

Second-order Semi-implicit Projection Methods for Landau-Lifshitz Equation

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September 21, 2019, CSIAM 2019, Foshan

Outline

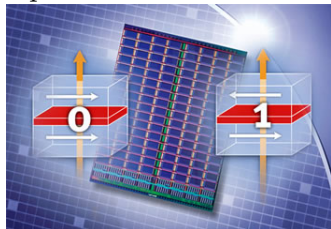
- 1 Background and motivation
- 2 Semi-implicit projection methods
- 3 Benchmark problem from NIST
- 4 Main theoretical results
 - Unconditional unique solvability
 - Optimal rate convergence analysis
- 5 Numerical examples
- 6 Conclusion

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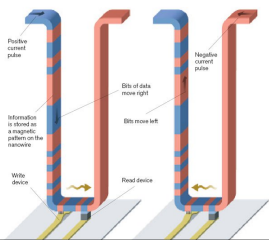
Magnetic recording devices and computer storages

- Spinvalues¹



Magnetoresistance random access memory (MRAM)

- Domain walls²



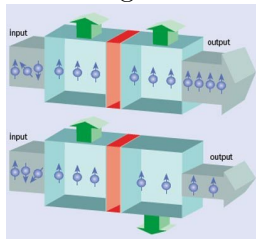
Racetrack memories

¹Science@Berkeley Lab: The Current Spin on Spintronics

²<http://www2.technologyreview.com/article/412189/tr10-racetrack-memory/>

Methodology for detecting the orientation

● Tunnel magnetoresistance ³

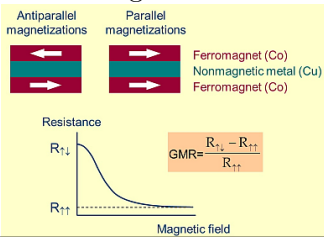


Julliere's model:
Constant tunneling
matrix

$$\text{TMR} \equiv \frac{G_{\text{AP}} - G_{\text{P}}}{G_{\text{AP}}} = \frac{2P_{\text{L}}P_{\text{R}}}{1 - P_{\text{L}}P_{\text{R}}}$$

$$P_{\text{L}} = \frac{n_{\text{L}}^{\uparrow} - n_{\text{L}}^{\downarrow}}{n_{\text{L}}^{\uparrow} + n_{\text{L}}^{\downarrow}} \quad P_{\text{R}} = \frac{n_{\text{R}}^{\uparrow} - n_{\text{R}}^{\downarrow}}{n_{\text{R}}^{\uparrow} + n_{\text{R}}^{\downarrow}}$$

● Gaint magnetoresistance ⁴



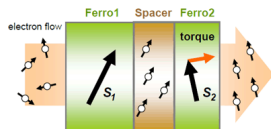
- ▶ Albert Fert and Peter Gruber: 2007 Nobel Prize in Physics
- ▶ Polarization and scattering

³<http://ducthe.wordpress.com/category/spintronics/>

⁴<http://physics.unl.edu/>

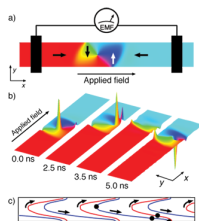
Methodology for rotating the orientation

- Spin transfer torque (STT) ⁵



- ▶ Two layers of different thickness: different switching fields
- ▶ The thin film is switched, and the resistance measured

- Current-driven domain wall motion ⁶



- ▶ Applied current supplies spin transfer torques

⁵http://www.wpi-aimr.tohoku.ac.jp/miyazaki_lab/spintorque.htm

⁶<http://physics.aps.org/articles/v2/11>

Micromagnetics: Landau-Lifshitz model

Basic quantity of interest:

$$\mathbf{m} : \Omega \longrightarrow \mathbb{R}^3; \quad |\mathbf{m}| = 1$$

Landau-Lifshitz energy functional:

$$\begin{aligned} F_{\text{LL}}[\mathbf{m}] &= \frac{K_u}{M_s} \int_{\Omega} \phi(\mathbf{m}) \, dx + \frac{C_{\text{ex}}}{M_s} \int_{\Omega} |\nabla \mathbf{m}|^2 \, dx \\ &\quad - \frac{\mu_0}{2} M_s \int_{\Omega} \mathbf{h}_s \cdot \mathbf{m} \, dx - \mu_0 M_s \int_{\Omega} \mathbf{h}_e \cdot \mathbf{m} \, dx \end{aligned}$$

- Continuum theory.
- Domain structure \longleftrightarrow Local minimizers.

- $\phi(\mathbf{m})$: Anisotropy Energy: Penalizes deviations from the easy directions. For uniaxial materials $\phi(\mathbf{m}) = (m_2^2 + m_3^2)$.
- $\frac{C_{\text{ex}}}{M_s} |\nabla \mathbf{m}|^2$: Exchange energy: Penalizes spatial variations.
- $-\mu_0 M_s \mathbf{h}_e \cdot \mathbf{m}$: External field (Zeeman) energy.
- $-\frac{\mu_0}{2} M_s \mathbf{h}_s \cdot \mathbf{m}$: Stray field (self-induced) energy.
- The stray field, $\mathbf{h}_s = -\nabla u$ is obtained by solving the magnetostatic equation:

$$\Delta u = \operatorname{div} \mathbf{m}, \quad \mathbf{x} \in \Omega, \quad \Delta u = 0, \quad \mathbf{x} \in \overline{\Omega}^c$$

with jump boundary conditions

$$[u]_{\partial\Omega} = 0, \quad \left[\frac{\partial u}{\partial \nu} \right]_{\partial\Omega} = -\mathbf{m} \cdot \boldsymbol{\nu}.$$

Landau-Lifshitz equation

- Torque balance

$$\mathbf{m}_t = -\mathbf{m} \times \mathbf{h} + \alpha \mathbf{m} \times \mathbf{m}_t,$$

or equivalently,

$$\mathbf{m}_t = -\frac{1}{1 + \alpha^2} \mathbf{m} \times \mathbf{h} - \frac{\alpha}{1 + \alpha^2} \mathbf{m} \times (\mathbf{m} \times \mathbf{h}),$$

where

$$\mathbf{h} = -\frac{\delta F_{LL}}{\delta \mathbf{m}} = -Q(m_2 \mathbf{e}_2 + m_3 \mathbf{e}_3) + \epsilon \Delta \mathbf{m} + \mathbf{h}_s + \mathbf{h}_e$$

and the second term is the Gilbert damping term.

- $\alpha \ll 1$: Damping coefficient

Model problem

$$\mathbf{m}_t = -\mathbf{m} \times \Delta \mathbf{m} + \alpha \mathbf{m} \times \mathbf{m}_t,$$

or

$$\mathbf{m}_t = -\mathbf{m} \times \Delta \mathbf{m} - \alpha \mathbf{m} \times (\mathbf{m} \times \Delta \mathbf{m})$$

with the Neumann boundary condition and the constraint $|\mathbf{m}| = 1$.

