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Chiral magnetic skyrmions and computational micromagnetism

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joint work with

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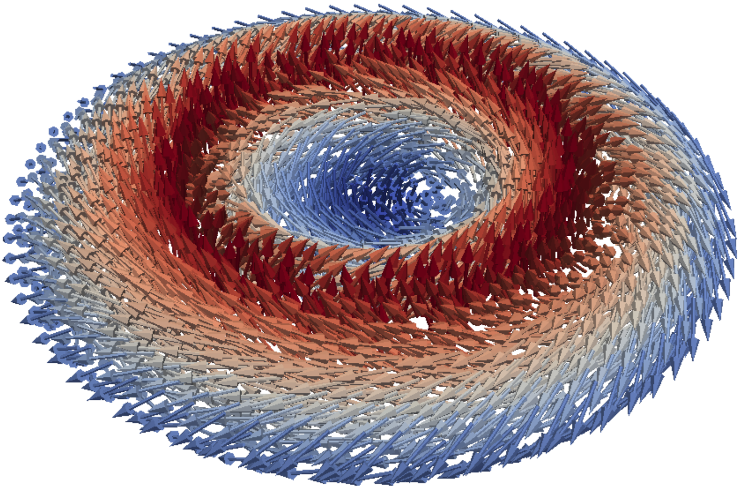
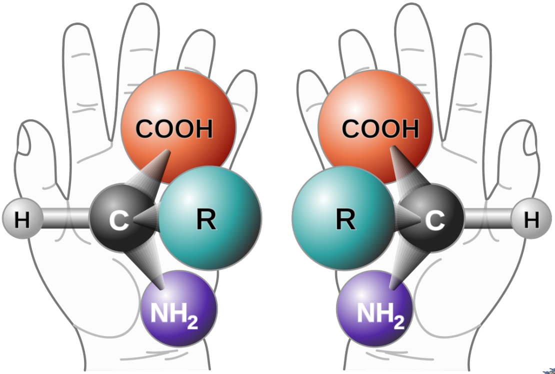
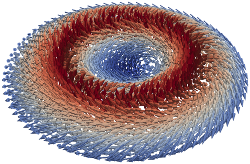
FWF

Introduction

Magnetic skyrmions

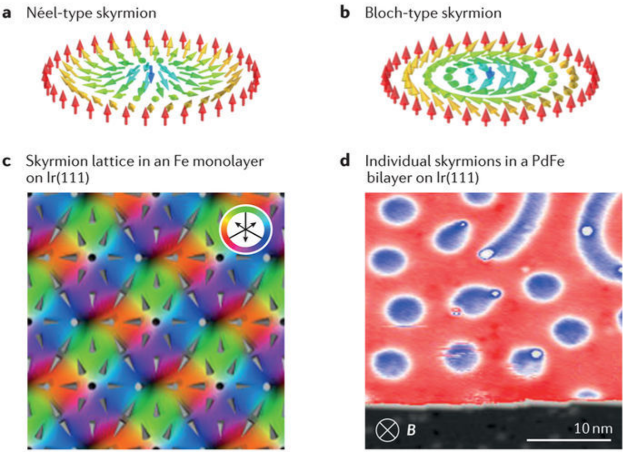




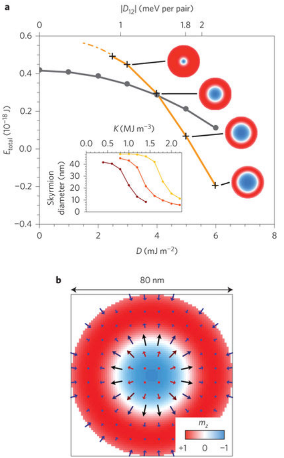


@ Wikipedia (https://en.wikipedia.org/wiki/Chirality)

Magnetic skyrmions



source: Fert et al. '17

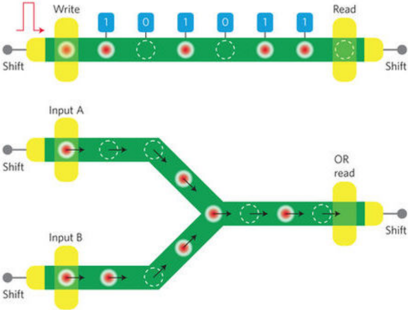


source: Sampaio et al. '13

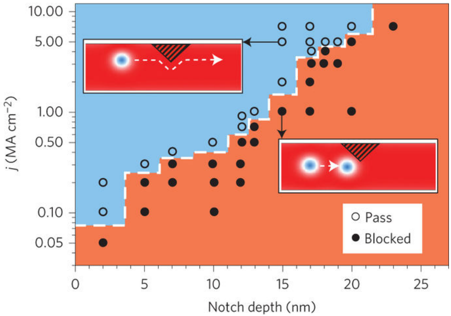
Sampaio, Cros, Rohart, Thiaville, Fert: Nat. Nanotechnol. 8 (2013)

Fert, Reyren, Cros: Nat. Rev. Mater. 2 (2017)

Skyrmionics



source: Krause et al. '16



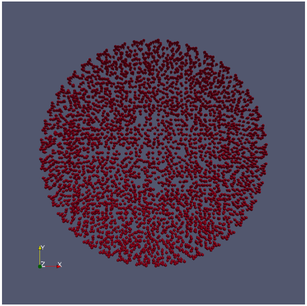
source: Fert et al. '17

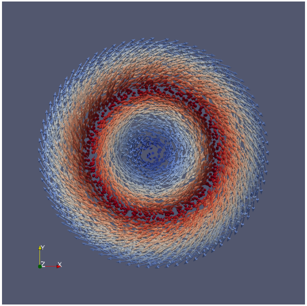
Krause, Wiesendanger: Nat. Mater. 15 (2016)

Fert, Reyren, Cros: Nat. Rev. Mater. 2 (2017)

Numerical experiment

- helimagnetic nanodisk of 140 nm diameter and thickness 10 nm
- material parameters of FeGe





Beg, Albert, Bisotti, Fangohr et al. Phys. Rev. B 95 (2017)

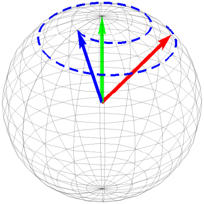
Outline

Landau–Lifshitz–Gilbert equation

Landau–Lifshitz form of LLG

- $\partial_t \boldsymbol{m} = -\dfrac{1}{1+\alpha^2}\,\boldsymbol{m} \times \boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m}) - \dfrac{\alpha}{1+\alpha^2}\,\boldsymbol{m} \times \big[\boldsymbol{m} \times \boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m})\big]$
- $\boldsymbol{m}(0) = \boldsymbol{m}^0 : \Omega \to \mathbb{S}^2$

- $\Omega \subset \mathbb{R}^3$ $\rightsquigarrow$ ferromagnet
- $\boldsymbol{m} : \Omega \times (0,T) \to \mathbb{S}^2$ $\rightsquigarrow$ magnetization
- $\alpha > 0$ $\rightsquigarrow$ Gilbert damping constant
- $\boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m})$ $\rightsquigarrow$ effective field



Dynamics preserves modulus

- $\partial_t \dfrac{1}{2}|\boldsymbol{m}|^2 = \boldsymbol{m} \cdot \partial_t \boldsymbol{m} = 0 \quad \Longrightarrow \quad |\boldsymbol{m}| = 1$

Effective field

- $\boldsymbol{h}_{\text{eff}}(\boldsymbol{m}) = -\dfrac{\delta\mathcal{E}(\boldsymbol{m})}{\delta\boldsymbol{m}}$
- induces natural boundary conditions on $\boldsymbol{m}$

- micromagnetic energy $\mathcal{E}(\boldsymbol{m}) \rightsquigarrow$ sum of several contributions
  - Heisenberg exchange $\quad +A\int_\Omega |\nabla\boldsymbol{m}|^2\,\mathrm{d}x$

