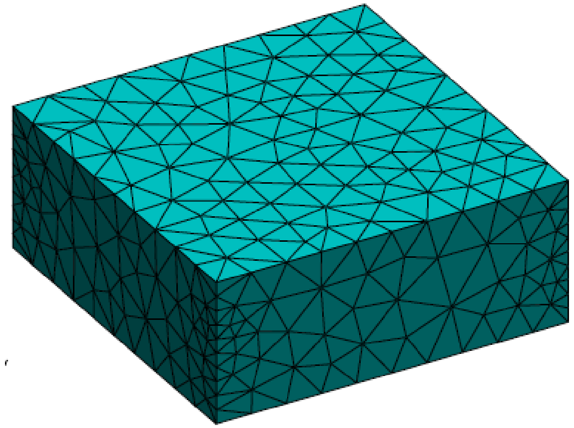
Finite difference approximation (FDA)



-regular mesh
-restrictive geometry

W.F. Brown Jr (1965)
Schabes et al., (1988)
Berkov et al.
Bertram et al.
Donahue et al.
Miltat et al.
Nakatani et al.
Toussaint et al.
Scheinfein et al.
J. -G. Zhu et al.…………

Finite element method (FEM / BEM)



-irregular meshes
-adaptive mesh refinement

Fredkin & Koehler
Fidler & Schrefl
Hertel & Kronmuller
Ramstöck et al.
…….

magpar

nmag

tetmag

MAGNUM fe

feeLLGood
finite element LLG object oriented development

FastMag

Micromagnetisme

Tomorrow's micromagnetic simulations

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Published Online: 10 May 2019

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J. Leliaert[a),b)] and J. Mulkers[a),c)]

AFFILIATIONS

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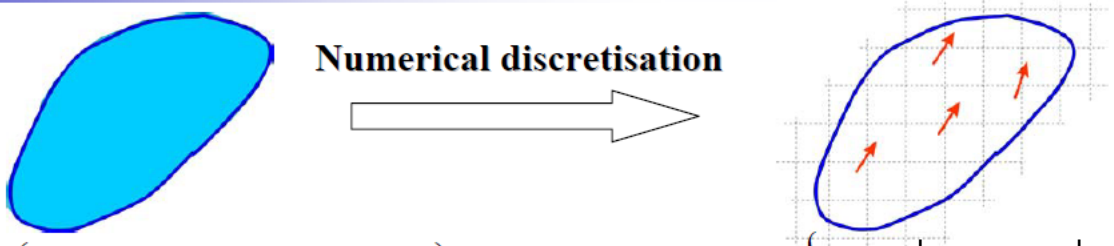
Name	Release	FE/FD	GPU capable?	Free?	References
LLG micromagnetics simulator	1997	FD	No	Commercial	29
OOMMF	1998	FD	No	Free	27
micromagus	2003[a]	FD	No	Commercial	30
magpar	2003	FE	No	Free	31
Nmag	2007	FE	No	Free	32
GPMagnet	2010	FD	Yes	Commercial	26
FEMME	2010	FE	No	Commercial	33
tetramag[b]	2010	FE	Yes	Commercial	34
finmag[c]	2011	FE	No	Free	35
Fastmag	2011	FE	Yes	Commercial	36
Mumax	2011	FD	Yes	Free	37
micromagnum	2012	FD	Yes	Free	38
magnum.fd[d]	2014	FD	Yes	Free	39
magnum.fe	2013	FE	No	Commercial	40
mumax3	2014	FD	Yes	Free	41
LLG micromagnetics simulator v4.	2015	FD	Yes	Commercial	29
Grace	2015	FD	Yes	Free	42,43
OOMMF (GPU version)	2016	FD	Yes	Free	44
fidimag	2018	FD	No	Free	45
commics	2018	FE	No	Free	46

Micromagnetisme

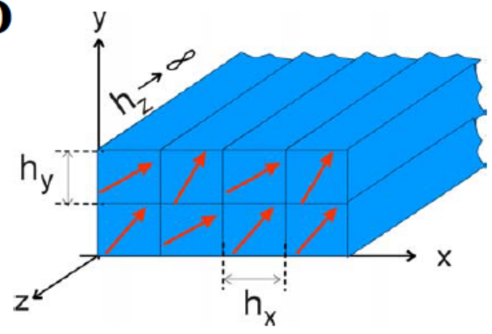


$$\vec{m} = \left\{ \vec{m}(\vec{r}) \mid \vec{r} \in V, |\vec{m}| = 1 \right\}$$
$$\vec{H}_{eff} = \left\{ \vec{H}_{eff}(\vec{r}) \mid \vec{r} \in V \right\}$$

$$\vec{m} = \left\{ \vec{m}_i \mid i = 1..N, |\vec{m}_i| = 1 \right\}$$
$$\vec{H}_{eff} = \left\{ \vec{H}_{eff,i} \mid i = 1..N \right\}$$

N – *total number of mesh nodes*

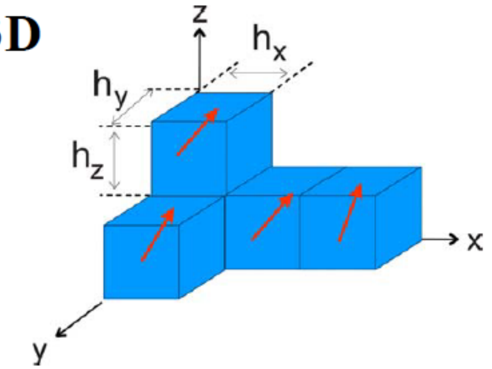
2D



-infinite prisms

: e.g. thin films

3D



-orthorhombic cells

: dots, wires, platelets, …

Micromagnetisme

Finite Difference Aproximation (FDA)

$$E[\vec{m}] = \int_V \left\{ \begin{array}{l} A_{ex}\left[\vec{\nabla}\vec{m}(\vec{r})\right]^2 + K_1\left[1-\left(\vec{u}_K\cdot\vec{m}(\vec{r})\right)^2\right] - \\ -\mu_0 M_s\left[\vec{m}(\vec{r})\cdot\vec{H}_{app}(\vec{r})\right] - \frac{1}{2}\mu_0 M_s\left[\vec{m}(\vec{r})\cdot\vec{H}_{dem}(\vec{m}(\vec{r}))\right] \end{array} \right\} dV$$

$$\vec{H}_{eff} = \frac{2A_{ex}}{\mu_0 M_s}\Delta\vec{m} + \frac{2K_1}{\mu_0 M_s}\left(\vec{u}_K\cdot\vec{m}\right)\vec{u}_K + \vec{H}_H + \vec{H}_D$$

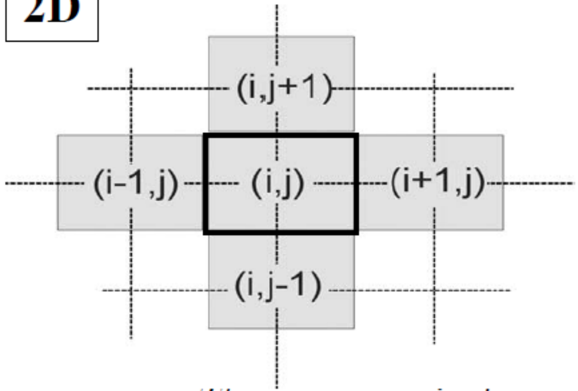
magnetic charges

$$\rho_m = -M_s\left(\vec{\nabla}\cdot\vec{m}\right)$$

$$\sigma_m = M_s\left(\vec{m}\cdot\vec{n}\right)$$

Taylor expansion

2D



$$m(i+1,j) = m(i,j) + \frac{\partial m}{\partial x}(i,j)h_x + \frac{1}{2}\frac{\partial^2 m}{\partial x^2}(i,j)h_x^2 + O(h_x^3)$$

$$m(i-1,j) = m(i,j) - \frac{\partial m}{\partial x}(i,j)h_x + \frac{1}{2}\frac{\partial^2 m}{\partial x^2}(i,j)h_x^2 + O(h_x^3)$$

