EPFL

MICRO-435 Quantum and Nanocomputing

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NML - LLG

MICROMAGNETIC SIMULATIONS

NANOMAGNETIC LOGIC

OBJECTIVES

MAGNETIZATION DYNAMICS - LLG

MICROMAGNETIC SIMULATIONS

GENERAL NANOMAGNETIC ELEMENTS

A BIT OF THEORY ON MAGNETIZATION DYNAMICS

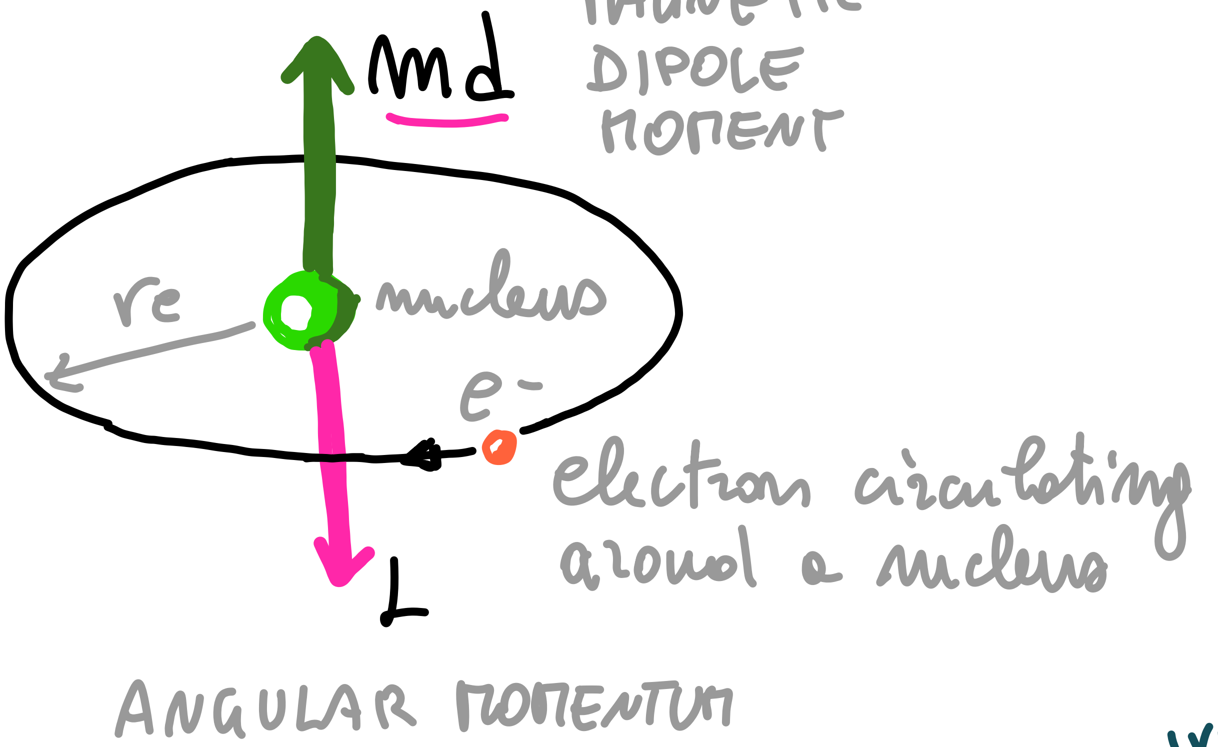
$$\frac{dM}{dt}$$

The goals are

1) to understand what happens to a general magnetic element when a magnetic field is applied

2) to see how this dynamic is analyzed in micromagnetic - simulations

3) to understand how the model is simplified when nanomagnets are the focus



IN A FERROMAGNETIC MATERIAL EVERY ATOM HAS A MAGNETIC DIPOLE MOMENT

USING BOHR MODEL, WHEN AN ELECTRON e^- CIRCLES AROUND THE NUCLEUS GENERATES A CIRCULAR CURRENT I_e

THE CURRENT I_e EMBRACING AREA A RESULTS IN A DIPOLE MOMENT AMPLITUDE

$$m_d = I_e \cdot A$$

- If the orbit radius is r_e $\quad A \to \pi r_e^2$
- If the motion around the nucleus has ROTATION FREQUENCY ω_0 $\quad I_e \to -\frac{e\omega_0}{2\pi}$

then

$$m_d = I_e A = -\frac{e\omega_0}{2\pi}\pi r_e^2 = \underbrace{-\frac{e\omega_0}{2} r_e^2}$$