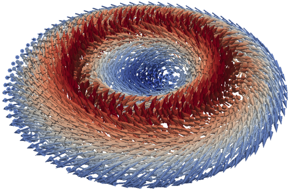
    $\rightsquigarrow \quad \boldsymbol{h}_{\text{eff}}(\boldsymbol{m}) = 2A\boldsymbol{\Delta}\boldsymbol{m} \quad \& \quad \partial_{\boldsymbol{n}}\boldsymbol{m} = \boldsymbol{0}$
  - magnetocrystalline anisotropy $\quad +\int_\Omega \phi(\boldsymbol{m})\,\mathrm{d}x$
  - Zeeman / applied external field $\quad -\int_\Omega \boldsymbol{f}\cdot\boldsymbol{m}\,\mathrm{d}x$
  - magnetostatic / stray field $\quad +\frac{1}{2}\int_\Omega \nabla u\cdot\boldsymbol{m}\,\mathrm{d}x$
  - chiral interactions

Chirality in micromagnetics

- Dzyaloshinskii–Moriya interaction (DMI)
- DMI energy $\rightsquigarrow$ linear combination of components of $\nabla \boldsymbol{m} \times \boldsymbol{m}$

$$m_i \, \partial_\ell m_j - m_j \, \partial_\ell m_i$$

- competition with Heisenberg exchange
- chiral interactions in ferromagnetic thin films $\rightsquigarrow$ magnetic skyrmions



Dzyaloshinskii: J. Phys. Chem. Solids 4 (1958)
Moriya: Phys. Rev. 120 (1960)
Bogdanov et al.: J. Magn. Magn. Mater. 138 (1994)
Bogdanov et al.: Phys. Rev. Lett. 87 (2001)

Dzyaloshinskii–Moriya interaction (DMI)

- bulk DMI $$+D\int_\Omega (\nabla\times\boldsymbol{m})\cdot\boldsymbol{m}\,\mathrm{d}x$$

  $\rightsquigarrow$ $\boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m}) = 2A\boldsymbol{\Delta m} - 2D\nabla\times\boldsymbol{m}$

  $\rightsquigarrow$ $2A\,\partial_{\boldsymbol{n}}\boldsymbol{m} + D\,\boldsymbol{m}\times\boldsymbol{n} = \boldsymbol{0}$

- interfacial DMI $$+D\int_\Omega [m_3(\partial_1 m_1 + \partial_2 m_2) - (m_1\,\partial_1 m_3 + m_2\,\partial_2 m_3)]\,\mathrm{d}x$$

  $\rightsquigarrow$ $\boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m}) = 2A\boldsymbol{\Delta m} - 2D\,\big[-\partial_1 m_3\,,\,-\partial_2 m_3\,,\,\partial_1 m_1 + \partial_2 m_2\big]^\top$

  $\rightsquigarrow$ $2A\,\partial_{\boldsymbol{n}}\boldsymbol{m} + D(\boldsymbol{e}_3\times\boldsymbol{n})\times\boldsymbol{m} = \boldsymbol{0}$

Solvability of LLG

Landau–Lifshitz form of LLG

- $\partial_t \boldsymbol{m} = -\frac{1}{1+\alpha^2}\, \boldsymbol{m} \times \boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m}) - \frac{\alpha}{1+\alpha^2}\, \boldsymbol{m} \times \big[\boldsymbol{m} \times \boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m})\big]$
- $\boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m}) = 2A\boldsymbol{\Delta m} - 2D\nabla \times \boldsymbol{m} + 2\boldsymbol{\pi}(\boldsymbol{m}) + \boldsymbol{f}$
- $2A\partial_{\boldsymbol{n}}\boldsymbol{m} + D\,\boldsymbol{m} \times \boldsymbol{n} = \boldsymbol{0}$ on $\partial\Omega \times (0,T)$
- $\boldsymbol{m}(0) = \boldsymbol{m}^0 \in \boldsymbol{H}^1(\Omega;\mathbb{S}^2)$ in Ω

Corresponding ferromagnetic bulk energy

- $\mathcal{E}(\boldsymbol{m}) = A\,\|\boldsymbol{\nabla m}\|_\Omega^2 + D\,\langle \nabla \times \boldsymbol{m}\,,\,\boldsymbol{m}\rangle_\Omega - \langle \boldsymbol{\pi}(\boldsymbol{m}) + \boldsymbol{f}\,,\,\boldsymbol{m}\rangle_\Omega$

Strong solutions

NumPDEs ASC TUWIEN

- satisfy $|\boldsymbol{m}| = 1$ in $\Omega_T = (0,T) \times \Omega$

Energy identity

- $$\mathcal{E}(\boldsymbol{m}(\tau)) + \alpha \int_0^\tau \|\partial_t \boldsymbol{m}\|_\Omega^2 \,\mathrm{d}t + \int_0^\tau \langle \partial_t \boldsymbol{f}\,,\, \boldsymbol{m}\rangle_\Omega \,\mathrm{d}t = \mathcal{E}(\boldsymbol{m}^0)$$

- existence + uniqueness locally in time, if $\boldsymbol{m}^0$ is smooth
  - $\boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m}) =$ exchange + stray field (or full Maxwell)

- existence + uniqueness + smoothness locally in time, if $\boldsymbol{m}^0 \approx \mathrm{const} \in \mathbb{S}^2$
  - $\boldsymbol{h}_{\mathrm{eff}}(\boldsymbol{m}) =$ exchange only

- so far: no results for general effective field

Carbou, Fabrie: Differential Integral Equations 14 (2001)

Feischl, Tran: SIAM J. Math. Anal. 49 (2017)

Weak solutions

Weak solution of LLG (global in time)

1. $\boldsymbol{m} \in L^\infty(\mathbb{R}_+; \boldsymbol{H}^1(\Omega;\mathbb{S}^2)) \cap \boldsymbol{H}^1(\Omega_T;\mathbb{S}^2)$ for all $T > 0$
2. $\boldsymbol{m}(0) = \boldsymbol{m}^0 \in \boldsymbol{H}^1(\Omega;\mathbb{S}^2)$ in sense of traces
3. variational formulation in $\boldsymbol{H}^1(\Omega_T)$ of Gilbert form of LLG

$$\partial_t \boldsymbol{m} = -\boldsymbol{m} \times \big[\boldsymbol{h}_{\rm eff}(\boldsymbol{m}) - \alpha\, \partial_t \boldsymbol{m}\big]$$

4. for a.e. $\tau \in (0,T)$

$$\mathcal{E}(\boldsymbol{m}(\tau)) + \alpha \int_0^\tau \|\partial_t \boldsymbol{m}\|_\Omega^2 \,\mathrm{d}t + \int_0^\tau \langle \partial_t \boldsymbol{f}\,,\, \boldsymbol{m}\rangle_\Omega \,\mathrm{d}t \le \mathcal{E}(\boldsymbol{m}^0)$$

- global-in-time existence
- possibly non-unique

Alouges, Soyeur: Nonlinear Anal. 18 (1992)

Strong-weak uniqueness

Theorem (Di Fratta, Innerberger, P. '19+)

- $\boldsymbol{h}_{\rm eff}(\boldsymbol{m}) = 2A\boldsymbol{\Delta m} - 2D\nabla \times \boldsymbol{m} + 2\boldsymbol{\pi}(\boldsymbol{m}) + \boldsymbol{f}$
- $\boldsymbol{m}_1 \in \boldsymbol{H}^3(\Omega_T)$ strong solution, $T > 0$
- $\boldsymbol{m}_2 \in L^\infty(\mathbb{R}_+; \boldsymbol{H}^1(\Omega)) \cap \boldsymbol{H}^1(\Omega_T)$ weak solution

$\Longrightarrow$ $\boldsymbol{m}_1 = \boldsymbol{m}_2$ on Ω_T

- first proof by Dumas & Sueur '14
  - $\Omega = \mathbb{R}^3$
  - $\boldsymbol{h}_{\rm eff}(\boldsymbol{m}) =$ exchange + stray field / Maxwell
- new / simplified / extended proof
  - $\Omega \subset \mathbb{R}^3$ Lipschitz domain
  - general effective field
  - imitates proof of strong-strong uniqueness
  - based on energy argument for difference $\boldsymbol{m}_2 - \boldsymbol{m}_1$ & Gronwall lemma

