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

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Outline

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

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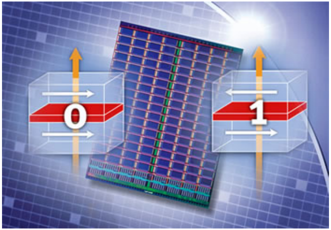
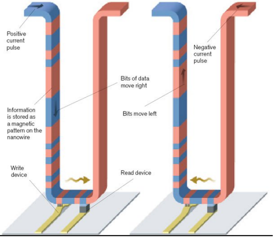
Magnetic recording devices and computer storages

- Spinvalues[1]



Magnetoresistance random access memory (MRAM)

- Domain walls [2]

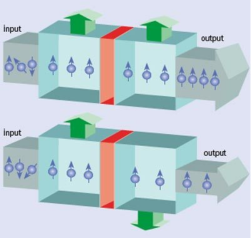


Racetrack memories

[1] Science@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]

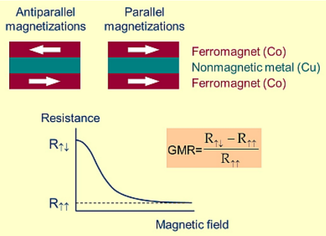


Julliere's model: Constant tunneling matrix

$$TMR \equiv \frac{G_{AP} - G_P}{G_{AP}} = \frac{2P_L P_R}{1 - P_L P_R}$$

$$P_L = \frac{n_L^{\uparrow} - n_L^{\downarrow}}{n_L^{\uparrow} + n_L^{\downarrow}} \qquad P_R = \frac{n_R^{\uparrow} - n_R^{\downarrow}}{n_R^{\uparrow} + n_R^{\downarrow}}$$

- Gaint magnetoresistance [4]

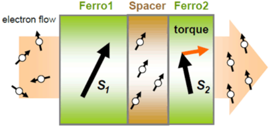


- Albert Fert and Peter Grüberg: 2007 Nobel Prize in Physics
- Polarization and scattering

[3] http://ducthe.wordpress.com/category/spintronics/
[4] http://physics.unl.edu/

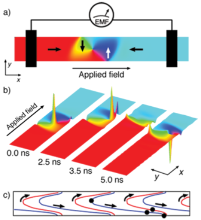
Methodology for rotating the orientation

- 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

[5] http://www.wpi-aimr.tohoku.ac.jp/miyazaki_ labo/spintorque.htm
[6] http://physics.aps.org/articles/v2/11

Micromagnetics: Landau-Lifshitz model

Basic quantity of interest:

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

Landau-Lifshitz energy functional:

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

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

Landau-Lifshitz equation

- Torque balance

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

or equivalently,

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

where

$$\boldsymbol{h} = -\frac{\delta F_{\mathrm{LL}}}{\delta \boldsymbol{m}} = -Q(m_2 \boldsymbol{e}_2 + m_2 \boldsymbol{e}_3) + \epsilon \Delta \boldsymbol{m} + \boldsymbol{h}_{\mathrm{s}} + \boldsymbol{h}_{\mathrm{e}}$$

and the second term is the Gilbert damping term.

- $\alpha << 1$: Damping coefficient

Model problem

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

or

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

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

Literature review: Numerical aspect

Review articles: [Kruzík 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].

Continued...

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];
- 2st 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;

Outline

Spatial discretization

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

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

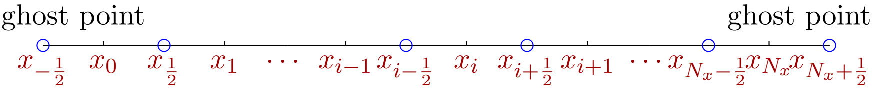


Figure 1: Illustration of the 1-D spatial mesh.

Semi-implicit projection methods [Xie, Garcia-Cervera, Wang, Zhou, and Chen, in progress, 2018]

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

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

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

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

- A projection step: $\boldsymbol{m}_h^{n+2} = \dfrac{\boldsymbol{m}_h^{n+2}}{|\boldsymbol{m}_h^{n+2}|}$.