THE NUCLEUS EXERTS A FORCE on the circulating $\underline{e}$ that has MASS m_e

This generates the ANGULAR MOMENTUM $\underline{L}$ having amplitude

$$\underbrace{L = \omega_0 m_e r_e^2}$$

ACCORDING TO BOHR MAGNETON AS:

→ the ENERGY LEVELS of an atom are discrete → the angular momentum is quantized

→ the magnetic dipole is consequently quantized, and ASSUMES VALUES that ARE INTEGER MULTIPLE of BOHR MAGNETON

$$\mu_B = \frac{e}{2m_e}\hbar$$ (← Planck's constant)

$$m_d = -m_L \cdot \mu_B \quad , \quad m_L = 0, \pm 1, \pm 2 \ldots$$

when the Bohr magneton represents the smallest dipole moment of an electron

DIPOLE MOMENT AND ANGULAR MOMENTUM ARE ASSOCIATED BY THE GIROMAGNETIC RATIO γ

$$\bar{m}_d = \gamma \cdot \bar{L}$$

if a single electron

$$\gamma = -\frac{e}{2m_e}$$

BUT ELECTRONS HAVE SPIN, THAT GENERATE A MAGNETIC MOMENT

→ THE RELATION IS CORRECTED TO

$$\overline{m}_d = g \cdot \gamma \cdot \overline{L} = -g \frac{e}{2m_e} \cdot \overline{L}$$

$g \Leftarrow$ LANDE GYROMAGNETIC SPLITTING FACTOR depending on the value

- only orbital momentum
- only spin momentum
- both and other contributions

are considered

IF AN EXTERNAL FIELD H_{eff} IS APPLIED, WITH A CERTAIN ANGLE α TO m_d $\Rightarrow$ A TORQUE T IS IMPOSED TO THE MAGNETIC MOMENT

DIPOLE

$$\bar{T} = \mu_0 \cdot \overline{m_d} \times \overline{H_{eff}}$$

TORQUE IS PERPENDICULAR TO m_d and H_{eff}

THE TORQUE DETERMINES A PRECESSION MOTION OF $\overline{m_d}$ AROUND THE DIRECTION of H_{eff}

(if $\alpha = 0$ then is no precession)

TORQUE REPRESENTS THE GRADIENT W.R.T. TIME

OF THE ANGULAR MOMENTUM

$$\overline{T} = \frac{d\overline{L}}{dt}.$$

$$\overline{m}_d = g\gamma\overline{L} \qquad \overline{L} = \frac{\overline{m}_d}{g\gamma}$$

substituting the value of $\overline{T}$ given before

$$T = \frac{d}{dt}\left(\frac{\overline{m}_d}{g\gamma}\right) = \underbrace{\frac{1}{g\gamma}\cdot\frac{d\overline{m}_d}{dt}} = \underbrace{\mu_0\,\overline{m}_d \times H_{eff}}$$

THEN THE GRADIENT OF m_d W.R.T. TIME IS

$$\frac{d\bar{m}_d}{dt} = \mu_0 \cdot g \gamma \bar{m}_d \times H_{eff} = \mu_0 \cdot g \cdot \frac{e}{2m_e} \cdot m_d \times H_{eff}$$

that is

$$\boxed{\frac{d\bar{m}_d}{dt} = \gamma_{LLG} \cdot m_d \times H_{eff}}$$

DESCRIBES THE MOTION OF AN UNDAMPED MAGNETIC MOMENT IN A FIELD

with $\gamma_{LLG} = \mu_0 g \frac{e}{2m_e} = 2.21 \cdot 10^5 \frac{m}{As}$

IS THE LANDAU-LIFSHITZ GYROMAGNETIC RATIO

IF A MAGNETIC MATERIAL IS CONSIDERED IN A CERTAIN VOLUME THE RESULTING MAGNETIC DIPOLE IS THE MAGNETIZATION M

$$\Downarrow$$

$$\rightarrow \quad \frac{d\,\underline{\bar{M}(r,t)}}{dt} = -\gamma_{LLG}\left[\underline{\bar{M}(r,t)} \times \bar{H}_{eff}(r,t)\right]$$