Dumas, Sueur: Commun. Math. Phys. 330 (2014)
Di Fratta, Innerberger, Praetorius: Preprint arXiv:1910.04630 (2019)

Computational micromagnetism

Challenges

- nonlinearities
- nonconvex pointwise constraint ⇝ $|\boldsymbol{m}| = 1$
- energy identity

$$\mathcal{E}(\boldsymbol{m}(\tau)) + \alpha \int_0^\tau \|\partial_t \boldsymbol{m}\|_\Omega^2 \, \mathrm{d}t + \int_0^\tau \langle \partial_t \boldsymbol{f} \, , \, \boldsymbol{m} \rangle_\Omega \, \mathrm{d}t = \mathcal{E}(\boldsymbol{m}^0)$$

- nonlocal effects ⇝ stray field
- coupling with other PDEs ⇝ Maxwell / spin diffusion / magnetostriction

Discretization of DMI ⇝ additional challenges

- neither self-adjoint nor positive definite energy contribution
- different boundary conditions $\quad \boldsymbol{0} \neq 2A \, \partial_{\boldsymbol{n}} \boldsymbol{m} = -D \, \boldsymbol{m} \times \boldsymbol{n}$

Tangent plane scheme: Alouges & Jaisson (2006), Bartels et al. (2008), Alouges (2008), Alouges et al. (2012), Le & Tran (2013), Praetorius et al. (2014ff.), Le et al. (2015), Feischl & Tran (2017)

Midpoint scheme: Bartels & Prohl (2006), Banas et al. (2008), Kim & Wilkening (2018), Praetorius et al. (2018)

Discretization

- time discretization $\rightsquigarrow$ $t_i = ik$ with uniform time-step size $k = T/N$
- spatial discretization $\rightsquigarrow$ $\mathcal{T}_h$ tetrahedral mesh of Ω with mesh size h
- $\mathcal{S}^1(\mathcal{T}_h) = \{\phi_h \in C(\overline{\Omega}) : \phi_h|_K \in \mathcal{P}^1(K)$ for all elements $K \in \mathcal{T}_h\}$

- $|\boldsymbol{m}| = 1$

Set of discrete magnetizations

$$\boldsymbol{m}(t_i) \approx \boldsymbol{m}_h^i \in \boldsymbol{\mathcal{M}}_h := \{\boldsymbol{\phi}_h \in \mathcal{S}^1(\mathcal{T}_h)^3 : |\boldsymbol{\phi}_h(\boldsymbol{z})| = 1 \text{ for all nodes } \boldsymbol{z}\}$$

- $\partial_t \boldsymbol{m} \cdot \boldsymbol{m} = 0$

Discrete tangent space

$$\partial_t \boldsymbol{m}(t_i) \approx \boldsymbol{v}_h^i \in \boldsymbol{\mathcal{K}}_h(\boldsymbol{m}_h^i) := \{\boldsymbol{\phi}_h \in \mathcal{S}^1(\mathcal{T}_h)^3 : \boldsymbol{m}_h^i(\boldsymbol{z}) \cdot \boldsymbol{\phi}_h(\boldsymbol{z}) = 0 \text{ for all } \boldsymbol{z}\}$$

Tangent plane scheme 1/2

NumPDEs ASC ▸ TUWIEN

Equivalent formulation of LLG

- $\alpha\, \boldsymbol{m}_t + \boldsymbol{m} \times \boldsymbol{m}_t = \boldsymbol{h}_{\text{eff}}(\boldsymbol{m}) - [\boldsymbol{h}_{\text{eff}}(\boldsymbol{m}) \cdot \boldsymbol{m}]\boldsymbol{m}$

- linear in $\boldsymbol{m}_t$ & $\boldsymbol{m}_t \cdot \boldsymbol{m} = 0$

Time-marching scheme

For all $0 \le i \le N-1$: given $\boldsymbol{m}_h^i \approx \boldsymbol{m}(t_i)$

- compute $\boldsymbol{v}_h^i \approx \partial_t \boldsymbol{m}(t_i)$ in $\boldsymbol{\mathcal{K}}_h(\boldsymbol{m}_h^i)$
- first-order time-stepping $\rightsquigarrow$ $\boldsymbol{m}_h^{i+1} \approx \boldsymbol{m}_h^i + k\boldsymbol{v}_h^i \approx \boldsymbol{m}(t_{i+1})$
- nodal projection to ensure $\boldsymbol{m}_h^{i+1} \in \boldsymbol{\mathcal{M}}_h$

Alouges: Discrete Contin. Dyn. Syst. Ser. S 1 (2008)

Bruckner, Praetorius, Ruggeri et al.: Math. Models Methods Appl. Sci. 24 (2014)

Tangent plane scheme 2/2

Equivalent formulation of LLG

- $\alpha\, \boldsymbol{m}_t + \boldsymbol{m} \times \boldsymbol{m}_t = \boldsymbol{h}_{\rm eff}(\boldsymbol{m}) - [\boldsymbol{h}_{\rm eff}(\boldsymbol{m}) \cdot \boldsymbol{m}]\boldsymbol{m}$
- $\boldsymbol{h}_{\rm eff}(\boldsymbol{m}) = 2A\boldsymbol{\Delta m} - 2D\nabla \times \boldsymbol{m} + 2\boldsymbol{\pi}(\boldsymbol{m}) + \boldsymbol{f}$
- $2A\, \partial_{\boldsymbol{n}}\boldsymbol{m} = -\, D\, \boldsymbol{m} \times \boldsymbol{n}$ on $\partial\Omega$

Algorithm (tangent plane scheme)

For all $0 \le i \le N-1$:

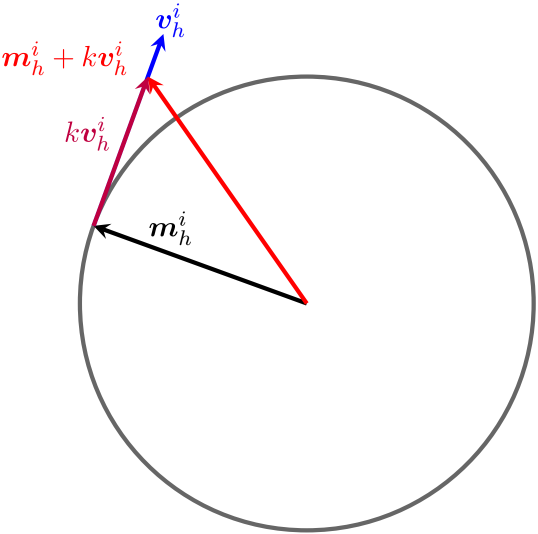
1. Compute $\boldsymbol{v}_h^i \in \boldsymbol{\mathcal{K}}(\boldsymbol{m}_h^i)$ such that, for all $\boldsymbol{\phi}_h \in \boldsymbol{\mathcal{K}}(\boldsymbol{m}_h^i)$, it holds that

$$\alpha\langle \boldsymbol{v}_h^i\,,\, \boldsymbol{\phi}_h\rangle + \langle \boldsymbol{m}_h^i \times \boldsymbol{v}_h^i\,,\, \boldsymbol{\phi}_h\rangle + 2Ak\langle \boldsymbol{\nabla v}_h^i\,,\, \boldsymbol{\nabla\phi}_h\rangle$$
$$= -2A\langle \boldsymbol{\nabla m}_h^i\,,\, \boldsymbol{\nabla\phi}_h\rangle - D\langle \nabla \times \boldsymbol{m}_h^i\,,\, \boldsymbol{\phi}_h\rangle - D\langle \boldsymbol{m}_h^i\,,\, \nabla \times \boldsymbol{\phi}_h\rangle$$
$$+ \langle 2\boldsymbol{\pi}_h(\boldsymbol{m}_h^i) + \boldsymbol{f}(t_i)\,,\, \boldsymbol{m}_h^i\rangle$$