1D test: Accuracy

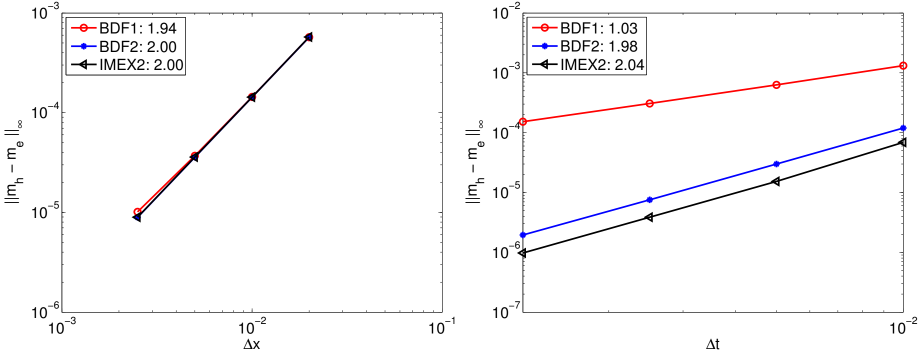


Figure 2: Accuracy of BDF1, BDF2, and IMEX2. They are all second-order accurate in space. BDF1 is first-order accurate in time. BDF2 and IMEX2 are second-order accurate in time.

1D test: Efficiency

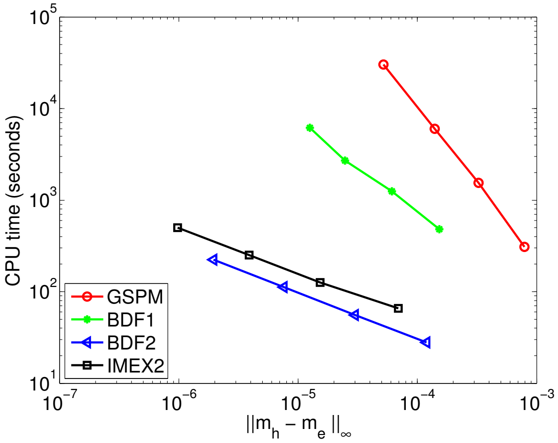


Figure 3: CPU time (in seconds) of GSPM, BDF1, BDF2, and IMEX2 versus error $\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_\infty$. For a given tolerance of error, costs of these schemes in the increasing order are: BDF2 $<$ IMEX2 $<$ BDF1 $<$ GSPM.

Semi-implicit projection methods revisited

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

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

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

1D test

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

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

k	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_\infty$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_2$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_{H^1}$
2.0D-2	4.990D-5	5.865D-5	1.060D-4
1.0D-2	1.262D-5	1.434D-5	2.666D-5
5.0D-3	3.167D-6	3.545D-6	6.762D-6
2.5D-3	7.927D-7	8.813D-7	1.699D-6
1.25D-3	1.983D-7	2.197D-7	4.257D-7
6.25D-4	4.961D-8	5.484D-8	1.065D-7
order	1.996	2.012	1.991

Outline

Unconditional unique solvability

Theorem

Given $\boldsymbol{p}_h$, $\hat{\boldsymbol{m}}_h$, *the numerical scheme*

$$\frac{\frac{3}{2}\tilde{\boldsymbol{m}}_h - \boldsymbol{p}_h}{k} = -\hat{\boldsymbol{m}}_h \times \Delta_h \tilde{\boldsymbol{m}}_h - \alpha \hat{\boldsymbol{m}}_h \times (\hat{\boldsymbol{m}}_h \times \Delta_h \tilde{\boldsymbol{m}}_h)$$

is uniquely solvable.