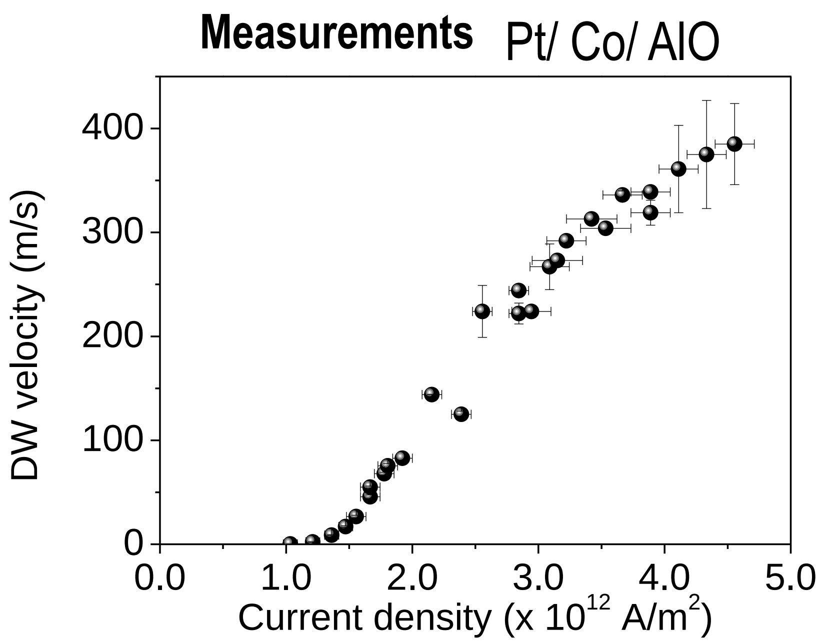
$$\frac{\partial m}{\partial x}(i,j) \cong \frac{m(i+1,j)-m(i-1,j)}{2h_x}$$

$$\frac{\partial^2 m}{\partial x^2}(i,j) \cong \frac{m(i+1,j)-2m(i,j)+m(i-1,j)}{h_x^2}$$

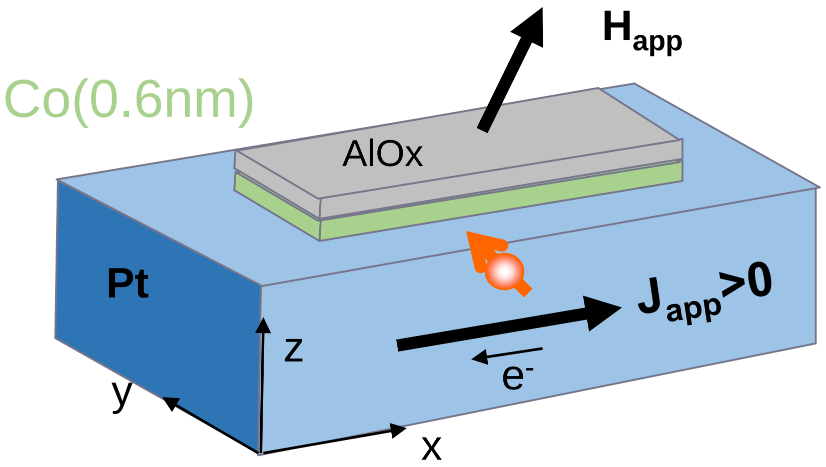
The accuracy is dependent on the Taylor expansion order !

M. Labrune, J. Miltat, JMMM **151**, 231 (1995).

Micromagnetism and spin related phenomena : DMI and domain walls



Miron et al, Nature Mater. **10**, 419 (2011)



1) Chiral exchange Dzyaloshinskii-Moriya

2) Spin polarized current //Oy (Spin Hall effect & Rashba effect

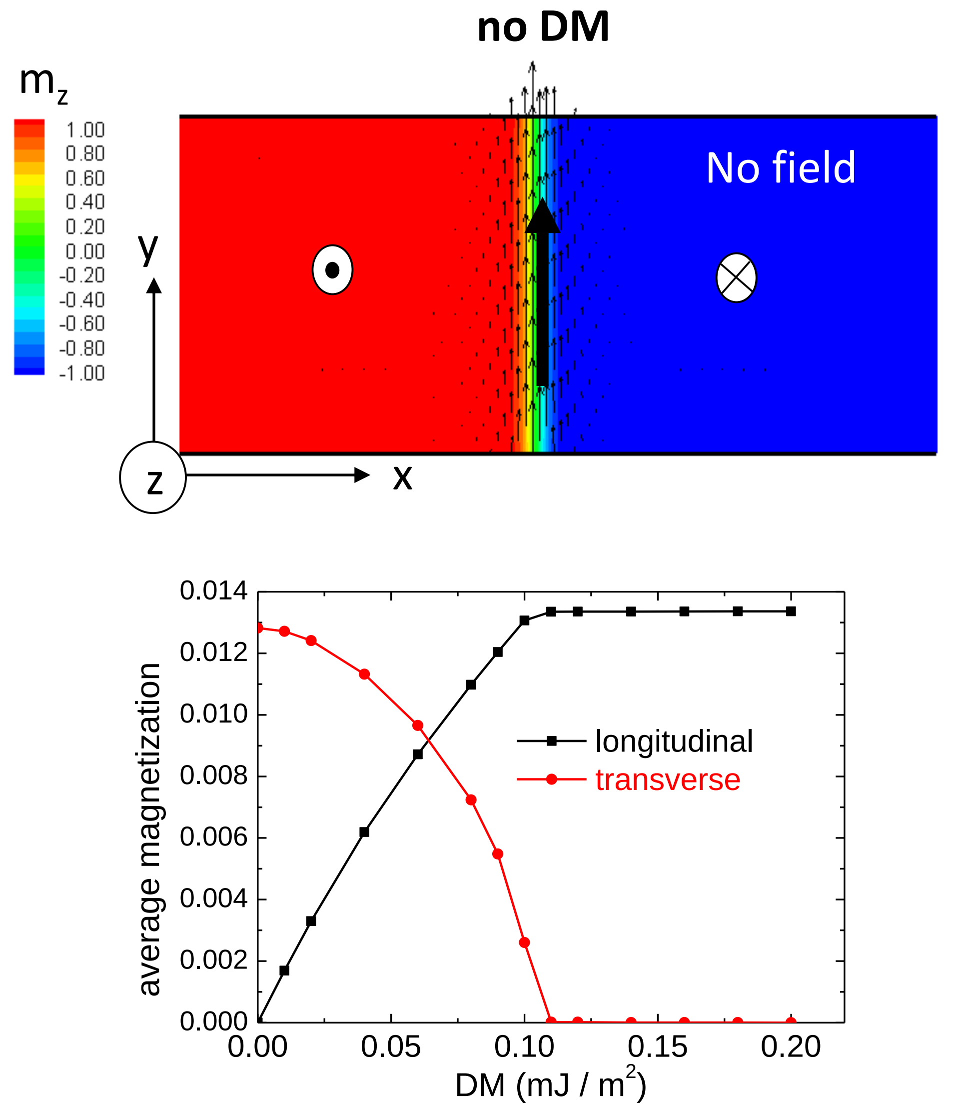
Eq. Landau-Lifshitz-Gilbert + DMI **+** **spin orbit torques**

$$\mathbf{H}_{\mathbf{DM}}(\mathbf{m}) = \frac{2D}{\mu_0 M_S}\left(\frac{\partial m_z}{\partial x}, \quad \frac{\partial m_z}{\partial y}, \quad -\frac{\partial m_x}{\partial x} - \frac{\partial m_y}{\partial y}\right)$$