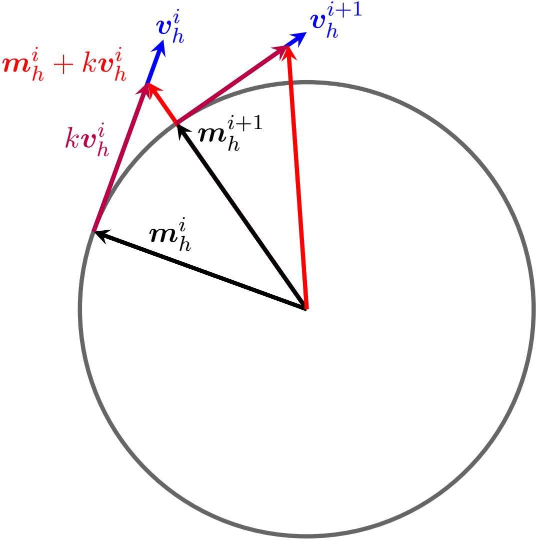
2. Define $\boldsymbol{m}_h^{i+1} \in \boldsymbol{\mathcal{M}}_h$ as nodal projection of $\boldsymbol{m}_h^i + k\boldsymbol{v}_h^i$

Hrkac, Pfeiler, Praetorius, Ruggeri, Segatti, Stiftner: Adv. Comp. Math. 398 (2019)

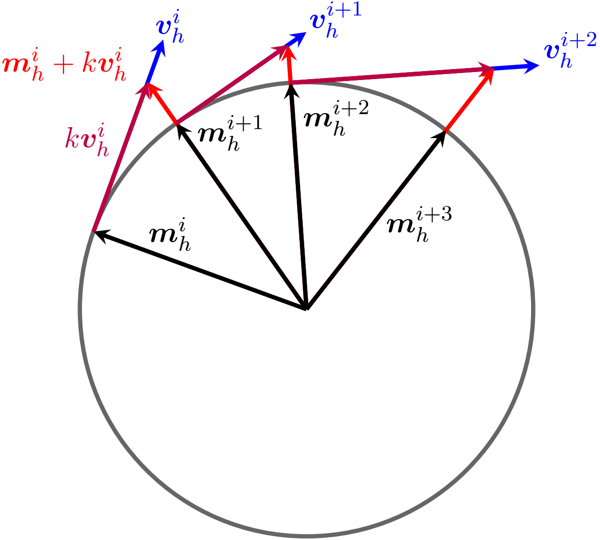
Sketch of TPS

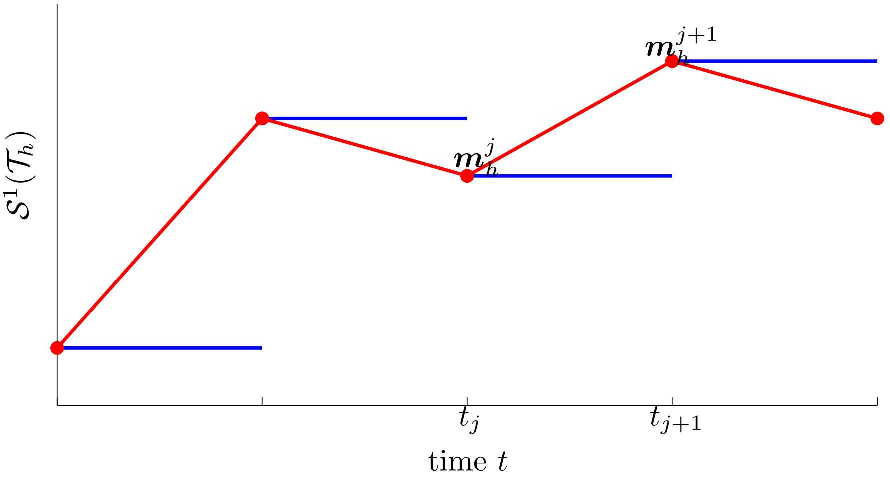


Sketch of TPS



Sketch of TPS





- continuous $\boldsymbol{m}_{hk}$
- piecewise constant $\boldsymbol{m}_{hk}^-$

Convergence theorem

Theorem (Hrkac et al. '19)

- $\boldsymbol{m}^0 \in \boldsymbol{H}^1(\Omega, \mathbb{S}^2)$ with $\boldsymbol{m}_h^0 \to \boldsymbol{m}^0$ as $h \to 0$.
- consistent convergence of $\boldsymbol{\pi}_h \to \boldsymbol{\pi}$
- $\mathcal{T}_h$ satisfies certain angle condition
- CFL condition $k = o(h)$

$\Longrightarrow$ exists weak solution $\boldsymbol{m}$ of LLG and $\boldsymbol{m}_{hk} \rightharpoonup \boldsymbol{m}$ in $\boldsymbol{H}^1(\Omega_T)$

- at least for subsequences

- numerical integrator also provides existence of weak solution
- angle condition ensures that $\|\boldsymbol{\nabla} \boldsymbol{m}_h^{i+1}\|_\Omega \le \|\boldsymbol{\nabla}(\boldsymbol{m}_h^i + k\boldsymbol{v}_h^i)\|_\Omega$
- CFL condition needed to estimate $\|\nabla \times [\boldsymbol{m}_h^{i+1} - (\boldsymbol{m}_h^i + k\boldsymbol{v}_h^i)]\|_\Omega$

Alouges: Discrete Contin. Dyn. Syst. Ser. S 1 (2008)

Hrkac, Pfeiler, Praetorius, Ruggeri, Segatti, Stiftner: Adv. Comp. Math. 398 (2019)

Sketch of proof (energy method)

1. boundedness of discrete energy
   - $\|\nabla \boldsymbol{m}_{hk}^-\|_{L^\infty(\boldsymbol{L}^2)}^2 + \|\boldsymbol{v}_{hk}^-\|_{L^2(\boldsymbol{L}^2)}^2 + \frac{k}{2}\,\|\nabla \boldsymbol{v}_{hk}^-\|_{L^2(\boldsymbol{L}^2)}^2 \le C$
   - $\|\boldsymbol{m}_{hk}^-\|_{L^\infty(\boldsymbol{L}^2)}^2 \lesssim \|\boldsymbol{m}_{hk}^-\|_{\boldsymbol{L}^\infty}^2 = 1$

2. abstract arguments provide convergent subsequences
   - $\boldsymbol{m}_{jk} \rightharpoonup \boldsymbol{m}$ in $\boldsymbol{H}^1(\Omega_T)$
   - $\boldsymbol{m}_{hk}, \boldsymbol{m}_{hk}^- \to \boldsymbol{m}$ in $\boldsymbol{L}^2(\Omega_T)$
   - $\boldsymbol{v}_{hk}^- \rightharpoonup \boldsymbol{v} \overset{!}{=} \partial_t \boldsymbol{m}$ in $\boldsymbol{L}^2(\Omega_T)$

3. prove that $\boldsymbol{m}$ is weak solution of LLG
   - $|\boldsymbol{m}| = 1$ a.e. in Ω_T
   - satisfies variational formulation
   - satisfies energy estimate

Projection-free TPS

- apply TPS without nodal projection $\rightsquigarrow$ $\boldsymbol{m}_h^{i+1} := \boldsymbol{m}_h^i + k\boldsymbol{v}_h^i$

Theorem (Hrkac et al. '19)

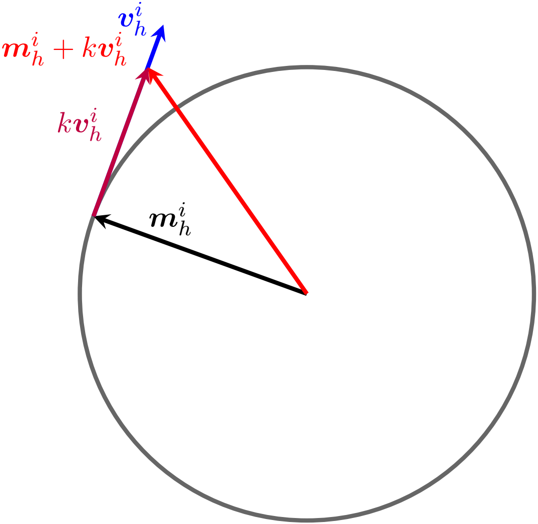
- $\boldsymbol{m}^0 \in \boldsymbol{H}^1(\Omega, \mathbb{S}^2)$ with $\boldsymbol{m}_h^0 \to \boldsymbol{m}^0$ as $h \to 0$.
- consistent convergence of $\boldsymbol{\pi}_h \to \boldsymbol{\pi}$
- ~~$\mathcal{T}_h$ satisfies certain angle condition~~
- ~~CFL condition $k = o(h)$~~