- ① Existence of weak solutions: [Alouges and Soyeur, 1992] in 3D whole space and [Guo and Hong, 1993] in 2D bounded domain;
- ② Nonuniqueness of weak solutions: [Alouges and Soyeur, 1992];
- ③ Local existence and uniqueness; global existence and uniqueness with small-energy initial data of strong solutions: [Carbou and Fabrie, 2001a] in 3D whole space; [Carbou and Fabrie, 2001b] in 2D bounded domain.

Review articles: [Kružík and Prohl, 2006; Cimrák, 2008]

- Finite element: [Bartels and Prohl, 2006; Alouges, 2008; Cimrák, 2009];
- Finite difference: [E and Wang, 2001; Fuwa et al., 2012; Kim and Lipnikov, 2017];

Linearity of the discrete system:

- Explicit scheme: [Jiang et al., 2001; Alouges and Jaisson, 2006];
- Fully implicit scheme: [Prohl, 2001; Bartels and Prohl, 2006; Fuwa et al., 2012];
- Semi-implicit scheme: [Wang, Garcia-Cervera, and E, 2001; E and Wang, 2001; Gao, 2014; Lewis and Nigam, 2003; Cimrák, 2005].

Time marching

- Splitting method: [Wang, Garcia-Cervera, and E, 2001];
- Mid-point method: [Bertotti et al., 2001, d'Aquino et al., 2005];
- Runge-Kutta methods: [Romeo et al., 2008];
- Geometric integration methods: [Jiang, Kaper, and Leaf, 2001];

Convergence analysis

- 1st order in time + 2nd order in space: [Alouges, 2008];
- 2nd order in time + 2nd order in space: [Bertotti et al., 2001, d'Aquino et al., 2005, Bartels and Prohl, 2006, Fuwa et al., 2012];
 - ▶ Unconditional stability;
 - ▶ Nonlinear solver at each time step (unavailable theoretical justification of the unique solvability);
 - ▶ Step-size condition $k = \mathcal{O}(h^2)$ with k the temporal stepsize and h the spatial stepsize;

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Spatial discretization

- $x_i = ih$, $i = 0, 1, 2, \dots, N_x$, with $x_0 = 0$, $x_{N_x} = 1$;
- $\hat{x}_i = x_{i-1/2} = (i - 1/2)h$, $i = 1, \dots, N_x$;
- $\mathbf{m}_i^n \approx \mathbf{m}(\hat{x}_i, t^n)$;
- $\Delta_h \mathbf{m}_i = \frac{\mathbf{m}_{i+1} - 2\mathbf{m}_i + \mathbf{m}_{i-1}}{h^2}$;
- Third order extrapolation for boundary condition:

$$\mathbf{m}_1 = \mathbf{m}_0, \quad \mathbf{m}_{N_x+1} = \mathbf{m}_{N_x}.$$

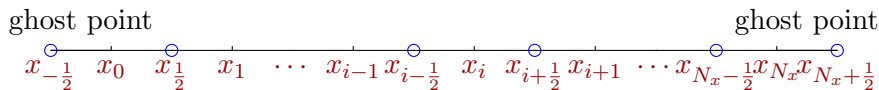


Figure 1: Illustration of the 1-D spatial mesh.

Semi-implicit projection methods [Xie, García-Cervera, Wang, Zhou, and Chen, submitted, 2019]

- $\mathbf{m}_t = -\mathbf{m} \times \Delta \mathbf{m} + \alpha \mathbf{m} \times \mathbf{m}_t$:

$$\begin{aligned} (1 - \alpha \hat{\mathbf{m}}_h^{n+2} \times) \frac{\frac{3}{2} \mathbf{m}_h^{n+2,*} - 2 \mathbf{m}_h^{n+1} + \frac{1}{2} \mathbf{m}_h^n}{k} &= -\hat{\mathbf{m}}_h^{n+2} \times \Delta_h \mathbf{m}_h^{n+2,*}, \\ \hat{\mathbf{m}}_h^{n+2} &= 2 \mathbf{m}_h^{n+1} - \mathbf{m}_h^n; \end{aligned}$$

- $\mathbf{m}_t = -\mathbf{m} \times \Delta \mathbf{m} - \alpha \mathbf{m} \times (\mathbf{m} \times \Delta \mathbf{m})$:

$$\begin{aligned} \frac{\frac{3}{2} \mathbf{m}_h^{n+2,*} - 2 \mathbf{m}_h^{n+1} + \frac{1}{2} \mathbf{m}_h^n}{k} &= -\hat{\mathbf{m}}_h^{n+2} \times \Delta_h \mathbf{m}_h^{n+2,*} \\ &\quad - \alpha \hat{\mathbf{m}}_h^{n+2} \times \left(\hat{\mathbf{m}}_h^{n+2} \times \Delta_h \mathbf{m}_h^{n+2,*} \right); \end{aligned}$$

- A projection step: $\mathbf{m}_h^{n+2} = \frac{\mathbf{m}_h^{n+2,*}}{|\mathbf{m}_h^{n+2,*}|}$.

1D test: Accuracy

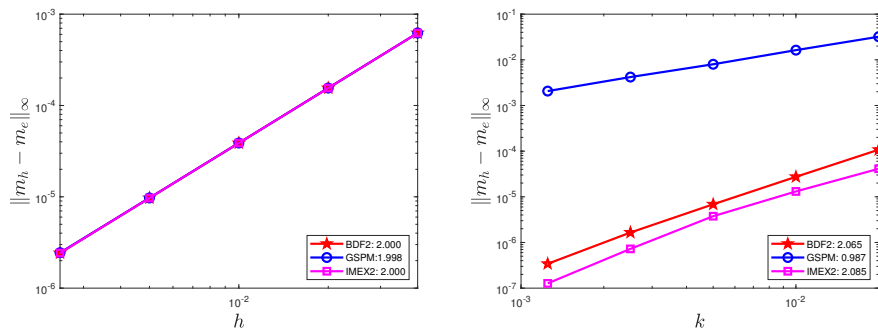


Figure 2: Accuracy of BDF2, GSPM and IMEX2. They are all second-order accurate in space. GSPM is first-order accurate in time. BDF2 and IMEX2 are second-order accurate in time.

1D test: Efficiency

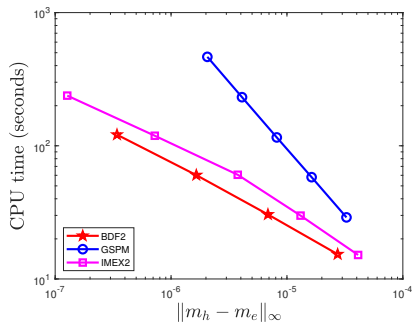


Figure 3: CPU time (in seconds) of BDF2, GSPM and IMEX2 versus error $\|m_h - m_e\|_\infty$. For a given tolerance of error, costs of these schemes in the increasing order are: BDF2 < IMEX2 < GSPM.