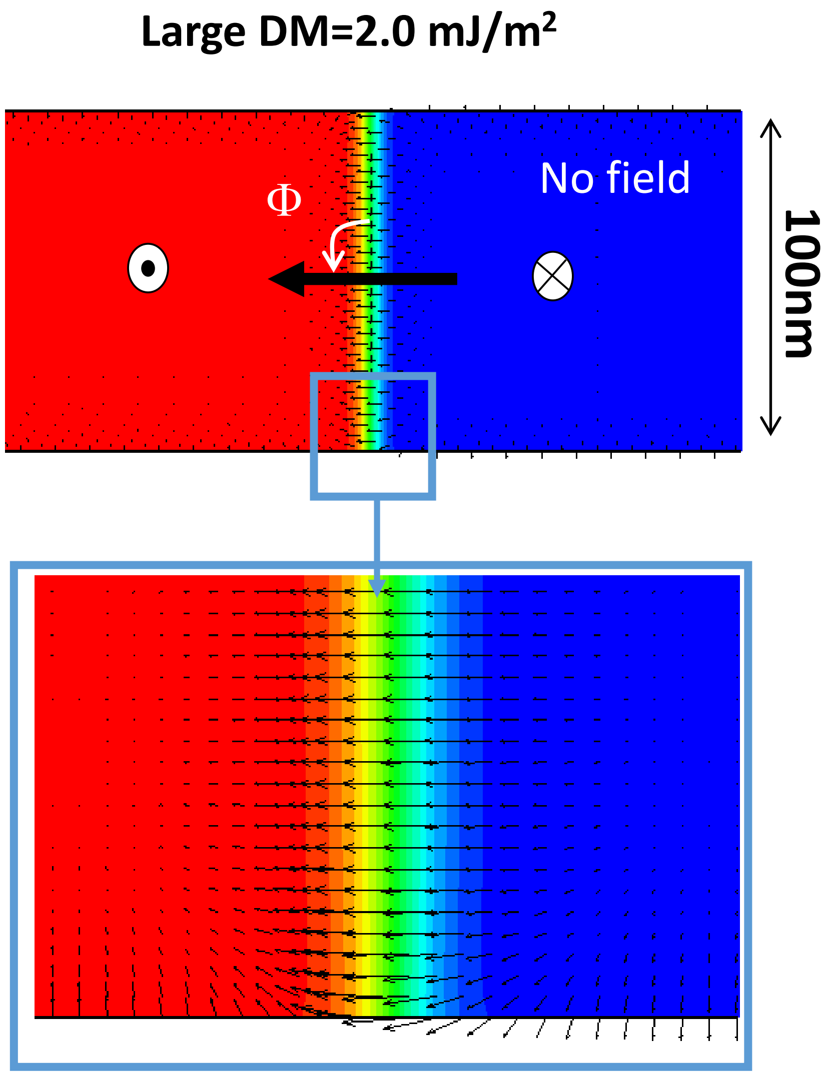
$$\left(\frac{\partial \mathbf{m}}{\partial t}\right)_{SOT} = \gamma_0 C_{FL} J_{app}\left[\mathbf{m}\times(\mathbf{u_J}\times\hat{\mathbf{z}})\right] + \gamma_0 C_{DL} J_{app}\mathbf{m}\times\left[\mathbf{m}\times(\mathbf{u_J}\times\hat{\mathbf{z}})\right]$$

A. Thiaville et al *Europhys*. Lett. 100, 57002 (2012)

Micromagnetism and spin related phenomena : DMI and domain walls

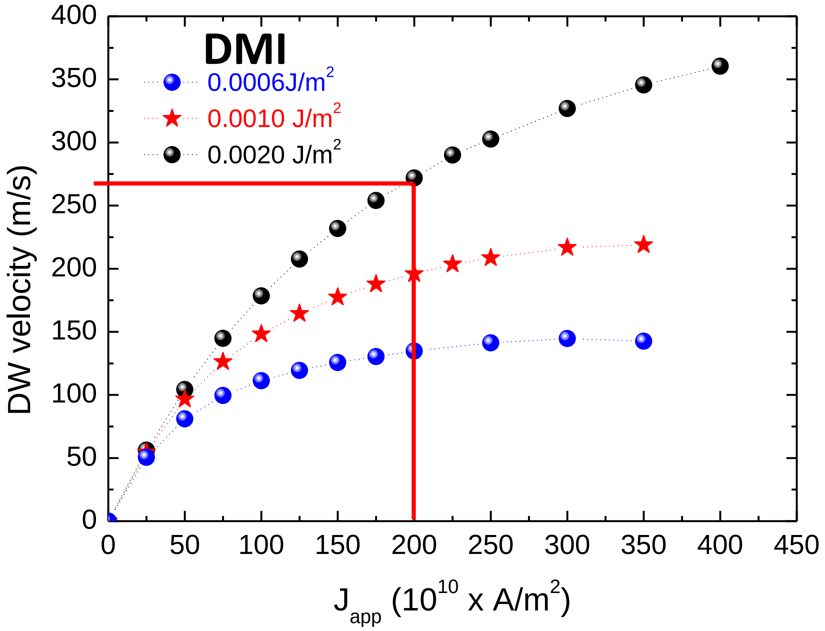


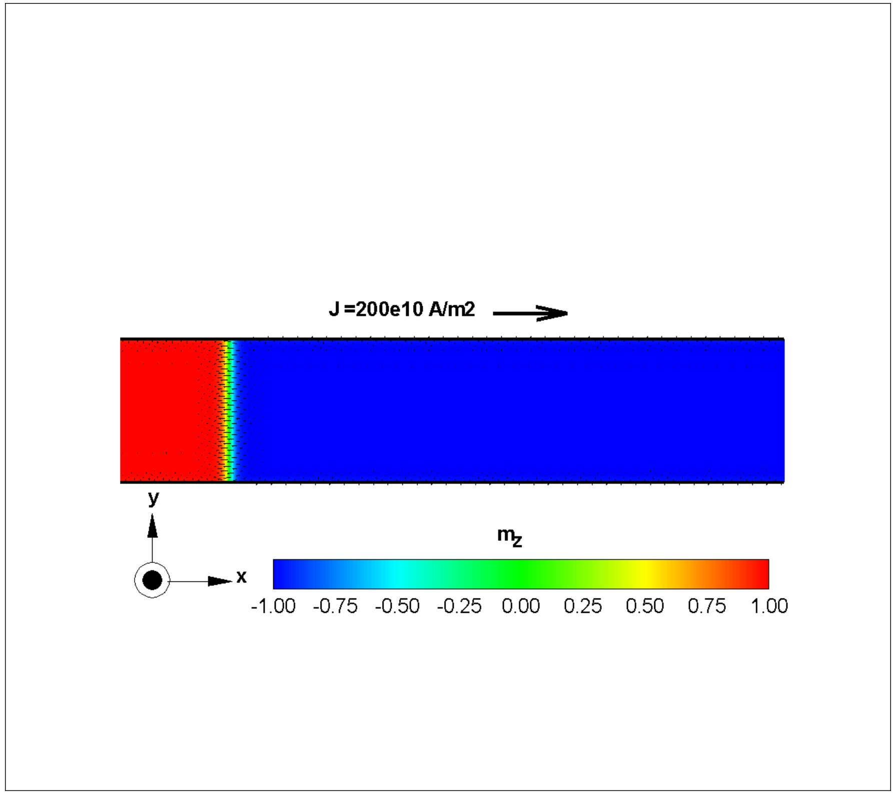
A. Thiaville et al., EPL, 100 (2013)