$\Longrightarrow$ exists weak solution $\boldsymbol{m}$ of LLG and $\boldsymbol{m}_{hk} \rightharpoonup \boldsymbol{m}$ in $\boldsymbol{H}^1(\Omega_T)$
  - at least for subsequences

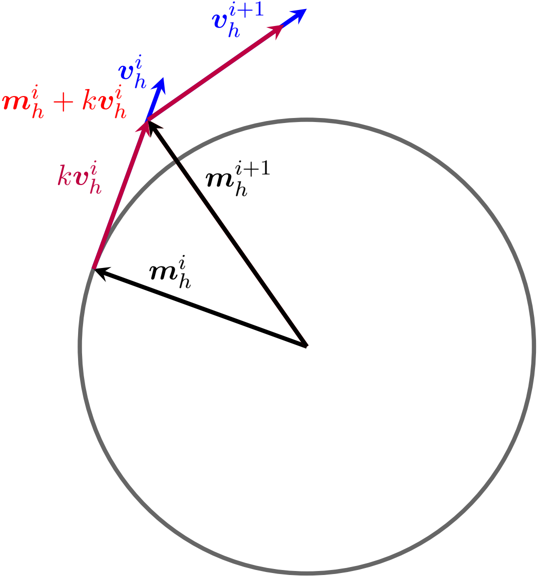
- angle condition only used for $\|\boldsymbol{\nabla} \boldsymbol{m}_h^{i+1}\|_\Omega \le \|\boldsymbol{\nabla}(\boldsymbol{m}_h^i + k\boldsymbol{v}_h^i)\|_\Omega$
- CFL condition only needed to control $\|\nabla \times [\boldsymbol{m}_h^{i+1} - (\boldsymbol{m}_h^i + k\boldsymbol{v}_h^i)]\|_\Omega$

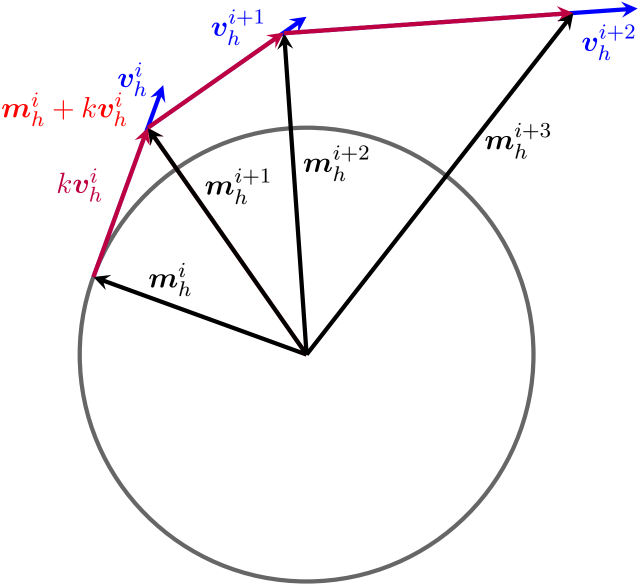
Hrkac, Pfeiler, Praetorius, Ruggeri, Segatti, Stiftner: Adv. Comp. Math. 398 (2019)

Sketch of projection-free TPS



Sketch of projection-free TPS




$\boldsymbol{v}_h^{i+1}$
$\boldsymbol{v}_h^{i+2}$
$\boldsymbol{v}_h^{i}$
$\boldsymbol{m}_h^i + k\boldsymbol{v}_h^i$
$\boldsymbol{m}_h^{i+3}$
$\boldsymbol{m}_h^{i+2}$
$k\boldsymbol{v}_h^i$
$\boldsymbol{m}_h^{i+1}$
$\boldsymbol{m}_h^{i}$

Sketch of proof (avoid normalization)

- as before: boundedness of discrete energy

$$\|\nabla \boldsymbol{m}_{hk}^-\|_{L^\infty(\boldsymbol{L}^2)}^2 + \|\boldsymbol{v}_{hk}^-\|_{L^2(\boldsymbol{L}^2)}^2 + \frac{k}{2}\,\|\nabla \boldsymbol{v}_{hk}^-\|_{L^2(\boldsymbol{L}^2)}^2 \le C$$

- essential question: how to bound $\|\boldsymbol{m}_{hk}^-\|_{L^\infty(\boldsymbol{L}^2)}$?

- recall $\boldsymbol{m}_h^j(\boldsymbol{z}) \cdot \boldsymbol{v}_h^j(\boldsymbol{z}) = 0$ for all nodes $\boldsymbol{z}$

$$\Longrightarrow \quad |\boldsymbol{m}_h^{j+1}(\boldsymbol{z})|^2 = |\boldsymbol{m}_h^j(\boldsymbol{z})|^2 + k^2\,|\boldsymbol{v}_h^j(\boldsymbol{z})|^2 = \cdots = 1 + k^2 \sum_{i=0}^{j} |\boldsymbol{v}_h^i(\boldsymbol{z})|^2$$

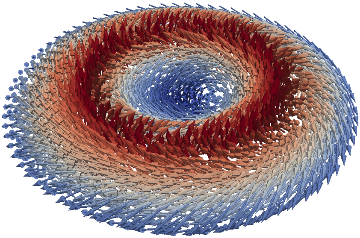
$$\Longrightarrow \quad \|\boldsymbol{m}_{hk}^-\|_{L^\infty(\boldsymbol{L}^2)}^2 \lesssim 1 + k\,\|\boldsymbol{v}_{hk}^-\|_{\boldsymbol{L}^2(\Omega_T)}^2$$

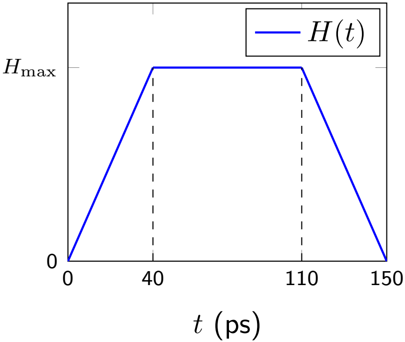
Bartels: Math. Comp. 85 (2016)

Numerical experiment

Numerical experiment

- goal: stability and dynamics of skyrmions in response to pulse field
- helimagnetic nanodisk of 140 nm diameter and thickness 10 nm
- Material parameters of FeGe (with bulk DMI)

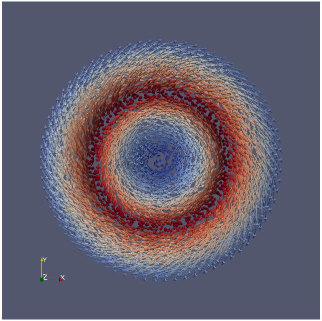


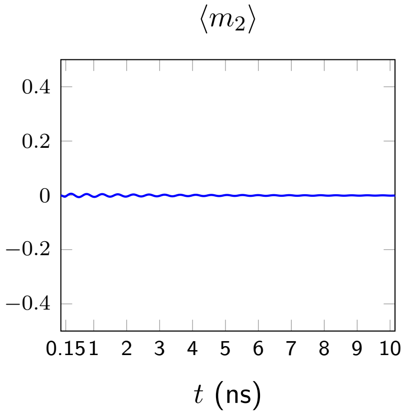


Beg, Albert, Bisotti, Fangohr et al. Phys. Rev. B 95 (2017)
Pfeiler, Praetorius, Ruggeri, Schöberl et al.: Comp. Phys. Comm. 248 (2020)