THIS TERM REPRESENTS THE PRECESSION MOVEMENT ($\underbrace{\text{LANDAU - LIFTSHITZ}}$ eq.) OF MAGNETIZATION VECTOR SUBJECTO TO FIELD Heff

IN A REAL MAGNETIC STRUCTURE ALSO DISSIPATION MUST BE CONSIDERED (OTHERWISE M WOULD NEVER STOP PRECESSING AROUND H!)

⇒ DISSIPATION IS INCLUDED (GILBERT & KELLY) WITH A DAMPING TERM

$$\left.\frac{d\bar{M}(r,t)}{dt}\right|_{\text{DISSI-PATION}} = \frac{\alpha}{M_s}\left[\bar{M}(r,t) \times \frac{dM(r,t)}{dt}\right]$$

α = GILBERT DAMPING $\quad$ M_s SATURATION MAGNETIZATION

SUMMING THE 2 TERMS GIVES

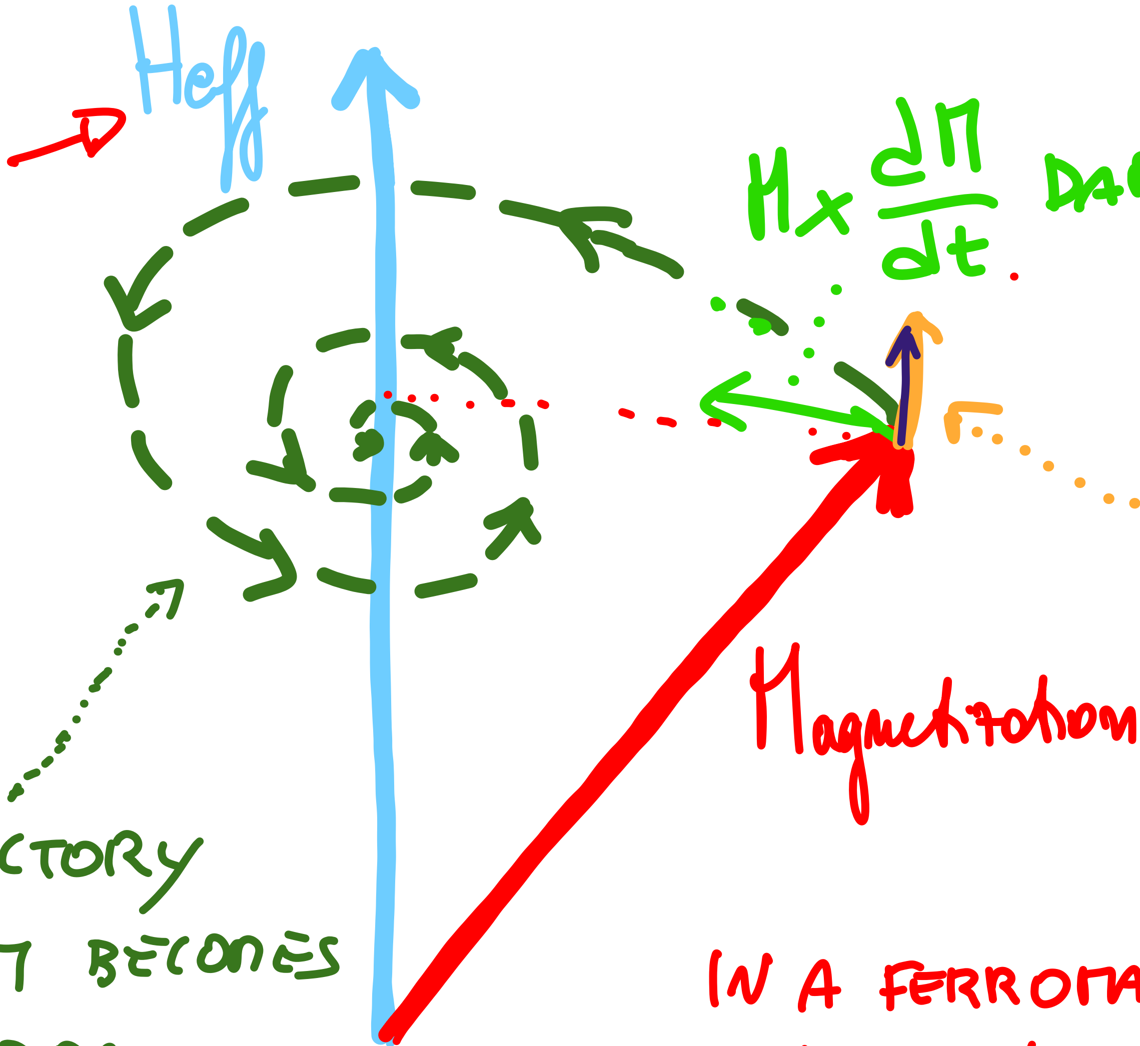
LANDAU - LIFSHITZ - GILBERT EQ.. (LLG)