O. Boulle et al, Phys. Rev. Lett (2013)

Micromagnetism and spin related phenomena : DMI and domain walls



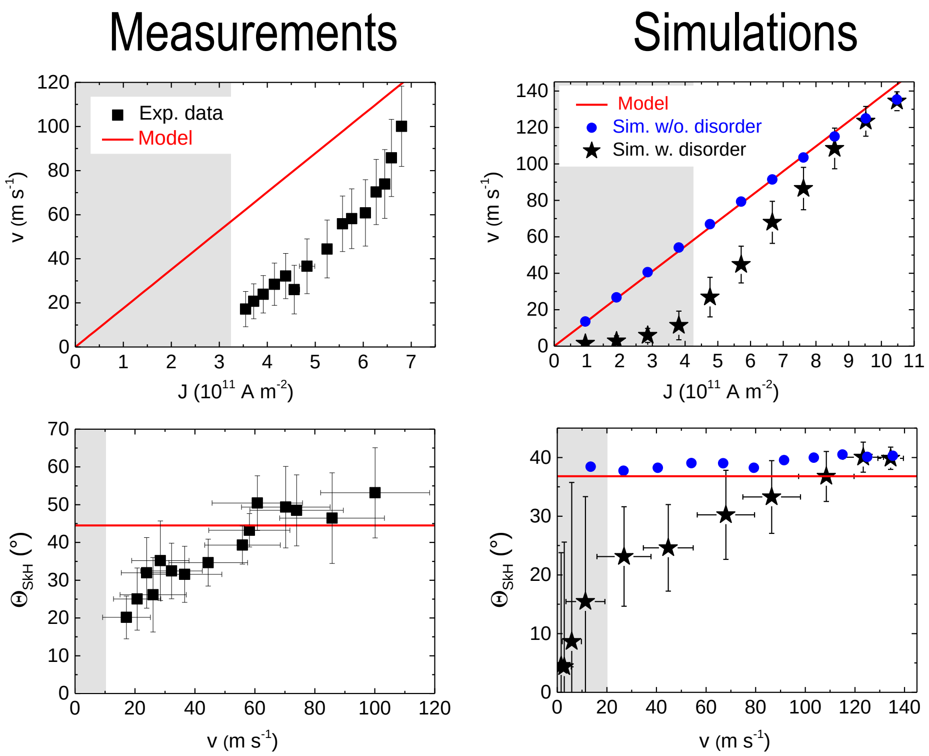


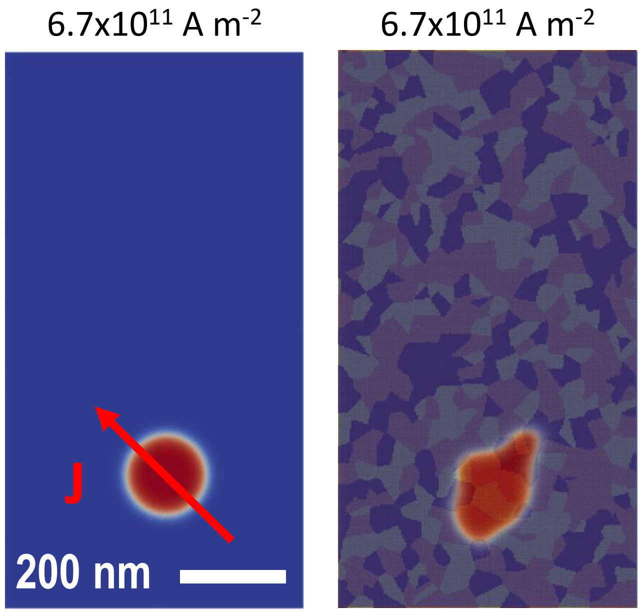
- ✓ **DMI+SOT : the key to explain the fast current induced DW motion in these materials**
- ✓ **DW velocity ~ J_{app}**

Micromagnetism and spin related phenomena : skyrmion Hall effect

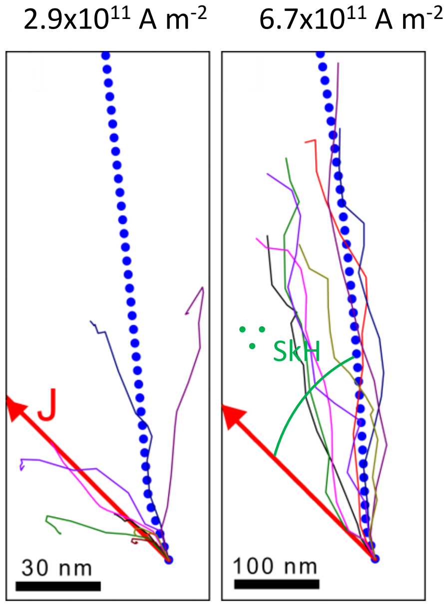
DARPA - TEE
Juge et al. PR Appl. (2019)
10.1103/PhysRevApplied.12.044007