In-plane pulse field

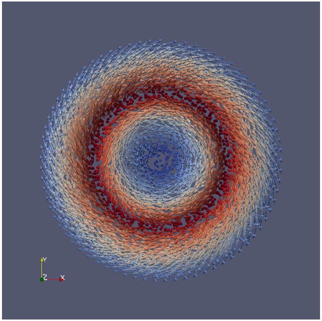
$\boldsymbol{H}_{\mathrm{ext}} = (H(t), 0, 0)$ with $\mu_0 H_{\max} = 1\,\mathrm{mT}$

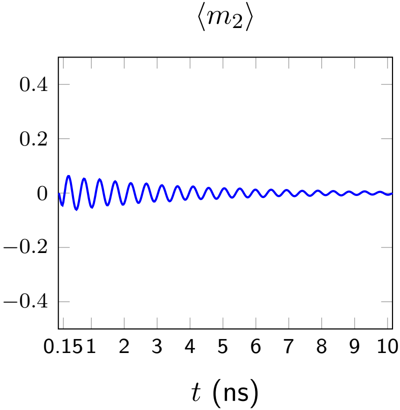




In-plane pulse field

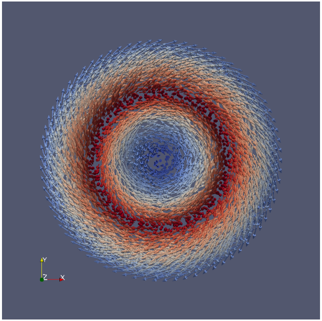
$\boldsymbol{H}_{\text{ext}} = (H(t), 0, 0)$ **with** $\mu_0 H_{\max} = 10\,\text{mT}$

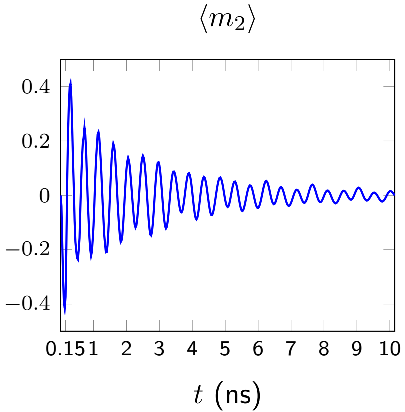




In-plane pulse field

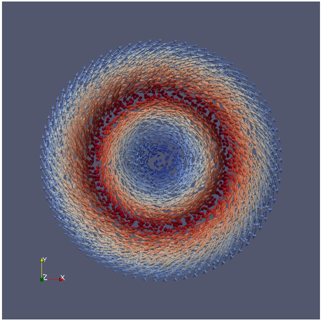
$\boldsymbol{H}_{\mathrm{ext}} = (H(t), 0, 0)$ **with** $\mu_0 H_{\max} = 100\,\mathrm{mT}$

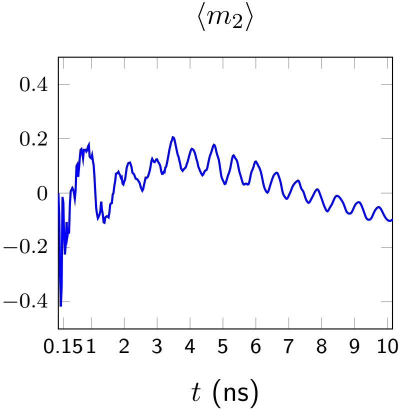




In-plane pulse field

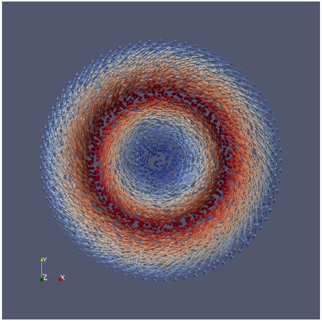
$\boldsymbol{H}_{\rm ext} = (H(t), 0, 0)$ **with** $\mu_0 H_{\max} = 200\,\mathrm{mT}$

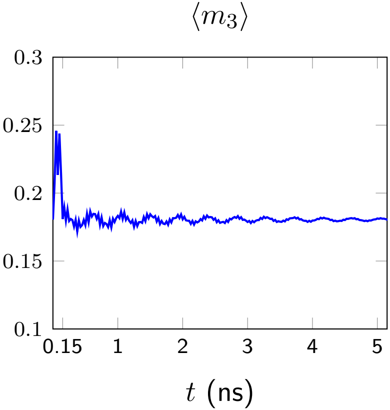




Out-of-plane pulse field

$\boldsymbol{H}_{\mathrm{ext}} = (0, 0, H(t))$ **with** $\mu_0 H_{\max} = 50\,\mathrm{mT}$





Discrete systems & preconditioning

Linear systems in TPS

- given $\boldsymbol{m}_h \in \boldsymbol{\mathcal{M}}_h$, compute $\boldsymbol{v}_h \in \boldsymbol{\mathcal{K}}(\boldsymbol{m}_h)$ such that, for all $\boldsymbol{\phi}_h \in \boldsymbol{\mathcal{K}}(\boldsymbol{m}_h)$,

$$\alpha\langle \boldsymbol{v}_h \,,\, \boldsymbol{\phi}_h\rangle + \langle \boldsymbol{m}_h \times \boldsymbol{v}_h \,,\, \boldsymbol{\phi}_h\rangle + 2Ak\langle \boldsymbol{\nabla}\boldsymbol{v}_h \,,\, \boldsymbol{\nabla}\boldsymbol{\phi}_h\rangle = \mathrm{RHS}(\boldsymbol{m}_h, \boldsymbol{f})$$

- $\{\boldsymbol{z}_1, \dots, \boldsymbol{z}_N\}$ nodes of $\mathcal{T}_h$ with scalar hat functions φ_j
- $\boldsymbol{\phi}_{3(j-1)+\ell} := \varphi_j \boldsymbol{e}_\ell$ vector-valued hat functions

- $\mathbf{M}_{ij} = \langle \boldsymbol{\phi}_j \,,\, \boldsymbol{\phi}_i\rangle$
- $\mathbf{S}[\boldsymbol{m}_h]_{ij} = \langle \boldsymbol{m}_h \times \boldsymbol{\phi}_j \,,\, \boldsymbol{\phi}_i\rangle$
- $\mathbf{L}_{ij} = \langle \boldsymbol{\nabla}\boldsymbol{\phi}_j \,,\, \boldsymbol{\nabla}\boldsymbol{\phi}_i\rangle$

$\Longrightarrow$ LHS w.r.t. $\mathcal{S}^1(\mathcal{T}_h)^3 \quad \rightsquigarrow \quad \mathbf{A} := \alpha\mathbf{M} + \mathbf{S}[\boldsymbol{m}_h] + 2Ak\mathbf{L} \in \mathbb{R}^{3N\times 3N}$

- restrict to subspace $\boldsymbol{\mathcal{K}}(\boldsymbol{m}_h) \subset \mathcal{S}^1(\mathcal{T}_h)^3$ with $\dim \boldsymbol{\mathcal{K}}(\boldsymbol{m}_h) = 2N$

FEM system on $\mathcal{K}_h(\boldsymbol{m}_h)$

Discrete tangent space

- recall $\mathcal{K}_h(\boldsymbol{m}_h) := \{\boldsymbol{\phi}_h \in \mathcal{S}^1(\mathcal{T}_h)^3 : \boldsymbol{m}_h(\boldsymbol{z}) \cdot \boldsymbol{\phi}_h(\boldsymbol{z}) = 0 \text{ for all } \boldsymbol{z}\}$

- choose Householder reflection $R_j \in O(3)$ s.t. $R_j \boldsymbol{e}_3 = \pm \boldsymbol{m}_h(\boldsymbol{z}_j)$
- $Q_j = [R_j \boldsymbol{e}_1 \, , \, R_j \boldsymbol{e}_2]$
  - ⇝ orthogonal basis of nodal tangent space at $\boldsymbol{m}_h(\boldsymbol{z}_j) \in \mathbb{R}^3$
- define $\mathbf{Q}[\boldsymbol{m}_h] := \mathrm{diag}(Q_1^\top, \ldots, Q_N^\top) \in \mathbb{R}^{2N \times 3N}$