3D test: Accuracy

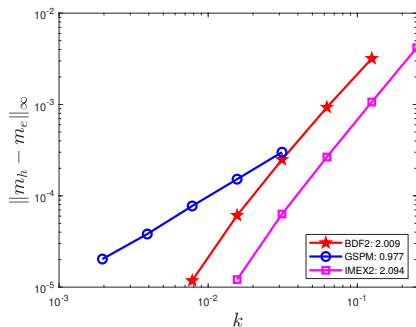
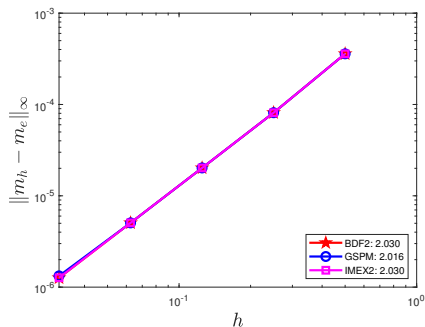


Figure 4: Accuracy of BDF2, GSPM and IMEX2. They are all second-order accurate in space. GSPM is first-order accurate in time. BDF2 and IMEX2 are second-order accurate in time.

3D test: Efficiency

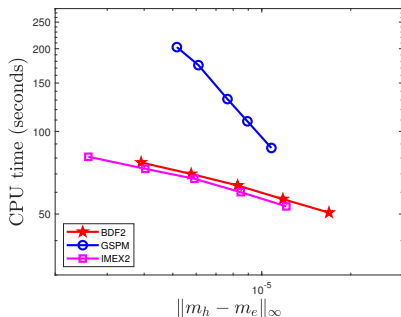


Figure 5: CPU time (in seconds) of BDF2, GSPM and IMEX2 versus error $\|m_h - m_e\|_\infty$. For a given tolerance of error, costs of $\text{BDF2} \approx \text{IMEX2} < \text{GSPM}$ when $h_x = h_y = h_z = 1/16$ in 3D.

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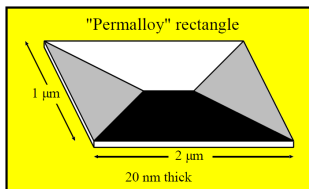
Mumag standard problem 1

Ask for simulating hysteresis loops.⁷

- Geometry: $1 \times 2 \times 0.02$ micron rectangle
- Material parameters: To mimic permalloy

Exchange constant: $C_{ex} = 1.3 \times 10^{-11}$ J/m
Saturation magnetization: $M_s = 8.0 \times 10^5$ A/m
Anisotropy constant: $K_u = 5.0 \times 10^2$ J/m³
Permeability of vacuum: $\mu_0 = 4\pi \times 10^{-7}$ N/A²
Damping parameter: $\alpha = 0.1$

Uniaxial, with easy axis nominally parallel to the long edges of the rectangle.



⁷<https://www.ctcms.nist.gov/~rdm/mumag.org.html>

Setup for our simulations

- The film of size: $1 \mu\text{m} \times 2 \mu\text{m} \times 200 \text{ \AA}$;
- The cell of size: $20 \text{ nm} \times 20 \text{ nm} \times 20 \text{ nm}$;
- Timescale: $k = 1 \text{ ps}$;
- # of field states: 133 for x - loop (or y - loop).
- For hysteresis loops simulation: the applied field H_0 (begin from 500 Oe) approximately parallel (canting angle $+1^\circ$) along y - (long) axis and x - (short) axis.

Semi-implicit projection methods for full LL equation

- $\mathbf{m}_t = -\mathbf{m} \times \mathbf{h} + \alpha \mathbf{m} \times \mathbf{m}_t$:

$$(1 - \alpha \hat{\mathbf{m}}_h^{n+2} \times) \frac{\frac{3}{2} \mathbf{m}_h^{n+2,*} - 2\mathbf{m}_h^{n+1} + \frac{1}{2} \mathbf{m}_h^n}{k} = -\hat{\mathbf{m}}_h^{n+2} \times (\epsilon \Delta_h \mathbf{m}_h^{n+2,*} + \hat{\mathbf{f}}_h^{n+2}),$$

$$\hat{\mathbf{m}}_h^{n+2} = 2\mathbf{m}_h^{n+1} - \mathbf{m}_h^n,$$

$$\hat{\mathbf{f}}_h^{n+2} = 2\mathbf{f}_h^{n+1} - \mathbf{f}_h^n,$$

$$\mathbf{f}_h^n = -Q(m_2^n \mathbf{e}_2 + m_3^n \mathbf{e}_3) + \mathbf{h}_s^n + \mathbf{h}_e^n;$$

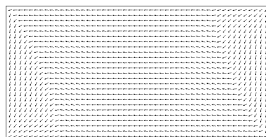
- $\mathbf{m}_t = -\mathbf{m} \times \mathbf{h} - \alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{h})$:

$$\frac{\frac{3}{2} \mathbf{m}_h^{n+2,*} - 2\mathbf{m}_h^{n+1} + \frac{1}{2} \mathbf{m}_h^n}{k} = -\hat{\mathbf{m}}_h^{n+2} \times (\epsilon \Delta_h \mathbf{m}_h^{n+2,*} + \hat{\mathbf{f}}_h^{n+2}) \\ - \alpha \hat{\mathbf{m}}_h^{n+2} \times \left(\hat{\mathbf{m}}_h^{n+2} \times (\epsilon \Delta_h \mathbf{m}_h^{n+2,*} + \hat{\mathbf{f}}_h^{n+2}) \right);$$

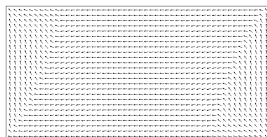
- A projection step: $\mathbf{m}_h^{n+2} = \frac{\mathbf{m}_h^{n+2,*}}{|\mathbf{m}_h^{n+2,*}|}$.

Magnetization profile

mo96a:

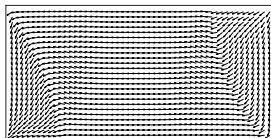


(a) $H_0 // y$ -axis

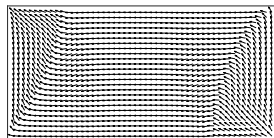


(b) $H_0 // x$ -axis

BDF2:



(c) $H_0 // y$ -axis



(d) $H_0 // x$ -axis

Figure 6: The in-plane magnetization components are represented by arrows.