Thin film of Pt / Co / MgO



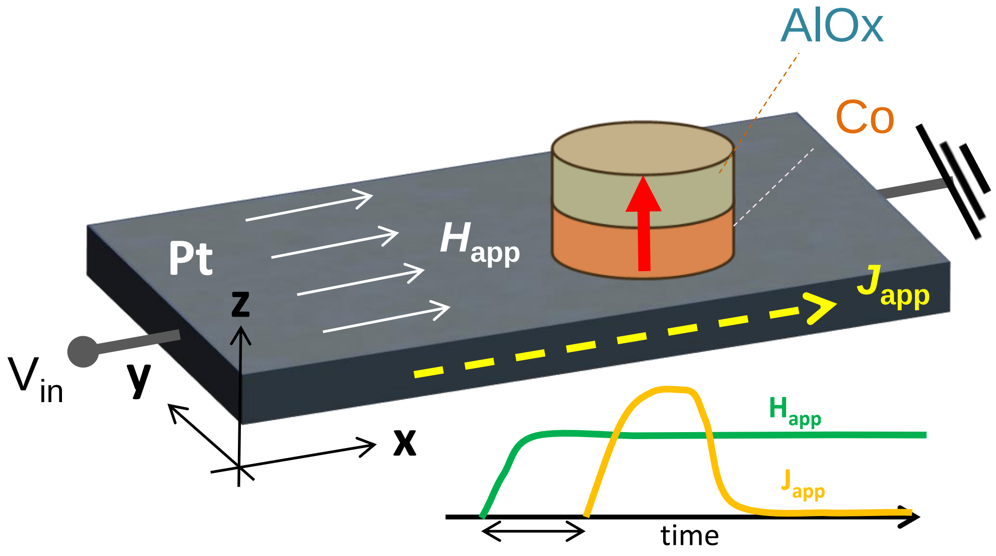


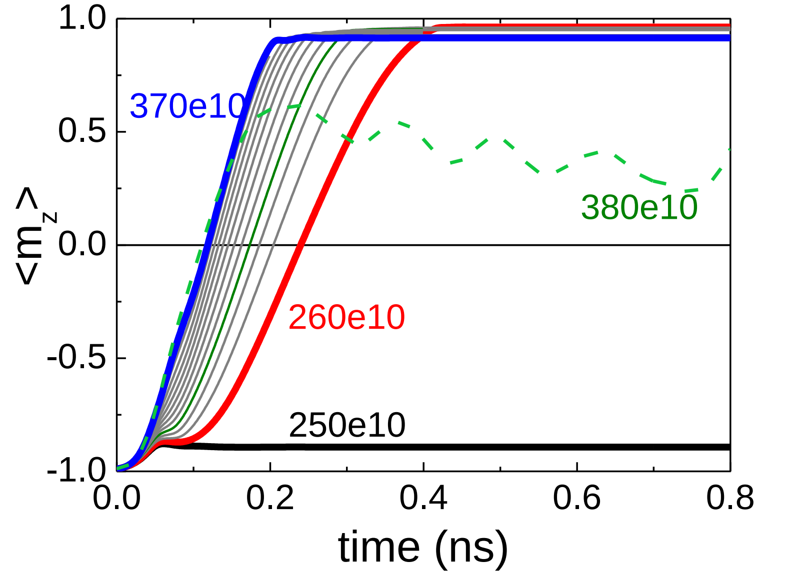
1 frame = 1 ns



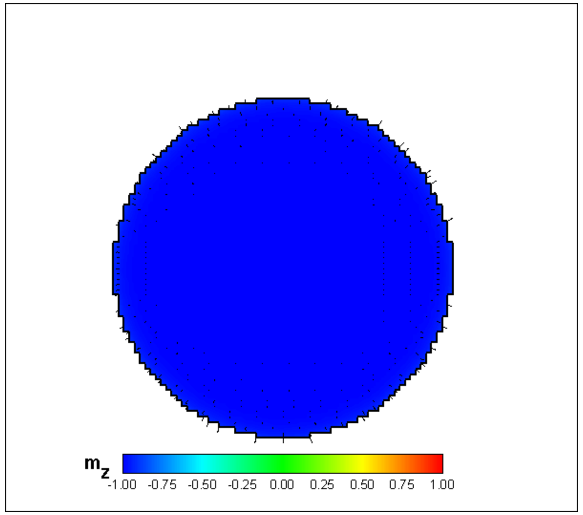
✓ **SOT current driven motion of the skyrmions depends strongly on the pinning**

Micromagnetism and spin related phenomena : SOT MRAM

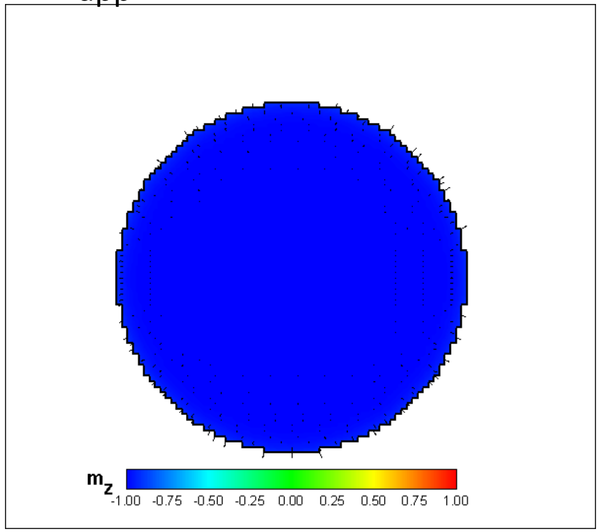




J_{app} = 260x10^{10} A/m^2



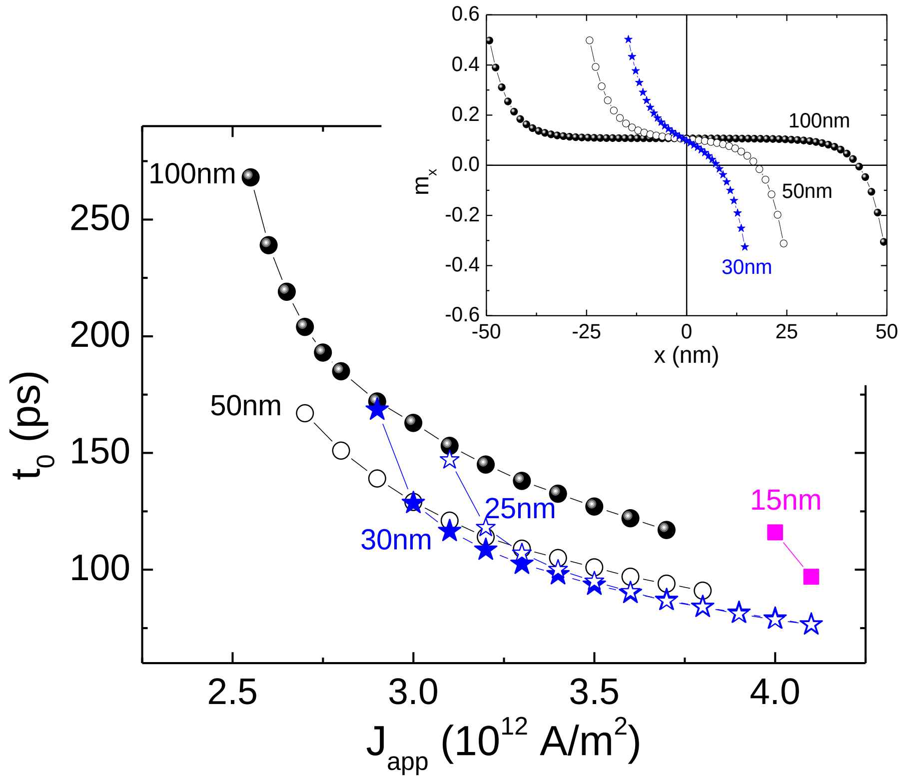
J_{app} = 350x10^{10} A/m^2 No field

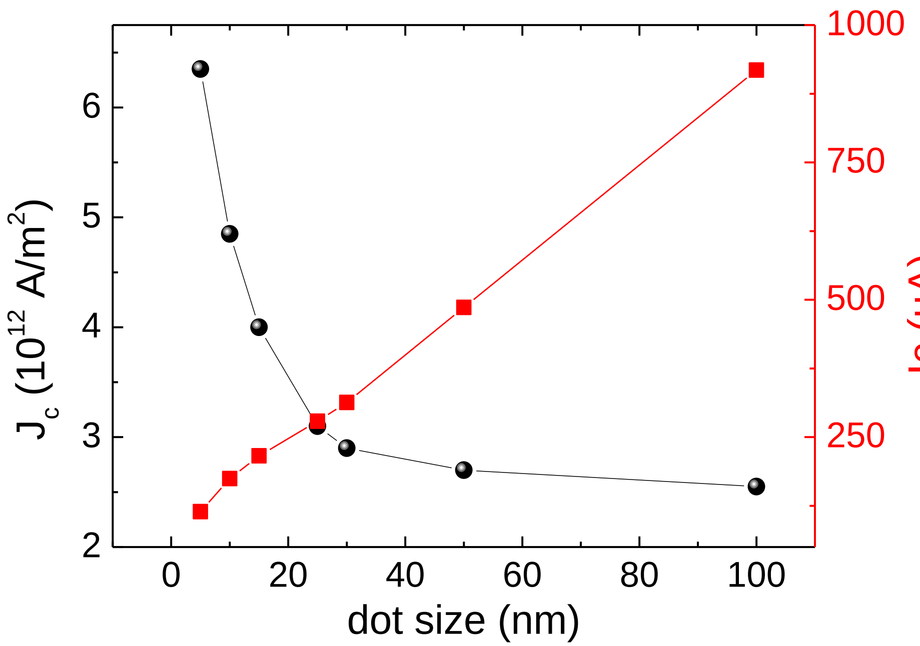


- ✓ **Bipolar switching**
- ✓ **Very short pulse < 250ps**
- ✓ **Reversal by nucleation/propagation of DW**