Linear systems in TPS

- given $\boldsymbol{m}_h \in \boldsymbol{\mathcal{M}}_h$, compute $\boldsymbol{v}_h \in \mathcal{K}(\boldsymbol{m}_h)$ such that, for all $\boldsymbol{\phi}_h \in \mathcal{K}(\boldsymbol{m}_h)$,

$$\alpha \langle \boldsymbol{v}_h \, , \, \boldsymbol{\phi}_h \rangle + \langle \boldsymbol{m}_h \times \boldsymbol{v}_h \, , \, \boldsymbol{\phi}_h \rangle + 2Ak \langle \boldsymbol{\nabla} \boldsymbol{v}_h \, , \, \boldsymbol{\nabla} \boldsymbol{\phi}_h \rangle = \mathrm{RHS}(\boldsymbol{m}_h, \boldsymbol{f})$$

$$\Longleftrightarrow \quad \mathbf{Q}[\boldsymbol{m}_h] \mathbf{A} \mathbf{Q}[\boldsymbol{m}_h]^\top \mathbf{x} = \mathbf{Q}[\boldsymbol{m}_h] \mathbf{b} \quad \text{with} \quad \mathbf{A} := \alpha \mathbf{M} + \mathbf{S} + 2Ak\mathbf{L}$$

Preconditioning

Linear systems in TPS

- $\mathbf{Q}[\boldsymbol{m}_h]\mathbf{A}\mathbf{Q}[\boldsymbol{m}_h]^\top\mathbf{x} = \mathbf{Q}[\boldsymbol{m}_h]\mathbf{b}$ with $\mathbf{A} := \alpha\mathbf{M} + \mathbf{S}[\boldsymbol{m}_h] + 2Ak\mathbf{L}$
- condition number $\sim (1 + k/h^2)$

- $\mathbf{P} := \mathbf{Q}[\boldsymbol{m}_h](\widetilde{\alpha}\mathbf{M} + 2Ak\mathbf{L})^{-1}\mathbf{Q}[\boldsymbol{m}_h]^\top$ essentially independent of $\boldsymbol{m}_h$

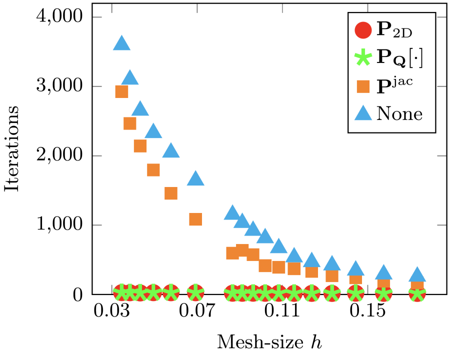
Theorem (Kraus, Pfeiler, P., Ruggeri, Stiftner '19)

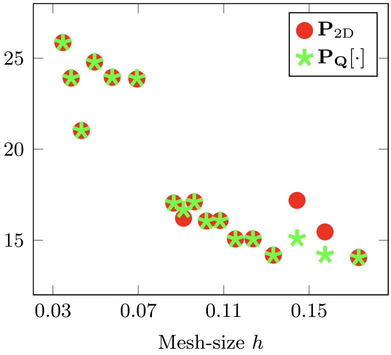
- linear convergence of GMRES for $\mathbf{P}\mathbf{Q}[\boldsymbol{m}_h]\mathbf{A}\mathbf{Q}[\boldsymbol{m}_h]^\top\mathbf{x} = \mathbf{P}\mathbf{Q}[\boldsymbol{m}_h]\mathbf{b}$
- h-independent rate depends only on $1 + \|\nabla\boldsymbol{m}_h\|_{\boldsymbol{L}^\infty(\Omega)}k/\widetilde{\alpha}$ (and $\widetilde{\alpha}/\alpha$)

- hence: linear GMRES convergence as long as no finite-time blow-up!
- empirical: $\widetilde{\alpha}/\alpha$ not visible, good choice $\widetilde{\alpha} = 1$, bad choice $\widetilde{\alpha} = \alpha$

Kraus, Pfeiler, Praetorius, Ruggeri, Stiftner: J. Comp. Phys. 398 (2019)

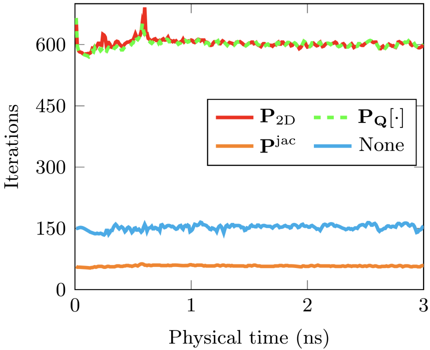
Academic example (unit cube)

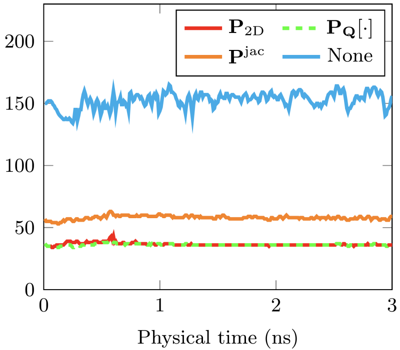




mumag#4 example (thin permalloy film)

left: $\widetilde{\alpha} = 0.02 = \alpha$ **vs.** **right:** $\widetilde{\alpha} = 1$





Thin-film model

LLG on thin film

- $\partial_t \boldsymbol{m}_\varepsilon = -\dfrac{1}{1+\alpha^2}\,\boldsymbol{m}_\varepsilon \times \boldsymbol{h}_{\rm eff}(\boldsymbol{m}_\varepsilon) - \dfrac{\alpha}{1+\alpha^2}\,\boldsymbol{m}_\varepsilon \times (\boldsymbol{m}_\varepsilon \times \boldsymbol{h}_{\rm eff}(\boldsymbol{m}_\varepsilon))$
- $\boldsymbol{h}_{\rm eff}(\boldsymbol{m}_\varepsilon) = 2A\boldsymbol{\Delta}\boldsymbol{m}_\varepsilon - 2D\nabla \times \boldsymbol{m}_\varepsilon - \nabla u[\boldsymbol{m}_\varepsilon] + \dots$
- $\boldsymbol{m}_\varepsilon(0) = \widehat{\boldsymbol{m}}^0 \in \boldsymbol{H}^1(\Omega_\varepsilon;\mathbb{S}^2)$ in Ω_ε
- $2A\partial_{\boldsymbol{n}}\,\boldsymbol{m}_\varepsilon + D\,\boldsymbol{m}_\varepsilon \times \boldsymbol{n} = \boldsymbol{0}$ on $\partial\Omega_\varepsilon \times (0,1)$

- $\omega \subset \mathbb{R}^2$ bounded Lipschitz domain
- $0 < \varepsilon \ll 1$ thickness of Ω
- $\Omega_\varepsilon = \omega \times (0,\varepsilon)$
- $\widehat{\boldsymbol{m}}_0(x,s) = \boldsymbol{m}_0(x)$ with $\boldsymbol{m}_0 \in \boldsymbol{H}^1(\omega;\mathbb{S}^2)$

- question: What happens for $\varepsilon \to 0$?

energy minimization: Gioia & James (1997), Carbou (2001), DeSimone et al. (2001, 2002), Kohn & Slastikov (2005)

thin-film dynamics: E & Garcia-Cervera (2001), Kohn & Slastikov (2005), Melcher (2010)

Rescaling & thin-film theorem

NumPDEs ASC TUWIEN

- $\Phi_\varepsilon : \mathbb{R}^2 \times \mathbb{R}_+ \to \mathbb{R}^3, \quad \Phi_\varepsilon(x,s) = (x, \varepsilon s)$
- $\widehat{\Omega} := \omega \times (0,1)$
- $\boldsymbol{m}_\varepsilon \in L^\infty(\mathbb{R}_+; \boldsymbol{H}^1(\Omega_\varepsilon; \mathbb{S}^2)) \cap \boldsymbol{H}^1(\Omega_{\varepsilon,T}; \mathbb{S}^2)$ weak solution of LLG