Magnetization profile (cont'd)

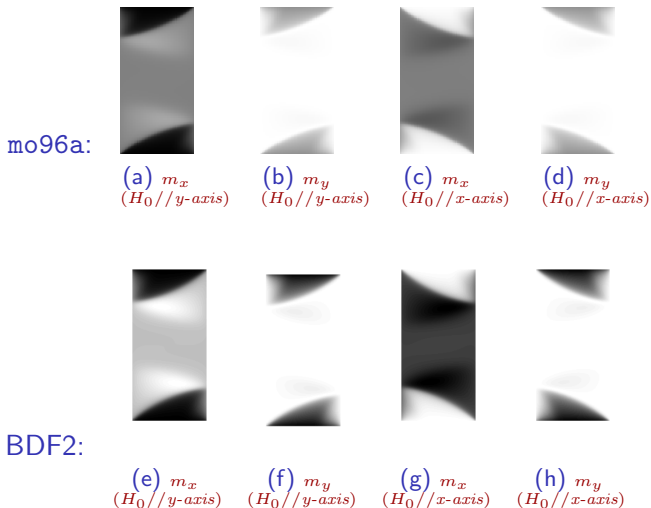
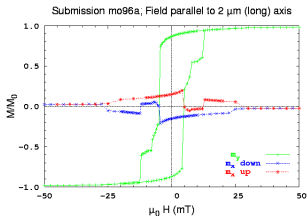


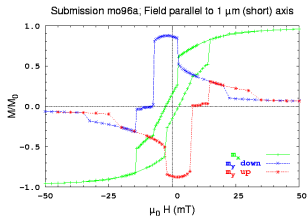
Figure 7: The x - and y - magnetization components are visualized by the gray value.

Hysteresis loop

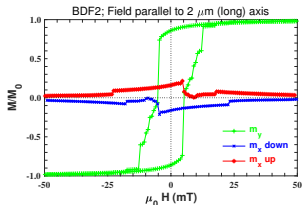


mo96a:

(a) $H_0 // y$ -axis

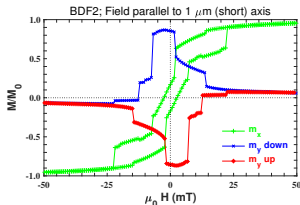


(b) $H_0 // x$ -axis



BDF2:

(c) $H_0 // y$ -axis



(d) $H_0 // x$ -axis

Semi-implicit projection methods revisited

- Lack of numerical stability of Lax-Richtmyer type;
- Separation of the time-marching step and the projection step:

$$\begin{aligned}\frac{\frac{3}{2}\tilde{\mathbf{m}}_h^{n+2} - 2\tilde{\mathbf{m}}_h^{n+1} + \frac{1}{2}\tilde{\mathbf{m}}_h^n}{k} &= -\hat{\mathbf{m}}_h^{n+2} \times \Delta_h \tilde{\mathbf{m}}_h^{n+2} \\ &\quad - \alpha \hat{\mathbf{m}}_h^{n+2} \times (\hat{\mathbf{m}}_h^{n+2} \times \Delta_h \tilde{\mathbf{m}}_h^{n+2}), \\ \hat{\mathbf{m}}_h^{n+2} &= 2\mathbf{m}_h^{n+1} - \mathbf{m}_h^n, \\ \mathbf{m}_h^{n+2} &= \frac{\tilde{\mathbf{m}}_h^{n+2}}{|\tilde{\mathbf{m}}_h^{n+2}|};\end{aligned}$$

- Two sets of approximations $\tilde{\mathbf{m}}_h^n$ and \mathbf{m}_h^n .

1D test

$$\mathbf{m}_e = (\cos(x^2(1-x)^2) \sin t, \sin(x^2(1-x)^2) \sin t, \cos t)^T$$

Table 1: Accuracy of our method on the uniform mesh when $h = k$ and $\alpha = 0.01$.

k	$\ \mathbf{m}_h - \mathbf{m}_e\ _\infty$	$\ \mathbf{m}_h - \mathbf{m}_e\ _2$	$\ \mathbf{m}_h - \mathbf{m}_e\ _{H^1}$
5.0D-3	3.867D-5	4.115D-5	1.729D-4
2.5D-3	7.976D-6	1.053D-5	4.629D-5
1.25D-3	2.135D-6	2.648D-6	1.177D-5
6.25D-4	5.765D-7	6.627D-7	2.949D-6
3.125D-4	1.447D-7	1.657D-7	7.370D-7
order	1.991	1.990	1.972

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- Inner product and $\|\cdot\|_2$ norm

$$\langle \mathbf{f}_h, \mathbf{g}_h \rangle = h^d \sum_{\mathcal{I} \in \Lambda_d} \mathbf{f}_{\mathcal{I}} \cdot \mathbf{g}_{\mathcal{I}},$$

$$\|\mathbf{f}_h\|_2 = (\langle \mathbf{f}_h, \mathbf{f}_h \rangle)^{1/2};$$

- Discrete $\|\cdot\|_{\infty}$ norm: $\|\mathbf{f}_h\|_{\infty} = \max_{\mathcal{I} \in \Lambda_d} \|\mathbf{f}_{\mathcal{I}}\|_{\infty}$;
- Average: $\bar{\mathbf{f}}_h = h^d \sum_{\mathcal{I} \in \Lambda_d} \mathbf{f}_{\mathcal{I}}$;
- Discrete H_h^{-1} -norm: $\|\mathbf{f}_h\|_{-1}^2 = \langle (-\Delta_h)^{-1} \mathbf{f}_h, \mathbf{f}_h \rangle$.

Preliminary estimates

- Inverse inequality:

$$\|\mathbf{e}_h^n\|_\infty \leq h^{-d/2} \|\mathbf{e}_h^n\|_2, \quad \|\nabla_h \mathbf{e}_h^n\|_\infty \leq h^{-d/2} \|\nabla_h \mathbf{e}_h^n\|_2;$$

- Summation by parts: $\langle -\Delta_h \mathbf{f}_h, \mathbf{g}_h \rangle = \langle \nabla_h \mathbf{f}_h, \nabla_h \mathbf{g}_h \rangle$;

- Discrete Gronwall inequality: Let $\{\alpha_j\}_{j \geq 0}$, $\{\beta_j\}_{j \geq 0}$ and $\{\omega_j\}_{j \geq 0}$ be sequences of real numbers such that

$$\alpha_j \leq \alpha_{j+1}, \quad \beta_j \geq 0, \quad \text{and} \quad \omega_j \leq \alpha_j + \sum_{i=0}^{j-1} \beta_i \omega_i, \quad \forall j \geq 0.$$

Then it holds that

$$\omega_j \leq \alpha_j \exp \left\{ \sum_{i=0}^{j-1} \beta_i \right\}, \quad \forall j \geq 0.$$