K. Garello et al Appl. Phys. Lett. (2014)
N. Mikuszeit et al. Phys. Rev. B (2015)

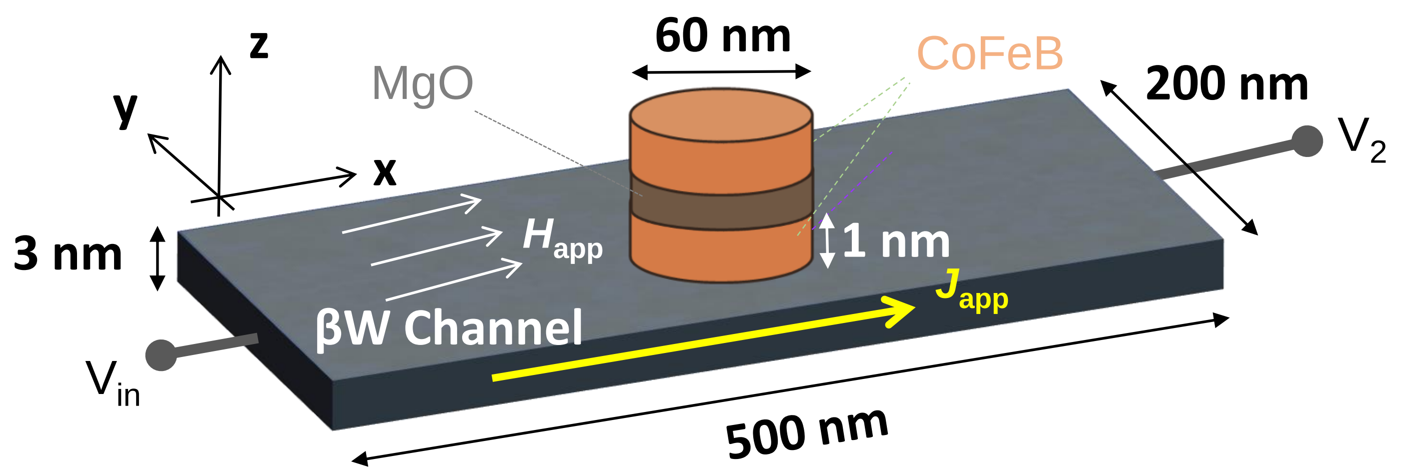
Micromagnetism and spin related phenomena : SOT MRAM





- ✓ **DW reversal mechanism if nanopillar size > 30nm**
- ✓ **Critical current varies linearly with nanopillar size**
- ✓ **Writing energy ~20fJ** $E_w = 1k\Omega \cdot (250\mu A)^2 \cdot 300\,ps = 20\,fJ$

Micromagnetism and spin related phenomena : SOT MRAM + heating



- **Key elements:**

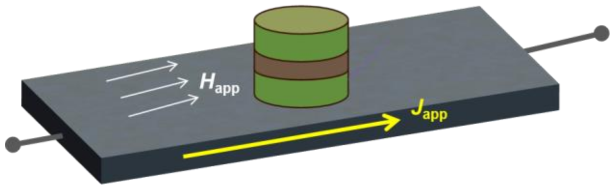
  Interfaces HM/FM and FM/Ox

  → perpendicular anisotropy – binary states & memory stability

  → Dzyaloshinskii-Moriya interaction

Spin orbit torques → to switch between the two stable states

Micromagnetism and spin related phenomena : SOT MRAM + heating



- **Intrinsic issues**
  - ✓ Parameters sensitive to temperature → $K_i(T)$, $M_s(T)$, $A_{ex}(T)$,…
  - ✓ Impact on the magnetization dynamics
  - ✓ Impact on the operation of the storage layer

Develop appropriate modelling approach

coupling : current → temperature → magnetization dynamics

Electric solver	Joule Heating
$\boldsymbol{J}_{app}(\boldsymbol{r},t)$	$\boldsymbol{T}(\boldsymbol{r},t)$
COMSOL	**3D**

LLG + SOT

$\boldsymbol{M}\left(\boldsymbol{J}_{app}(\boldsymbol{r},t),\boldsymbol{T}(\boldsymbol{r},t)\right)$