$$\frac{dM(r,t)}{dt} = \underbrace{-\gamma_{LLG}\left[M(r,t) \times H_{eff}(r,t)\right]}_{} + \quad \text{PRECESSION}$$

$$\text{DAMPING} \quad \underbrace{-\frac{\alpha\,\gamma_{LLG}}{M_s}\left[M(r,t) \times \left(M(r,t) \times H_{eff}(r,t)\right)\right]}_{}$$

AFTER AWHILE THE PRECESSION STOPS AND THE MAGNETIZATION TURNS TO THE DIRECTION H_{eff}

DISSIPATION DESCRIBES ENERGY TRANSFER FROM MOTION TO HEAT



OSCILLATIONS ARE REDUCED

$M \times \frac{dM}{dt}$ DAMPING → WLLG

$M \times [M \times H_{eff}]$

$-M \times H_{eff}$ PRECESSION

VARIATION OF DIRECTION OF ROT. AXIS

TRAJECTORY OF M BECOMES A SPIRAL FORCED BY H_{eff}.

IN A FERROMAGNET IN PRESENCE OF A FIEDS MAGNETIZATION EVOLVES AS A SPIRAL TOWARD H_{eff}.

H_{eff} REPRESENTS IN EACH MOMENT THE EFFECTIVE FIELD (CONSIDERED CONSTANT) AND INCLUDES SEVERAL COMPONENTS

$$H_{eff} = H_{exc} + H_{ANIS} + H_{ZEEM} + H_{DEM} + H_{ADD} + H_{THERM}$$

Depending on the situation some are negligible

H_{exc} : EXCHANGE ENERGY IS RESPONSIBLE OF THE MAGNETIC ORDERING SETTING, INCLUDES → QUANTUM EFFECT BETWEEN CONTIGUOUS SPINS THAT ALIGN IN A PARALLEL MAGNETIZATION DIRECTION → LOCAL CONTRIB., few Tens of nm

H_{ANIS}: MAGNETO CRISTALLINE ANISOTROPY, TENDS TO BLOCK ATOM IN A CERTAIN M, DUE TO PROPERTY OF MATERIAL

H_{ZEEM} : external magnetic field applied

H_{DEM} : demagnetization due to magnetostatic energy (stray field energy) due to interaction among the magnetic moments around; called demagn. because it tends to reduce M for minimizing energy; contribute to shape anisotropy

H_{ADD}: ADDITIONAL TERMS THAT MIGHT BE PRESENT (e.g. MAGNETOSTRICTION, SPIN TRANSFER TORQUE...)