Discrete gradient acting on cross product

Lemma

For grid functions \mathbf{f}_h and \mathbf{g}_h over the uniform numerical grid, we have

$$\|\nabla_h(\mathbf{f} \times \mathbf{g})_h\|_2^2 \leq C \left(\|\mathbf{f}_h\|_\infty^2 \cdot \|\nabla_h \mathbf{g}_h\|_2^2 + \|\mathbf{g}_h\|_\infty^2 \cdot \|\nabla_h \mathbf{f}_h\|_2^2 \right),$$

$$\langle (\mathbf{f}_h \times \Delta_h \mathbf{g}_h) \times \mathbf{f}_h, \mathbf{g}_h \rangle = \langle \mathbf{f}_h \times (\mathbf{g}_h \times \mathbf{f}_h), \Delta_h \mathbf{g}_h \rangle,$$

$$\langle \mathbf{f}_h \times (\mathbf{f}_h \times \mathbf{g}_h), \mathbf{g}_h \rangle = -\|\mathbf{f}_h \times \mathbf{g}_h\|_2^2.$$

Unconditional unique solvability

Theorem

Given \mathbf{p}_h , $\tilde{\mathbf{p}}_h$ and $\hat{\mathbf{m}}_h$, the numerical schemes

$$\left(\frac{3}{2}I_h - \frac{3}{2}\alpha\hat{\mathbf{m}}_h \times I_h + k\hat{\mathbf{m}}_h \times \Delta_h\right)\mathbf{m}_h = \mathbf{p}_h,$$

$$\left(\frac{3}{2}I_h + k\hat{\mathbf{m}}_h \times \Delta_h + \alpha k\hat{\mathbf{m}}_h \times (\hat{\mathbf{m}}_h \times \Delta_h)\right)\mathbf{m}_h = \tilde{\mathbf{p}}_h,$$

are uniquely solvable.

Denote $\mathbf{q}_h = -\Delta_h\mathbf{m}_h$. Then

$$\mathbf{m}_h = (-\Delta_h)^{-1}\mathbf{q}_h + C_{\mathbf{q}_h}^* \quad \text{with} \quad C_{\mathbf{q}_h}^* = \frac{2}{3}\left(\tilde{\mathbf{p}}_h + k\overline{\hat{\mathbf{m}}_h \times \mathbf{q}_h} + \alpha k\overline{\hat{\mathbf{m}}_h \times (\hat{\mathbf{m}}_h \times \mathbf{q}_h)}\right)$$

and

$$G(\mathbf{q}_h) := \frac{3}{2}\left((- \Delta_h)^{-1}\mathbf{q}_h + C_{\mathbf{q}_h}^*\right) - \tilde{\mathbf{p}}_h - k\hat{\mathbf{m}}_h \times \mathbf{q}_h - \alpha k\hat{\mathbf{m}}_h \times (\hat{\mathbf{m}}_h \times \mathbf{q}_h) = \mathbf{0}.$$

Observe that

$$\begin{aligned} A &:= \frac{3}{2}\alpha\hat{\mathbf{m}}_h \times I_h + k\hat{\mathbf{m}}_h \times (-\Delta_h) \\ &= k\hat{\mathbf{m}}_h \times \left(-\Delta_h + \frac{3\alpha}{2k}I_h \right) \\ &=: kMS. \end{aligned}$$

- I_h : identity matrix; M : antisymmetric matrix;
- $S = -\Delta_h + \frac{3\alpha}{2k}I_h$: symmetric positive definite matrix;
- $S = C^T C$ with C being nonsingular;
- $|\lambda I - MS| = |\lambda I - MC^T C| = |\lambda I - CM C^T|$;
- $(CM C^T)^T = -CM C^T$;

Lemma (spectral lemma for antisymmetric matrices)

Each eigenvalue of the real skew-symmetric matrix is either 0 or purely imaginary number.

By the lemma, $\det(\frac{3}{2}I_h - \frac{3}{2}\alpha\hat{\mathbf{m}}_h \times I_h + k\hat{\mathbf{m}}_h \times \Delta_h) \neq 0$ since the matrix has $\frac{3}{2}$ as real parts, and thus the corresponding linear system of equations has a unique solution.

For any $\mathbf{q}_{1,h}, \mathbf{q}_{2,h}$ with $\overline{\mathbf{q}_{1,h}} = \overline{\mathbf{q}_{2,h}} = 0$, we denote $\tilde{\mathbf{q}}_h = \mathbf{q}_{1,h} - \mathbf{q}_{2,h}$

$$\begin{aligned}
 & \langle G(\mathbf{q}_{1,h}) - G(\mathbf{q}_{2,h}), \mathbf{q}_{1,h} - \mathbf{q}_{2,h} \rangle \\
 &= \frac{3}{2k} \left(\langle (-\Delta_h)^{-1} \tilde{\mathbf{q}}_h, \tilde{\mathbf{q}}_h \rangle + \langle C_{\mathbf{q}_{1,h}}^* - C_{\mathbf{q}_{2,h}}^*, \tilde{\mathbf{q}}_h \rangle \right) \\
 & \quad - \langle \hat{\mathbf{m}}_h \times \tilde{\mathbf{q}}_h, \tilde{\mathbf{q}}_h \rangle - \alpha \langle \hat{\mathbf{m}}_h \times (\hat{\mathbf{m}}_h \times \tilde{\mathbf{q}}_h), \tilde{\mathbf{q}}_h \rangle \\
 & \geq \frac{3}{2k} \left(\langle (-\Delta_h)^{-1} \tilde{\mathbf{q}}_h, \tilde{\mathbf{q}}_h \rangle + \langle C_{\mathbf{q}_{1,h}}^* - C_{\mathbf{q}_{2,h}}^*, \tilde{\mathbf{q}}_h \rangle \right) \\
 &= \frac{3}{2k} \langle (-\Delta_h)^{-1} \tilde{\mathbf{q}}_h, \tilde{\mathbf{q}}_h \rangle = \frac{3}{2k} \|\tilde{\mathbf{q}}_h\|_{-1}^2 \geq 0.
 \end{aligned}$$

Moreover, for any $\mathbf{q}_{1,h}, \mathbf{q}_{2,h}$ with $\overline{\mathbf{q}_{1,h}} = \overline{\mathbf{q}_{2,h}} = 0$, we get

$$\langle G(\mathbf{q}_{1,h}) - G(\mathbf{q}_{2,h}), \mathbf{q}_{1,h} - \mathbf{q}_{2,h} \rangle \geq \frac{3}{2k} \|\tilde{\mathbf{q}}_h\|_{-1}^2 > 0, \quad \text{if } \mathbf{q}_{1,h} \neq \mathbf{q}_{2,h},$$

and the equality only holds when $\mathbf{q}_{1,h} = \mathbf{q}_{2,h}$.

Lemma (Browder-Minty lemma [Browder, 1963, Minty, 1963])

Let X be a real, reflexive Banach space and let $T : X \rightarrow X'$ (the dual space of X) be bounded, continuous, coercive (i.e., $\frac{(T(u), u)}{\|u\|_X} \rightarrow +\infty$, as $\|u\|_X \rightarrow +\infty$) and monotone. Then for any $g \in X'$ there exists a solution $u \in X$ of the equation $T(u) = g$. Furthermore, if the operator T is strictly monotone, then the solution u is unique.