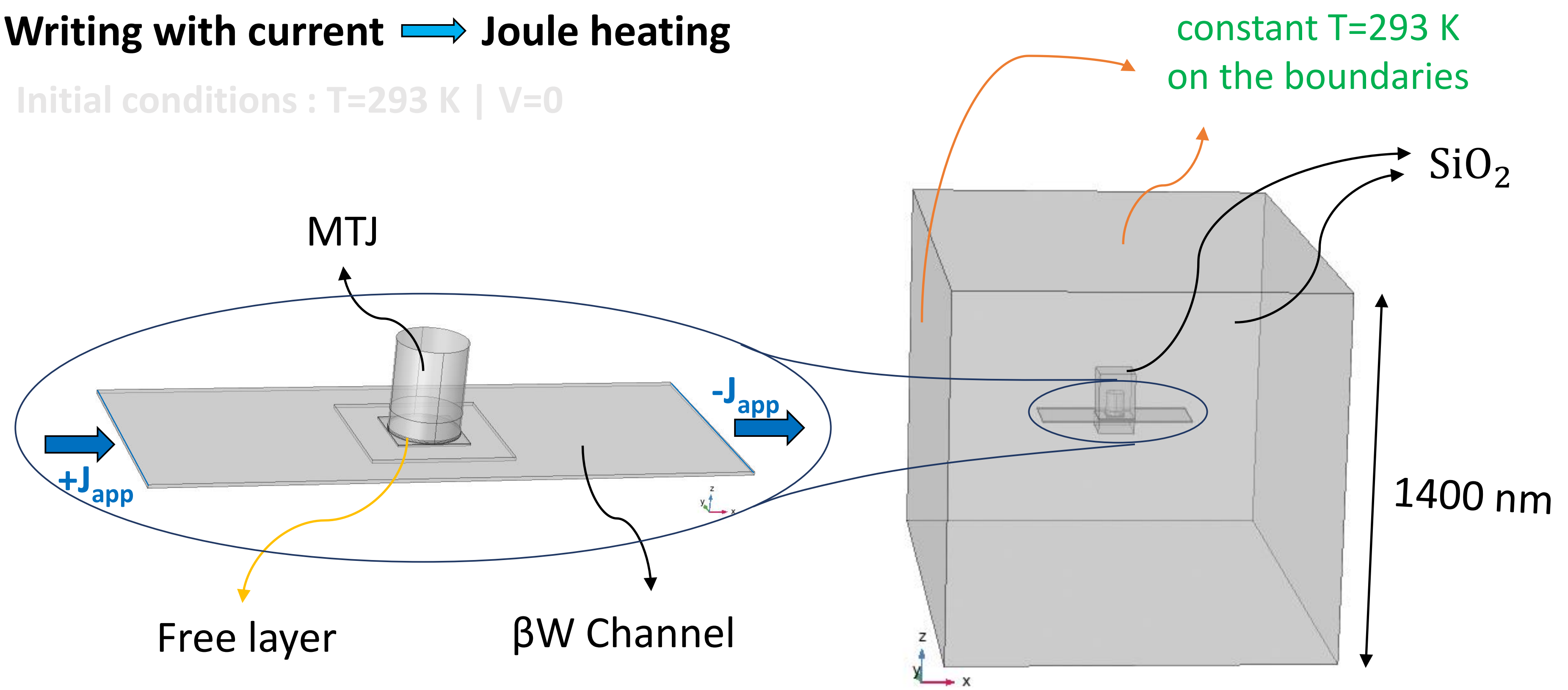
micromagnetic model

E. Grimaldi et al, Nature Nanotechnology (2020)

Micromagnetism and spin related phenomena : SOT MRAM + heating

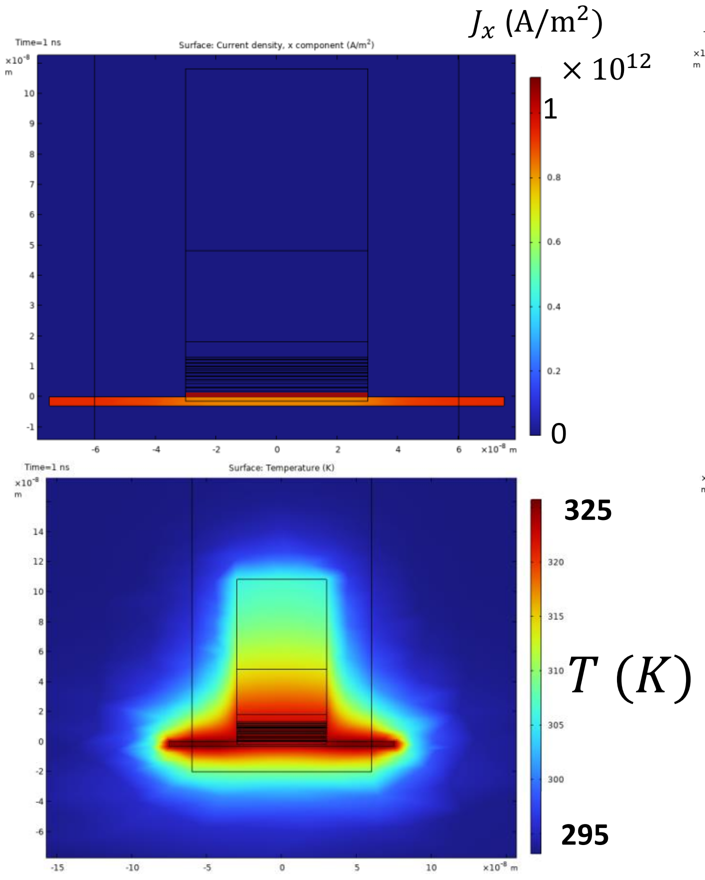
Writing with current ⟶ Joule heating

Initial conditions : T=293 K | V=0

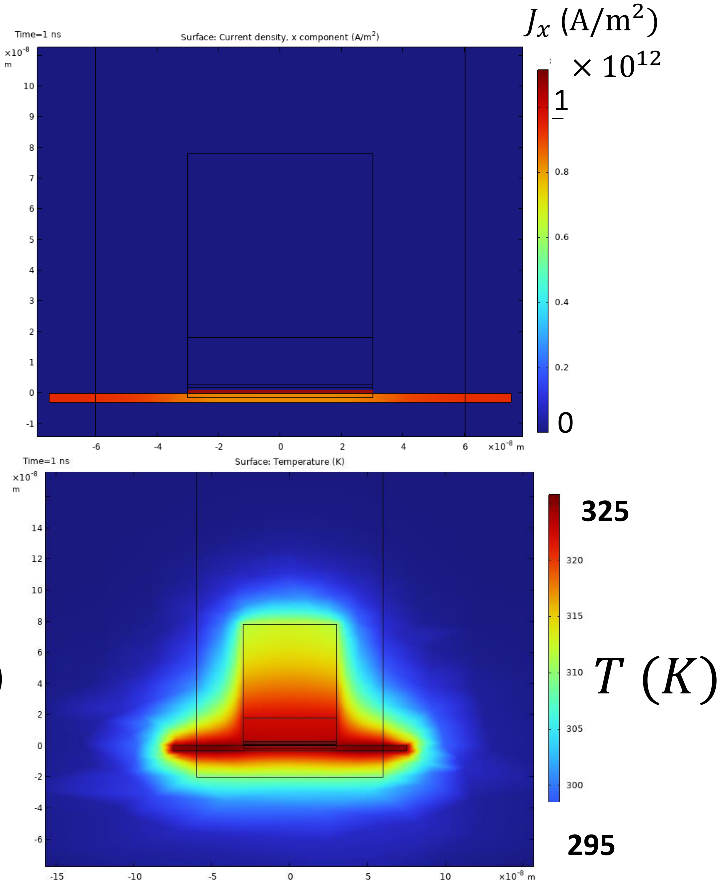


Micromagnetism and spin related phenomena : SOT MRAM + heating

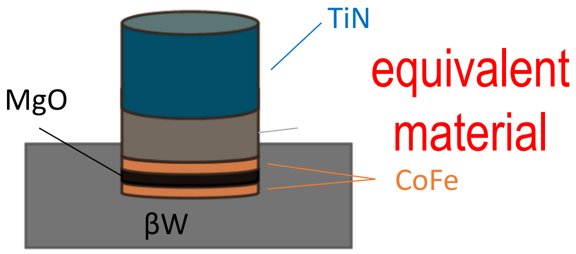
Full structure MTJ



Equivalent MTJ



t=1 ns



Micromagnetism and spin related phenomena : SOT MRAM + heating

Material parameters follow Callen-Callen laws

ΔT=30 K

Spontaneous magnetization

M_{s0} the value at 0K

T_C – critical temperature

$$M_s(T) = M_{s0}\left[1 - \left(\frac{T}{T_C}\right)^a\right]^b$$

7 % variation

Magnetocrystalline anisotropy

interface & bulk

$$K(T) = K_0\left[\frac{M_s(T)}{M_{s0}}\right]^p$$

16 % variation

Exchange stiffness

$$A_{ex}(T) = A_{ex_0}\left[\frac{M_s(T)}{M_{s0}}\right]^q$$

11 % variation

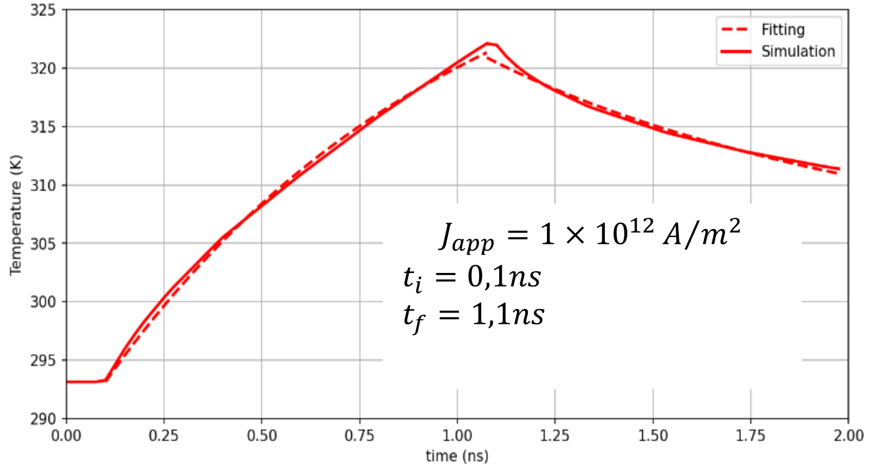
FeCoB

M_{s0} (A/m)	1.09e6
K_0 (J/m^3)	1.25e6
A_{ex_0} (J/m)	1.5e-11
a	1
b	1
p	2.5
q	1.7
T_C (K)	750
DMI (J/m^2)	1.5e-4
H_{app} (T)	0.06