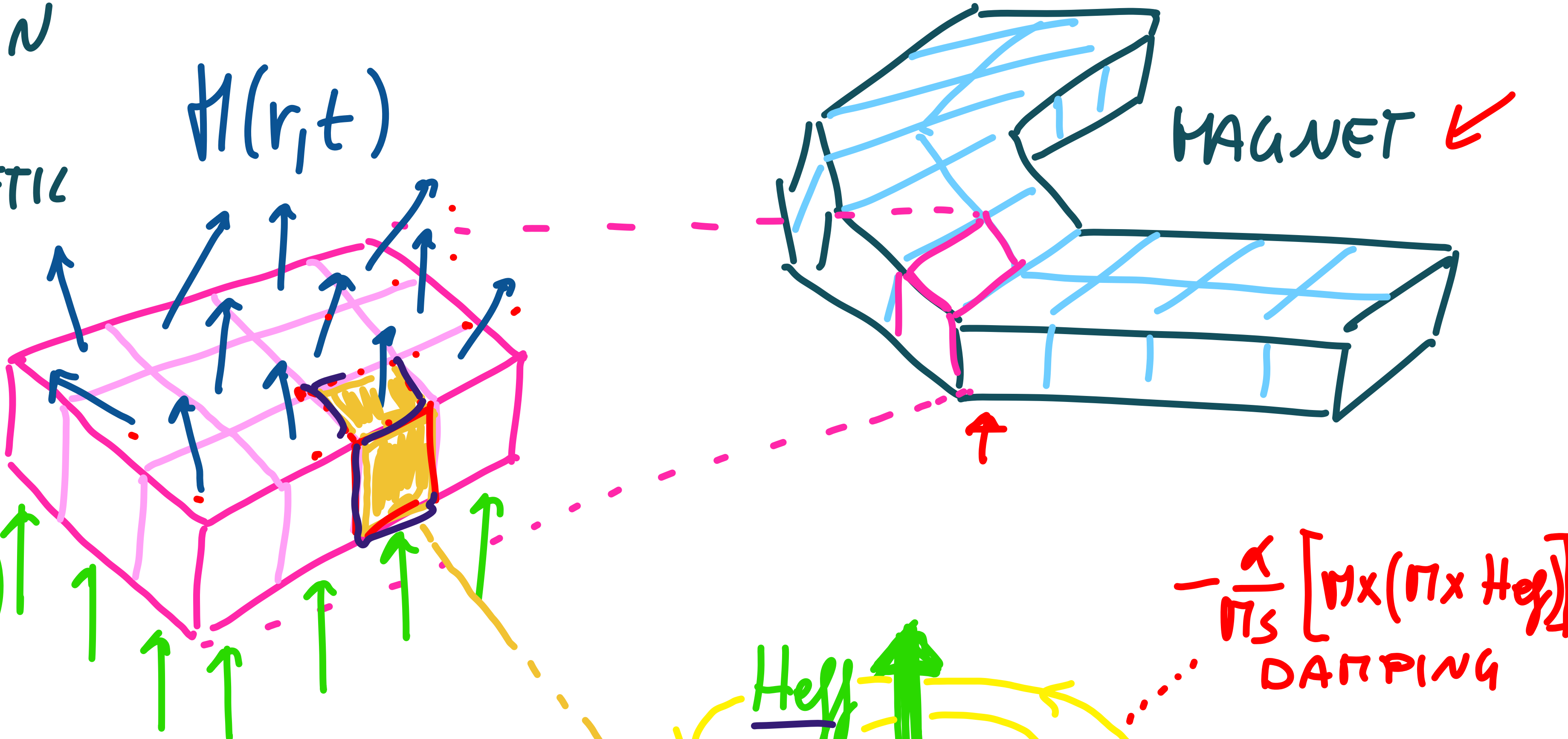
H_{THERM} To be considered when $T \neq 0$ AND CONSIDER T_1, $T_{2,1}$ and thermal noise