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

$$\tilde{\boldsymbol{m}}_h = (-\Delta_h)^{-1}\boldsymbol{q}_h + C^*_{\boldsymbol{q}_h} \quad \text{with } C^*_{\boldsymbol{q}_h} = \frac{2}{3}\Big(\overline{\boldsymbol{p}_h} + k\overline{\hat{\boldsymbol{m}}_h \times \boldsymbol{q}_h} + \alpha k \overline{\hat{\boldsymbol{m}}_h \times (\hat{\boldsymbol{m}}_h \times \boldsymbol{q}_h)}\Big)$$

and

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

Continued ...

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

Let X be a real, reflexive Banach space and let $T : X \to X'$ (the dual space of X) be bounded, continuous, coercive (i.e., $\frac{(T(u),u)}{\|u\|_X} \to +\infty$, as $\|u\|_X \to +\infty$) 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

Theorem

Let $\boldsymbol{m}_e \in C^3([0,T];C^0) \cap L^\infty([0,T];C^4)$ be a smooth solution with the initial data $\boldsymbol{m}_e(\boldsymbol{x},0) = \boldsymbol{m}_e^0(\boldsymbol{x})$ and $\boldsymbol{m}_h$ be the numerical solution with the initial data $\boldsymbol{m}_h^0 = \boldsymbol{m}_{e,h}^0$ and $\boldsymbol{m}_h^1 = \boldsymbol{m}_{e,h}^1$. Suppose that the initial error satisfies
$\|\boldsymbol{m}_{e,h}^\ell - \boldsymbol{m}_h^\ell\|_2 + \|\nabla_h(\boldsymbol{m}_{e,h}^\ell - \boldsymbol{m}_h^\ell)\|_2 = \mathcal{O}(k^2+h^2)$, $\ell = 0,1$, *and* $k \le \mathcal{C}h$.
Then the following convergence result holds as h and k goes to zero:

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

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

Idea of the proof

$$
\begin{array}{ccccccccc}
 & & \|\tilde{\boldsymbol{e}}_h^2\|, \|\nabla_h \tilde{\boldsymbol{e}}_h^2\| & \searrow & \|\tilde{\boldsymbol{e}}_h^3\|, \|\nabla_h \tilde{\boldsymbol{e}}_h^3\| & \searrow & \|\tilde{\boldsymbol{e}}_h^4\|, \|\nabla_h \tilde{\boldsymbol{e}}_h^4\| & & \cdots \\
 & & \uparrow & & \uparrow & & \uparrow & & \\
\|\boldsymbol{e}_h^0\|, \|\nabla_h \boldsymbol{e}_h^0\| & \dashrightarrow & \|\boldsymbol{e}_h^1\|, \|\nabla_h \boldsymbol{e}_h^1\| & \dashrightarrow & \|\boldsymbol{e}_h^2\|, \|\nabla_h \boldsymbol{e}_h^2\| & \dashrightarrow & \|\boldsymbol{e}_h^3\|, \|\nabla_h \boldsymbol{e}_h^3\| & & \cdots
\end{array}
$$

Blue arrow (Lemma)
Red arrow (Discrete Gronwall Inequality)
Dashed arrow (Combine these terms)

Lemma

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

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

$$\|\boldsymbol{m}_h\|_\infty + \|\nabla_h \boldsymbol{m}_h\|_\infty \le M, \quad \|\tilde{\boldsymbol{m}}_h\|_\infty + \|\nabla_h \tilde{\boldsymbol{m}}_h\|_\infty \le M,$$

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

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

Verification of assumptions.

$$
\begin{aligned}
&|\tilde{\boldsymbol{m}}_h| \geq \frac{1}{2}, \quad \text{at a point-wise level,} \\
&\|\boldsymbol{m}_h\|_\infty + \|\nabla_h \boldsymbol{m}_h\|_\infty \leq M, \quad \|\tilde{\boldsymbol{m}}_h\|_\infty + \|\nabla_h \tilde{\boldsymbol{m}}_h\|_\infty \leq M, \\
&\|\boldsymbol{e}_h^n\|_\infty \leq \frac{1}{6}, \quad \|\nabla_h \boldsymbol{e}_h^n\|_\infty \leq \frac{1}{6}, \\
&\|\tilde{\boldsymbol{e}}_h^n\|_\infty \leq \frac{1}{6}, \quad \|\nabla_h \tilde{\boldsymbol{e}}_h^n\|_\infty \leq \frac{1}{6}.
\end{aligned}
$$