Lee et al., AIP Adv., (2017)

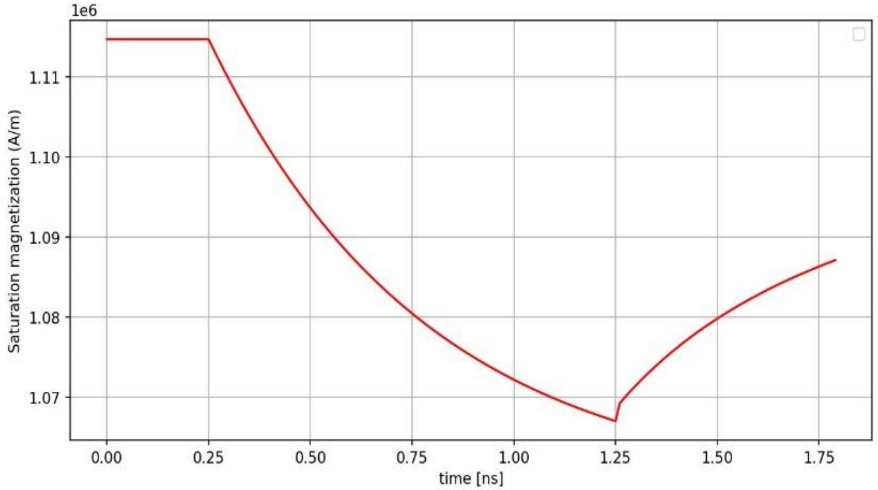
Micromagnetism and spin related phenomena : SOT MRAM + heating

$T(t)$



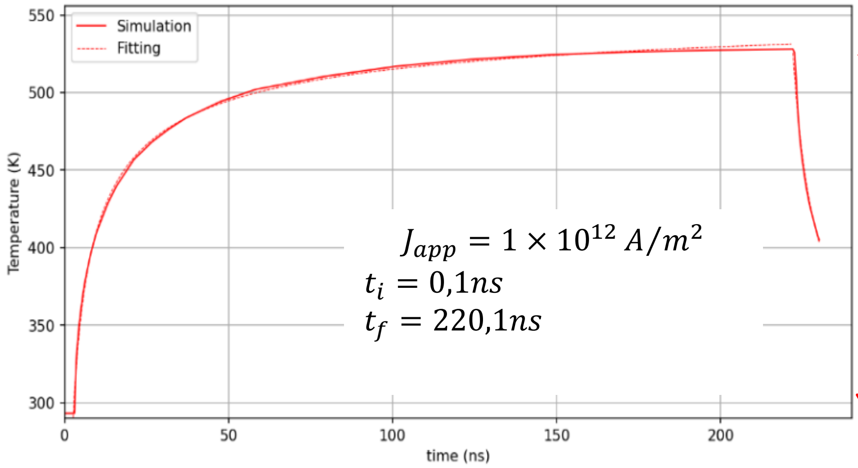
30°

$M_S(T(t))$



Fitting parameters : c, t', T_r, u and t^* depend on the simulation conditions

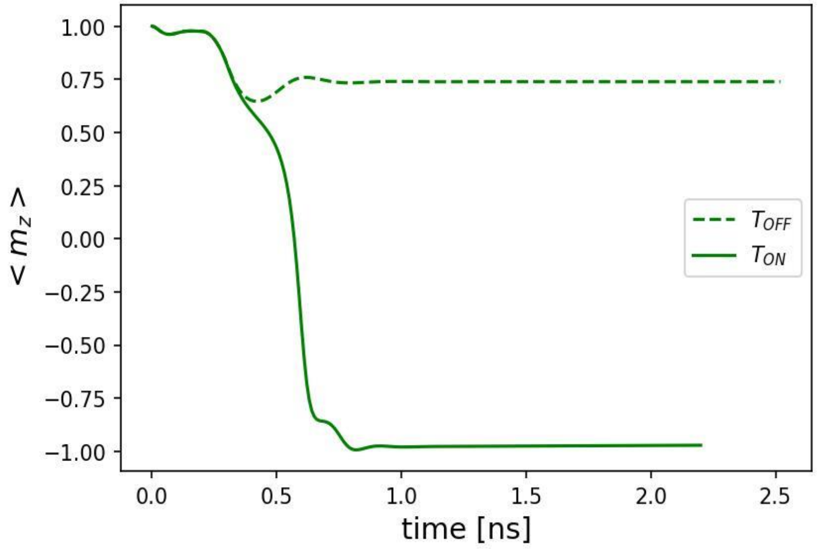
$$T(t) = \begin{cases} -\dfrac{c}{\sqrt{t - t'}} + T_r & t_i < t < t_f \\ -\dfrac{u}{t - t^*} + 293 & t > t_f \end{cases}$$



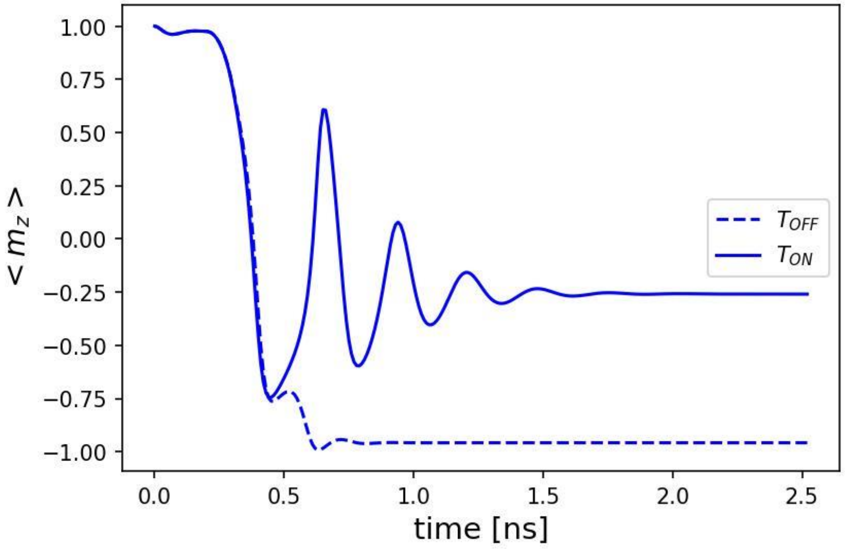
240°

Given current pulse → $T(t)$ → fitting → micromagnetics

$J = 0.9 \times 10^{12}\ A/m^2$



$J = 1.2 \times 10^{12}\ A/m^2$



Modelling – take home messages

- Model versus Reality
  - Validity of the model
  - Utility of the model

- Critical thinking on numerical solutions

  A solver gives always a solution!

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