By the Browder-Minty lemma, the semi-implicit scheme admits a unique solution.

Optimal rate convergence analysis [Chen, Wang and Xie, submitted, 2019]

Theorem

Let $\mathbf{m}_e \in C^3([0, T]; C^0) \cap L^\infty([0, T]; C^4)$ be a smooth solution with the initial data $\mathbf{m}_e(\mathbf{x}, 0) = \mathbf{m}_e^0(\mathbf{x})$ and \mathbf{m}_h be the numerical solution with the initial data $\mathbf{m}_h^0 = \mathbf{m}_{e,h}^0$ and $\mathbf{m}_h^1 = \mathbf{m}_{e,h}^1$. Suppose that the initial error satisfies

$$\|\mathbf{m}_{e,h}^\ell - \mathbf{m}_h^\ell\|_2 + \|\nabla_h(\mathbf{m}_{e,h}^\ell - \mathbf{m}_h^\ell)\|_2 = \mathcal{O}(k^2 + h^2), \quad \ell = 0, 1, \text{ and } k \leq Ch.$$

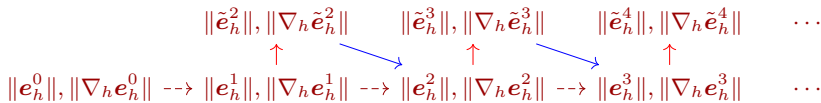
Then the following convergence result holds as h and k goes to zero:

$$\|\mathbf{m}_{e,h}^n - \mathbf{m}_h^n\|_2 + \|\nabla_h(\mathbf{m}_{e,h}^n - \mathbf{m}_h^n)\|_2 \leq \mathcal{C}(k^2 + h^2), \quad \forall n \geq 2,$$

in which the constant $\mathcal{C} > 0$ is independent of k and h .

Idea of the proof

- Initial error: e_h^0 and e_h^1 ;
- Alternative estimate: Using discrete Gronwall inequality and another lemma to evaluate \tilde{e}_h and $\nabla_h \tilde{e}_h$; Again by the lemma to estimate e_h and $\nabla_h e_h$. Illustrated by the following schematic:



- To guarantee the assumptions in the recursive demonstration.

Sketch of the proof

Step 1: Construction of an approximate solution $\underline{\mathbf{m}}$:

$$\underline{\mathbf{m}} = \mathbf{m}_e + h^2 \mathbf{m}^{(1)},$$

in which the auxiliary field $\mathbf{m}^{(1)}$ satisfies

$$\Delta \mathbf{m}^{(1)} = \hat{C} \quad \text{with} \quad \hat{C} = \frac{1}{|\Omega|} \int_{\partial\Omega} \partial_\nu^3 \mathbf{m}_e \, ds,$$

$$\partial_z \mathbf{m}^{(1)}|_{z=0} = -\frac{1}{24} \partial_z^3 \mathbf{m}_e|_{z=0}, \quad \partial_z \mathbf{m}^{(1)}|_{z=1} = \frac{1}{24} \partial_z^3 \mathbf{m}_e|_{z=1}.$$

Then

$$\begin{aligned} \mathbf{m}_e(\hat{x}_i, \hat{y}_j, \hat{z}_0) &= \mathbf{m}_e(\hat{x}_i, \hat{y}_j, \hat{z}_1) - \frac{h^3}{24} \partial_z^3 \mathbf{m}_e(\hat{x}_i, \hat{y}_j, 0) + \mathcal{O}(h^5), \\ \mathbf{m}^{(1)}(\hat{x}_i, \hat{y}_j, \hat{z}_0) &= \mathbf{m}^{(1)}(\hat{x}_i, \hat{y}_j, \hat{z}_1) + \frac{h}{24} \partial_z^3 \mathbf{m}_e(\hat{x}_i, \hat{y}_j, 0) + \mathcal{O}(h^3), \\ \underline{\mathbf{m}}(\hat{x}_i, \hat{y}_j, \hat{z}_0) &= \underline{\mathbf{m}}(\hat{x}_i, \hat{y}_j, \hat{z}_1) + \mathcal{O}(h^5), \\ \Delta_h \underline{\mathbf{m}}_{i,j,k} &= \Delta \mathbf{m}_e(\hat{x}_i, \hat{y}_j, \hat{z}_k) + \mathcal{O}(h^2), \quad \forall 1 \leq i, j, k \leq N. \end{aligned}$$

Step 2: Error function evolution system for

$$\tilde{e}_h^n = \underline{m}_h^n - \tilde{m}_h^n, \quad e_h^n = \underline{m}_h^n - m_h^n,$$

$$\begin{aligned} \frac{\frac{3}{2}\tilde{e}_h^{n+2} - 2\tilde{e}_h^{n+1} + \frac{1}{2}\tilde{e}_h^n}{k} &= - (2m_h^{n+1} - m_h^n) \times \Delta_h \tilde{e}_h^{n+2} - (2e_h^{n+1} - e_h^n) \times \Delta_h \underline{m}_h^{n+2} \\ &\quad - \alpha (2m_h^{n+1} - m_h^n) \times ((2m_h^{n+1} - m_h^n) \times \Delta_h \tilde{e}_h^{n+2}) \\ &\quad - \alpha (2m_h^{n+1} - m_h^n) \times ((2e_h^{n+1} - e_h^n) \times \Delta_h \underline{m}_h^{n+2}) \\ &\quad - \alpha (2e_h^{n+1} - e_h^n) \times ((2\underline{m}_h^{n+1} - \underline{m}_h^n) \times \Delta_h \underline{m}_h^{n+2}) + \tau^{n+2} \end{aligned}$$

with $\|\tau^{n+2}\|_2 \leq C(k^2 + h^2)$.

- Discrete L^2 error estimate: Inner product with $\tilde{e}_h^{\ell+2}$

$$\begin{aligned} &\|\tilde{e}_h^{\ell+2}\|_2^2 - \|\tilde{e}_h^{\ell+1}\|_2^2 + \|2\tilde{e}_h^{\ell+2} - \tilde{e}_h^{\ell+1}\|_2^2 - \|2\tilde{e}_h^{\ell+1} - \tilde{e}_h^\ell\|_2^2 \\ &\leq Ck(\|\nabla_h \tilde{e}_h^{\ell+2}\|_2^2 + \|\tilde{e}_h^{\ell+2}\|_2^2 + \|e_h^{\ell+1}\|_2^2 + \|e_h^\ell\|_2^2) + Ck(k^4 + h^4). \end{aligned}$$

Remark: Discrete Gronwall inequality is not applicable due to the presence of H_h^1 norms of the error function.