□

Outline

Numerical examples

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

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

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

k	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_\infty$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_2$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_{H^1}$
2.0D-2	4.990D-5	5.865D-5	1.060D-4
1.0D-2	1.262D-5	1.434D-5	2.666D-5
5.0D-3	3.167D-6	3.545D-6	6.762D-6
2.5D-3	7.927D-7	8.813D-7	1.699D-6
1.25D-3	1.983D-7	2.197D-7	4.257D-7
6.25D-4	4.961D-8	5.484D-8	1.065D-7
order	1.996	2.012	1.991

Example 2

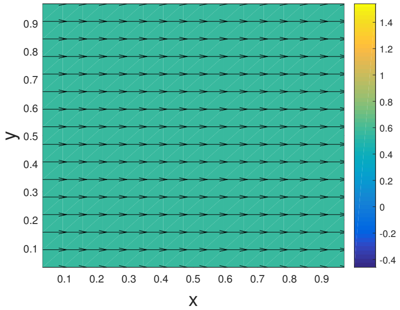
Table 3: Temporal accuracy of our method on the uniform mesh when $h = 5D-5$ and $\alpha = 0.01$.

k	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_\infty$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_2$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_{H^1}$
4.0D-2	5.778D-4	5.284D-4	0.00168
2.0D-2	1.456D-4	1.347D-4	4.095D-4
1.0D-2	3.652D-5	3.399D-5	1.010D-4
5.0D-3	9.147D-6	8.535D-6	2.523D-5
2.5D-3	2.287D-6	2.136D-6	6.640D-6
order	1.996	1.988	1.999

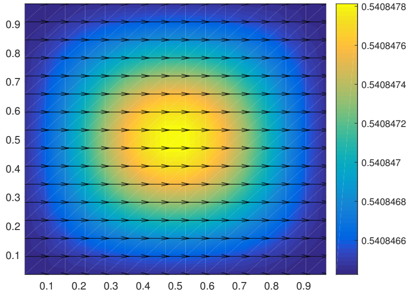
Table 4: Spatial accuracy of our method on the uniform mesh when $k = 1D-4$ and $\alpha = 0.01$.

h	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_\infty$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_2$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_{H^1}$
$1/3^2$	0.00546	0.00577	0.01336
$1/3^3$	6.101D-4	6.430D-4	0.0016
$1/3^4$	6.783D-5	7.147D-5	1.821D-4
$1/3^5$	7.536D-6	7.940D-6	2.038D-5
$1/3^6$	8.363D-7	8.811D-7	2.268D-6
order	1.999	2.000	1.978

Example 3



(a) Exact magnetization profile



(b) Numerical magnetization profile

Figure 4: Profiles of the exact and the numerical magnetization in the $xy-$plane with $z = 1/2$ when $k = 1/16$, $h_x = h_y = h_z = 1/16$, and $\alpha = 0.01$.

Table 5: Temporal accuracy in the 3-D case when $h_x = h_y = h_z = 1/16$ and $\alpha = 0.01$.

k	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_\infty$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_2$	$\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_{H^1}$
1/8	0.00360	0.00237	0.00233
1/16	9.983D-4	6.544D-4	6.612D-4
1/32	2.583D-4	1.691D-4	1.708D-4
1/64	6.256D-5	4.077D-4	4.164D-5
1/128	1.234D-5	7.846D-6	8.663D-6
order	2.047	2.059	2.018

Outline

Conclusion

What we have done

1. Several second-order semi-implicit schemes for LL equation;
2. Convergence analysis for one of the schemes.

To-do list

1. Benchmark problem from NIST (in progress);
2. Generalization of the technique for other implicit scheme;
3. Current-driven magnetization dynamics [Chen, Garcia-Cervera, and Yang, 2015].

Thank you for your attention!