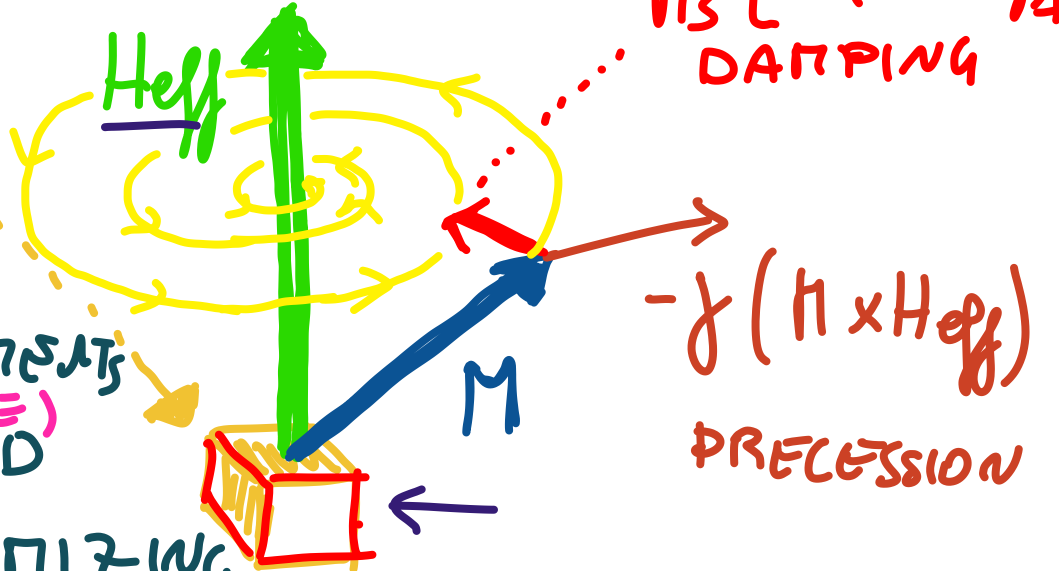
LLG IN MICROMAGNETIC ANALYSIS

LLG ARE USED AS MODEL FOR ALL MAGNETIC SYSTEMS EVOLVING IN TIME UNDER THE INFLUENCE OF A MAGNETIC FIELD

NORMALLY IN MICROMAGNETIC SIMULATIONS THE MULTIDOMAIN LLG VERSION IS APPLIED

MULTIDOMAIN
LLG
MICROMAGNETIC
SIMULATION.





THE MAGNETIC STRUCTURE IS
DISCRETIZED INTO FINITE ELEMENTS (IN TIME)
IN A 3DGRID, LLG ARE SOLVED
FOR EACH ELEMENT, MINIMIZING
THE TOTAL ENERGY —D 3D PARTIAL DIFFERENTIAL
CONSIDERING ALL THE INTERACTIONS EQUATIONS

MOST POPULAR SIMULATORS

OOMF (CPU) / MUMAX (GPU) USED IN PRO

↓

USED IN LAB

NOTE: THE NANOMAGNET, EVEN IF SINGLE DOMAIN IS SIMULATED USING THE MULTIDOMAIN P.D.D.EQ.

IMPORTANT FOR CORRECTLY READING THE SIM. RESULTS!!

$$\frac{\partial M(r,t)}{\partial t} = \overbrace{-\gamma M(r,t) \times H_{eff}(r,t)}^{\text{PRECESSION}} - \overbrace{\frac{\alpha\gamma}{M_s}\left\{ M(r,t) \times \left[M(r,s) \times H_{eff}(r,t) \right] \right\}}^{\text{DAMPING}}$$

PARTIAL DERIVATIVE DIFFERENTIAL EQ.

MAGNETIZATION VECTOR NORMALIZED W.R.T. M_s

time

VECTOR x, y, z IN SPACE

VECTOR PRODUCT

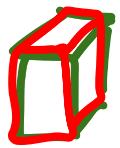
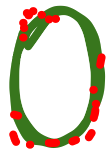
LLG MULTI DOMAIN

IF WE WANT TO MODEL THE SINGLE DOMAIN TO MORE RAPIDLY CALCULATE THE INFLUENCE BETWEEN SINGLE NANOMAGNET $\longrightarrow$ SINGLE DOMAIN APPROXIMATION $\downarrow$