$\Longrightarrow \quad \widehat{\boldsymbol{m}}_\varepsilon := \boldsymbol{m}_\varepsilon \circ \Phi_\varepsilon \in L^\infty(\mathbb{R}_+; \boldsymbol{H}^1(\widehat{\Omega}; \mathbb{S}^2)) \cap \boldsymbol{H}^1(\widehat{\Omega}_T; \mathbb{S}^2)$

Theorem (Davoli, Di Fratta, Praetorius, Ruggeri '20++)

- exists $\boldsymbol{m}_0 \in L^\infty(\mathbb{R}_+; \boldsymbol{H}^1(\omega; \mathbb{S}^2)) \cap \boldsymbol{H}^1(\omega_T; \mathbb{S}^2)$ such that
  - $\widehat{\boldsymbol{m}}_0(t,(x,s)) := \boldsymbol{m}_0(t,x)$
  - $\widehat{\boldsymbol{m}}_\varepsilon \rightharpoonup \widehat{\boldsymbol{m}}_0$ weakly* in $L^\infty(\mathbb{R}_+; \boldsymbol{H}^1(\widehat{\Omega}; \mathbb{S}^2))$ as $\varepsilon \to 0$
- moreover, $\boldsymbol{m}_0$ solves a fully local 2D LLG equation

  $\rightsquigarrow$ next slide

Gioia, James: Proc. Royal Soc. A 453 (1997)

Davoli, Di Fratta, Praetorius, Ruggeri: work in progress (2020)

Thin-film theorem (ctd.)

NumPDEs ASC TUWIEN

Theorem (Davoli, Di Fratta, Praetorius, Ruggeri '20++)

- limit $\boldsymbol{m}_0 \in L^\infty(\mathbb{R}_+; \boldsymbol{H}^1(\omega;\mathbb{S}^2)) \cap \boldsymbol{H}^1(\omega_T;\mathbb{S}^2)$ solves
  - $\partial_t \boldsymbol{m}_0 = -\frac{1}{1+\alpha^2}\boldsymbol{m}_0 \times \boldsymbol{h}_{\text{eff}}(\boldsymbol{m}_0) - \frac{\alpha}{1+\alpha^2}\boldsymbol{m}_0 \times [\boldsymbol{m}_0 \times \boldsymbol{h}_{\text{eff}}(\boldsymbol{m}_0)]$
  - $\boldsymbol{h}_{\text{eff}}(\boldsymbol{m}_0) = 2A\boldsymbol{\Delta}_{2d}\boldsymbol{m}_0 - 2D\,\nabla_{2d} \times \boldsymbol{m}_0 - (1+D^2)(\boldsymbol{m}_0\cdot\boldsymbol{e}_3)\boldsymbol{e}_3$
  - $\boldsymbol{m}_0(0) = \boldsymbol{m}^0 \in \boldsymbol{H}^1(\omega;\mathbb{S}^2)$ in ω
  - $2A\partial_{\boldsymbol{n}}\,\boldsymbol{m}_0 + D\,\boldsymbol{m}_0 \times \boldsymbol{n} = \boldsymbol{0}$ on $\partial\omega \times (0,1)$

- $\boldsymbol{h}_{\text{eff}}(\boldsymbol{m}_0) = -\dfrac{\delta\mathcal{E}_0(\boldsymbol{m}_0)}{\delta\boldsymbol{m}_0}$
- $\mathcal{E}_0(\boldsymbol{m}_0) = A\|\nabla_{2d}\boldsymbol{m}_0\|_\omega^2 + D\langle\nabla_{2d}\times\boldsymbol{m}_0\,,\,\boldsymbol{m}_0\rangle_\omega + \dfrac{1+D^2}{2}\|\boldsymbol{m}_0\cdot\boldsymbol{e}_3\|_\omega^2$
- despite stray field, $\boldsymbol{h}_{\text{eff}}(\boldsymbol{m}_0)$ is fully local
  - $\rightsquigarrow$ results into artificial in-plane anisotropy

Gioia, James: Proc. Royal Soc. A 453 (1997)

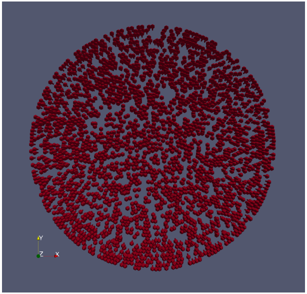
Davoli, Di Fratta, Praetorius, Ruggeri: work in progress (2020)

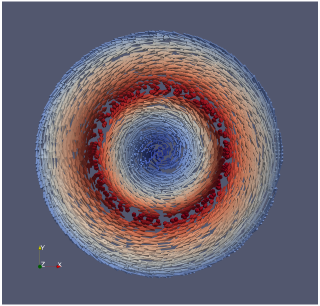
Numerical integration of thin-film LLG

- can formulate TPS also in 2D
- same convergence theorem as for 3D
- very attractive from computational point of view
  - dimension reduction (reduction of dofs)
  - 3D stray field is nonlocal + computationally expensive
  - replaced by local + cheap anisotropy contribution

"Cheating" 2D computation

- helimagnetic nanodisk of 140 nm diameter and thickness 10 nm
- material parameters of FeGe

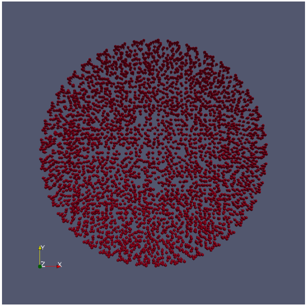


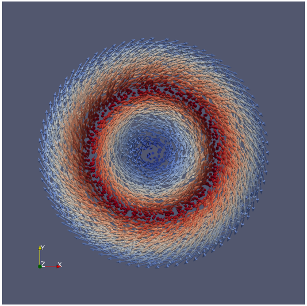


Beg, Albert, Bisotti, Fangohr et al. Phys. Rev. B 95 (2017)

Previous 3D computation

- helimagnetic nanodisk of 140 nm diameter and thickness 10 nm
- material parameters of FeGe

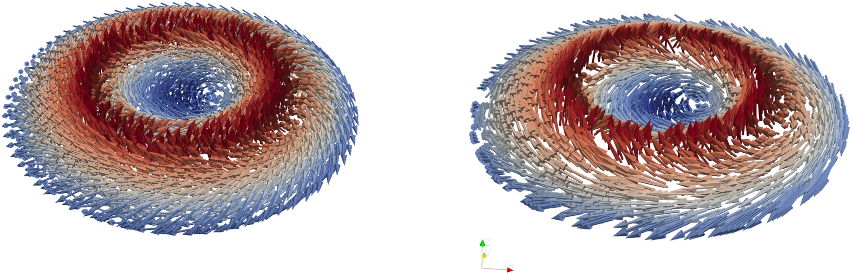




Beg, Albert, Bisotti, Fangohr et al. Phys. Rev. B 95 (2017)

Comparison

3D left vs. 2D right



Conclusion

Conclusion

- LLG with DMI leads to emergence of magnetic skyrmions
- numerical integration by (unconditionally) convergent TPS
  - our Python code is freely available online
- global-in-time existence of weak solutions for LLG (with DMI)
- strong-weak uniqueness for solutions of LLG
- thin-film limit for LLG with DMI
- reduced TPS integrator still has to be implemented

Pfeiler, Ruggeri, Schöberl, Praetorius et al.: Comp. Phys. Comm. 248 (2020)

Thank you for your attention!

Save the dates & see you at TU Wien:

- CMAM 2020 – 9th Computational Methods in Applied Mathematics
  July 13–17, 2020
- 20th GAMM Seminar on Microstructures
  January 29–30, 2021 (+ January 28)
- HMM 2021 – Symposium on Hysteresis Modeling and Micromagnetics
  May 31 —- June 02, 2021

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NumPDEs
Work group on Numerics of PDEs