- Discrete inner product with $-\Delta_h \tilde{\mathbf{e}}_h^{\ell+2}$

$$\begin{aligned} & \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 - \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|2\nabla_h \tilde{\mathbf{e}}_h^{\ell+2} - \nabla_h \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 - \|2\nabla_h \tilde{\mathbf{e}}_h^{\ell+1} - \nabla_h \tilde{\mathbf{e}}_h^\ell\|_2^2 \\ & \leq Ck \left(\|\nabla_h \tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 + \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|\nabla_h \mathbf{e}_h^\ell\|_2^2 + \|\mathbf{e}_h^{\ell+1}\|_2^2 + \|\mathbf{e}_h^\ell\|_2^2 \right) + Ck(k^4 + h^4). \end{aligned}$$

- Combination of both

$$\begin{aligned} & \|\tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 - \|\tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|2\tilde{\mathbf{e}}_h^{\ell+2} - \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 - \|2\tilde{\mathbf{e}}_h^{\ell+1} - \tilde{\mathbf{e}}_h^\ell\|_2^2 \\ & + \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 - \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|\nabla_h (2\tilde{\mathbf{e}}_h^{\ell+2} - \tilde{\mathbf{e}}_h^{\ell+1})\|_2^2 - \|\nabla_h (2\tilde{\mathbf{e}}_h^{\ell+1} - \tilde{\mathbf{e}}_h^\ell)\|_2^2 \\ & \leq Ck \left(\|\nabla_h \tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 + \|\tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 + \|\nabla_h \mathbf{e}_h^{\ell+1}\|_2^2 + \|\nabla_h \mathbf{e}_h^\ell\|_2^2 + \|\mathbf{e}_h^{\ell+1}\|_2^2 + \|\mathbf{e}_h^\ell\|_2^2 \right) \\ & + Ck(k^4 + h^4). \end{aligned}$$

Lemma

Consider $\underline{\mathbf{m}}_h = \mathbf{m}_e + h^2 \mathbf{m}^{(1)}$ with \mathbf{m}_e the exact solution and $|\mathbf{m}_e| = 1$ at a point-wise level, and $\|\mathbf{m}^{(1)}\|_\infty + \|\nabla_h \mathbf{m}^{(1)}\|_\infty \leq \mathcal{C}$. For any numerical solution $\tilde{\mathbf{m}}_h$, we define $\mathbf{m}_h = \frac{\tilde{\mathbf{m}}_h}{|\tilde{\mathbf{m}}_h|}$. Suppose both numerical profiles satisfy the following $W_h^{1,\infty}$ bounds

$$|\tilde{\mathbf{m}}_h| \geq \frac{1}{2}, \quad \text{at a point-wise level,}$$

$$\|\mathbf{m}_h\|_\infty + \|\nabla_h \mathbf{m}_h\|_\infty \leq M, \quad \|\tilde{\mathbf{m}}_h\|_\infty + \|\nabla_h \tilde{\mathbf{m}}_h\|_\infty \leq M,$$

and we denote the numerical error functions as $\mathbf{e}_h = \underline{\mathbf{m}}_h - \mathbf{m}_h$, $\tilde{\mathbf{e}}_h = \underline{\mathbf{m}}_h - \tilde{\mathbf{m}}_h$. Then the following estimate is valid

$$\|\mathbf{e}_h\|_2 \leq 2\|\tilde{\mathbf{e}}_h\|_2 + \mathcal{O}(h^2), \quad \|\nabla_h \mathbf{e}_h\|_2 \leq \mathcal{C}(\|\nabla_h \tilde{\mathbf{e}}_h\|_2 + \|\tilde{\mathbf{e}}_h\|_2) + \mathcal{O}(h^2).$$

- Using the Lemma

$$\begin{aligned}
& \|\tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 - \|\tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|2\tilde{\mathbf{e}}_h^{\ell+2} - \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 - \|2\tilde{\mathbf{e}}_h^{\ell+1} - \tilde{\mathbf{e}}_h^\ell\|_2^2 \\
& + \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 - \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|\nabla_h (2\tilde{\mathbf{e}}_h^{\ell+2} - \tilde{\mathbf{e}}_h^{\ell+1})\|_2^2 - \|\nabla_h (2\tilde{\mathbf{e}}_h^{\ell+1} - \tilde{\mathbf{e}}_h^\ell)\|_2^2 \\
\leq & \mathcal{C}k \left(\|\nabla_h \tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 + \|\nabla_h \tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|\nabla_h \tilde{\mathbf{e}}_h^\ell\|_2^2 + \|\tilde{\mathbf{e}}_h^{\ell+2}\|_2^2 + \|\tilde{\mathbf{e}}_h^{\ell+1}\|_2^2 + \|\tilde{\mathbf{e}}_h^\ell\|_2^2 \right) \\
& + \mathcal{C}k(k^4 + h^4).
\end{aligned}$$

- Discrete Gronwall inequality

$$\begin{aligned}
\|\tilde{\mathbf{e}}_h^n\|_2^2 + \|\nabla_h \tilde{\mathbf{e}}_h^n\|_2^2 & \leq \mathcal{C}T e^{\mathcal{C}T} (k^4 + h^4), \quad \text{for all } n : n \leq \left\lfloor \frac{T}{k} \right\rfloor, \\
\|\tilde{\mathbf{e}}_h^n\|_2 + \|\nabla_h \tilde{\mathbf{e}}_h^n\|_2 & \leq \mathcal{C}(k^2 + h^2).
\end{aligned}$$

Lemma

Assume the numerical error function:

$$\|\mathbf{e}_h^k\|_\infty + \|\nabla_h \mathbf{e}_h^k\|_\infty \leq \frac{1}{3}, \quad \|\tilde{\mathbf{e}}_h^k\|_\infty + \|\nabla_h \tilde{\mathbf{e}}_h^k\|_\infty \leq \frac{1}{3}, \quad \text{for } k = \ell, \ell + 1.$$

Such an assumption will be recovered by the convergence analysis at time step $t^{\ell+2}$. Then numerical solutions \mathbf{m}_h and $\tilde{\mathbf{m}}_h$:

$$\|\mathbf{m}_h^k\|_\infty = \|\underline{\mathbf{m}}_h^k - \mathbf{e}_h^k\|_\infty \leq \|\underline{\mathbf{m}}_h^k\|_\infty + \|\mathbf{e}_h^k\|_\infty \leq \mathcal{C} + \frac{1}{3},$$

$$\|\nabla_h \mathbf{m}_h^k\|_\infty = \|\nabla_h \underline{\mathbf{m}}_h^k - \nabla_h \mathbf{e}_h^k\|_\infty \leq \|\nabla_h \underline{\mathbf{m}}_h^k\|_\infty + \|\nabla_h \mathbf{e}_h^k\|_\infty \leq \mathcal{C} + \frac{1}{3},$$

$$\|\tilde{\mathbf{m}}_h^k\|_\infty \leq \mathcal{C} + \frac{1}{3}, \quad \|\nabla_h \tilde{\mathbf{m}}_h^k\|_\infty \leq \mathcal{C} + \frac{1}{3} \quad (\text{similar derivation}).$$