SINGLE DOMAIN APPROXIMATION

IN ORDER TO SIMPLIFY

a) <u>1 DOMAIN</u> ASSOCIATED TO <u>1 MESH ELEMENT</u>

b). THE ELEMENT  is approximated with an ELLIPSOIDAL ELEMENT  i <u>index</u> of current ellipsoidal approximation

c) $H_{eff} \longrightarrow H_{eff}^{(i)}(t)$ is simplified to what is sufficient ↓

$$H_{eff}^{(i)}(t) = H_{zeem}^{(i)} + \overbrace{N^{(i)} \cdot M^{(i)} + \sum_{\substack{j \in NEIGHBOURS \\ j \neq i}} C^{(i,j)} \cdot M^{(j)}}^{H_{dem}}$$

EXTERNAL FIELD

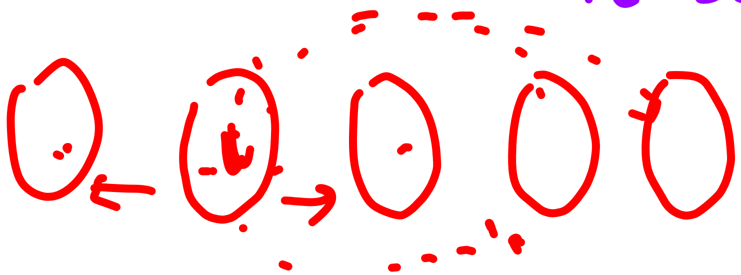
SELF (DE)MAGNETIZATION

→ SELF-INFLUENCE

MAGNETOSTATIC ENERGY DUE TO NEIGHBOURS

$N^{(i)}$ MAGNETIC DEMAGNETIZATION TENSOR

$C^{(i)}$ COUPLING TENSOR



H_{anis}, H_{exec} ARE NORMALLY NEGLECTED IN THIS APPROX.

AS A CONSEQUENCE THE SIMPLIFIED LLG $\Big|_{\text{SINGLE DOMAIN}}$ BECOMES

$$\frac{d\,M^{(i)}(t)}{dt} = \overbrace{-\gamma\, M^{(i)}(t) \times H_{eff}^{(i)}(t)}^{\text{precession}} + \underbrace{- \frac{\alpha\gamma}{M_s}\left\{ M^{(i)}(t) \times \left[M^{(i)}(t) \times H_{eff}^{(i)}(t) \right] \right\}}_{\text{damping}}$$

MAGNETIZATION OF A SINGLE ELIPSOIDAL ELEMENT NORMALIZED W.R.T. M_S

TO SOLVE THE SYSTEM IN TIME EVOLUTION FOR ALL THE SINGLE-MAGNETS

↳ MAGNETIC FCN-LOOP BASED ON SINGLE-DOMAIN LLG eq.

CONSIDERS

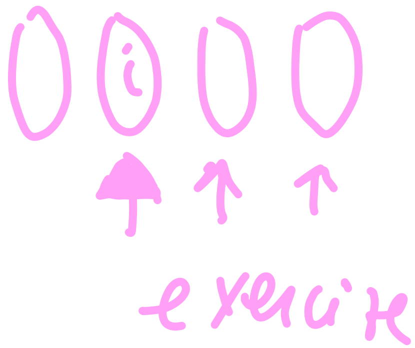
→ TIME VECTOR :

$$t_k \in \{t_0, t_1, \ldots\ldots t_{max}\}$$

• CONVERGENCY using

$\varepsilon_{STABILITY}$

INIT : t_0, $M_0^{(i)}$ STATUS



- $\forall t_k \in t_1 \dots t_{MAX}$
  - $\forall i$ element in the system

    SOLVE $\frac{dM^i(t)}{dt}$, FIND $M^i_{t_k}$
  - USE $M^i_{t_k}$ to FIND $M^i_{t_{k+1}}$ in next time step

UNTIL

→ t_{MAX} IS REACHED

OR

$\boxed{\overline{M^i_{t_{k+1}} - M^i_{t_k}} < \varepsilon_{STABILITY}}$ FOR EVERY i IN THE SYSTEM

CRISTALLIZATION

- LLG : MAGNETIZATION DYNAMIC
- MULTIDOMAIN LLG
- SINGLEDOMAIN LLG