- Inverse inequality with time step constraint $k \leq \mathcal{C}h$

$$\|\tilde{\mathbf{e}}_h^n\|_\infty \leq \frac{\|\tilde{\mathbf{e}}_h^n\|_2}{h^{d/2}} \leq \frac{\mathcal{C}(k^2 + h^2)}{h^{d/2}} \leq \frac{1}{6},$$

$$\|\nabla_h \tilde{\mathbf{e}}_h^n\|_\infty \leq \frac{\|\nabla_h \tilde{\mathbf{e}}_h^n\|_2}{h^{d/2}} \leq \frac{\mathcal{C}(k^2 + h^2)}{h^{d/2}} \leq \frac{1}{6}.$$

- Convergence estimate for e_h^n :

$$\|e_h^n\|_2 \leq 2\|\tilde{e}_h^n\|_2 + \mathcal{O}(h^2) \leq \mathcal{C}(k^2 + h^2),$$

$$\|\nabla_h e_h^n\|_2 \leq \mathcal{C}(\|\nabla_h \tilde{e}_h^n\|_2 + \|\tilde{e}_h^n\|_2) + \mathcal{O}(h^2) \leq \mathcal{C}(k^2 + h^2).$$

Verification of assumptions.

$$|\tilde{m}_h| \geq \frac{1}{2}, \quad \text{at a point-wise level,}$$

$$\|\mathbf{m}_h\|_\infty + \|\nabla_h \mathbf{m}_h\|_\infty \leq M, \quad \|\tilde{m}_h\|_\infty + \|\nabla_h \tilde{m}_h\|_\infty \leq M,$$

$$\|e_h^n\|_\infty \leq \frac{1}{6}, \quad \|\nabla_h e_h^n\|_\infty \leq \frac{1}{6},$$

$$\|\tilde{e}_h^n\|_\infty \leq \frac{1}{6}, \quad \|\nabla_h \tilde{e}_h^n\|_\infty \leq \frac{1}{6}.$$



Outline

- 1 Background and motivation
- 2 Semi-implicit projection methods
- 3 Benchmark problem from NIST
- 4 Main theoretical results
 - Unconditional unique solvability
 - Optimal rate convergence analysis
- 5 Numerical examples**
- 6 Conclusion

Homogenous Neumann boundary condition

- 1 1-D example with a forcing term and the given exact solution
- 2 1-D example without the exact solution
- 3 3-D example with a forcing term and the given exact solution

Example 1

$$\mathbf{m}_e = (\cos(x^2(1-x)^2) \sin t, \sin(x^2(1-x)^2) \sin t, \cos t)^T$$

Table 2: Accuracy of our method on the uniform mesh when $h = k$ and $\alpha = 0.01$.

k	$\ \mathbf{m}_h - \mathbf{m}_e\ _\infty$	$\ \mathbf{m}_h - \mathbf{m}_e\ _2$	$\ \mathbf{m}_h - \mathbf{m}_e\ _{H^1}$
5.0D-3	3.867D-5	4.115D-5	1.729D-4
2.5D-3	7.976D-6	1.053D-5	4.629D-5
1.25D-3	2.135D-6	2.648D-6	1.177D-5
6.25D-4	5.765D-7	6.627D-7	2.949D-6
3.125D-4	1.447D-7	1.657D-7	7.370D-7
order	1.991	1.990	1.972

Example 2

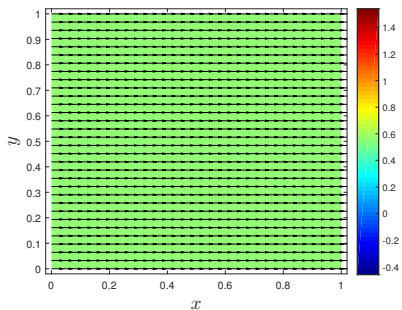
Table 3: Temporal accuracy of our method on the uniform mesh when $h = 1D - 4$ and $\alpha = 0.01$.

k	$\ m_h - m_c\ _\infty$	$\ m_h - m_c\ _2$	$\ m_h - m_c\ _{H^1}$
5.0D-3	2.949D-5	3.250D-5	1.633D-4
2.5D-3	8.116D-6	8.429D-6	4.393D-5
1.25D-3	2.125D-6	2.114D-6	1.118D-5
6.25D-4	4.851D-7	5.190D-7	2.791D-6
3.125D-4	1.129D-7	1.196D-7	6.875D-7
order	2.012	2.019	1.976

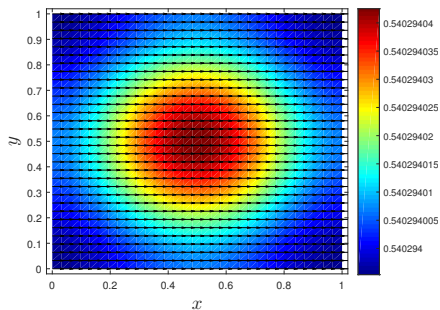
Table 4: Spatial accuracy of our method on the uniform mesh when $k = 1D - 4$ and $\alpha = 0.01$.

h	$\ m_h - m_c\ _\infty$	$\ m_h - m_c\ _2$	$\ m_h - m_c\ _{H^1}$
$1/3^2$	0.00546	0.00577	0.01336
$1/3^3$	6.101D-4	6.430D-4	0.00160
$1/3^4$	6.782D-5	7.146D-5	1.820D-4
$1/3^5$	7.527D-6	7.930D-6	2.036D-5
$1/3^6$	8.271D-7	8.714D-7	2.243D-6
order	2.001	2.002	1.980

Example 3



(e) Exact magnetization profile



(f) Numerical magnetization profile

Figure 8: Profiles of the exact and the numerical magnetization in the xy -plane with $z = 1/2$ when $k = 1/256$, $h_x = h_y = h_z = 1/32$, and $\alpha = 0.01$.

Table 5: Temporal accuracy in the 3-D case when $h_x = h_y = h_z = 1/32$ and $\alpha = 0.01$.

k	$\ m_h - m_e\ _\infty$	$\ m_h - m_e\ _2$	$\ m_h - m_e\ _{H^1}$
1/16	1.685D-3	1.098D-3	1.211D-3
1/32	4.411D-4	2.964D-4	3.082D-4
1/64	1.128D-4	7.730D-5	7.772D-5
1/128	2.966D-5	2.024D-5	2.051D-5
1/256	8.311D-6	5.693D-6	5.812D-6
order	1.922	1.906	1.932

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Conclusion

What we have done

- ① Two second-order semi-implicit schemes for LL equation;
- ② Benchmark problem from NIST;
- ③ Unique solvability for two schemes;
- ④ Convergence analysis for one of the schemes.

To-do list

- ① Generalization of the technique for other implicit scheme;
- ② Current-driven magnetization dynamics [Chen, García-Cervera, and Yang, 2015];
- ③ Application to Landau-Lifshitz-Maxwell equations.

Thank you