Second-order Semi-implicit Projection Methods And Analysis for Micromagnetics Simulations

Changjian Xie

Department of Mathematics, National University of Singapore

Joint work with

Jingrun Chen (*USTC*)
Carlos García-Cervera (*UC, Santa Barbara*)
Cheng Wang (*University of Massachusetts*)
Zhennan Zhou (*Peking University*)

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Outline

1. Semi-implicit projection methods
2. Applications for micromagnetics simulations
3. Main theoretical results

Recording devices and computer storages

- MRAM, SRAM, DRAM, FLASH, FeRAM[1]

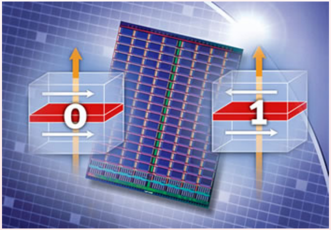
	MRAM	SRAM	DRAM	Flash	FeRam
Read Speed	Fast	Fastest	Medium	Fast	Fast
Write Speed	Fast	Fastest	Medium	Low	Medium
Array Efficiency	Med/High	High	High	Med/Low	Medium
Future Scalability	Good	Good	Limited	Limited	Limited
Cell Density	Med/High	Low	High	Medium	Medium
Non-Volatility	Yes	No	No	Yes	Yes
Endurance	Infinite	Infinite	Infinite	Limited	Limited
Cell Leakage	Low	Low/High	High	Low	Low
Low Voltage	Yes	Yes	Limited	Limited	Limited
Complexity	Medium	Low	Medium	Medium	Medium

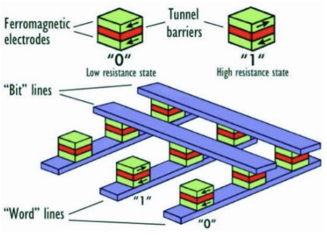
- MRAM: High speed performance; Infinite endurance; Non-volatility; Smaller size; Low-power consumption; Low cost.

[1] doi:10.20944/preprints201607.0093.v1

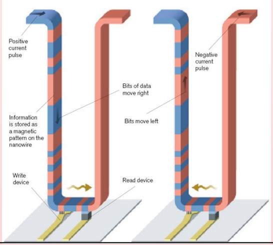
MRAM

- Spinvalues[2]





- Domain walls [3]



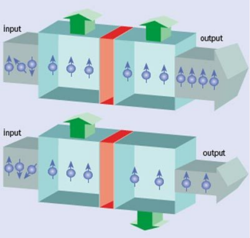
Racetrack memories

- Recording: Electric pulse 0 and 1, local magnetization;
- Reading: Inductive EMF 0 and 1, magnetoresistance effect.

[2] Science@Berkeley Lab: The Current Spin on Spintronics
[3] http://www2.technologyreview.com/article/412189/tr10-racetrack-memory/

Methodology for detecting the orientation

- Tunnel magnetoresistance [4]

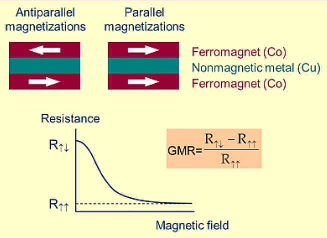


- Ferromagnetic electrode;
- Julliere's model:

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

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

- Gaint magnetoresistance [5]



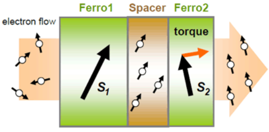
- Discovery: Albert Fert and Peter Grünberg: 2007 Nobel Prize in Physics;
- Application: Stuart Parkin (IBM);
- Explanation: Spin-polarized current (Mott theory);
- Capacity: $M \longrightarrow G$.

[4] http://ducthe.wordpress.com/category/spintronics/

[5] http://physics.unl.edu/

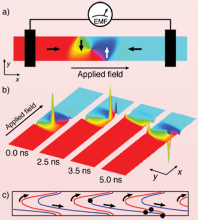
Methodology for rotating the orientation

- Spin transfer torque (Current induced magnetic switching) [6]



  - No applied magnetic field;
  - Utilizes heavily spin polarized current;

- Current-driven domain wall motion [7]



  - Applied current supplies spin transfer torques

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

Micromagnetics: statics

Basic quantity of interest:

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

Gibbs free energy functional:

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

Local minimizers of energy:

- $\boldsymbol{h}_s = 0, \boldsymbol{h}_e = 0$, $\min F_{LL}[m] \longleftrightarrow \underset{\longrightarrow}{\longrightarrow} 0, \ \underset{\longrightarrow}{\longleftarrow} 1;$
- Domain structure.

Dynamics: Landau-Lifshitz equation

- Torque balance and artificial dissipation

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

where

$$\boldsymbol{h} = -\frac{\delta F_{\mathrm{LL}}}{\delta \boldsymbol{m}} = -Q(m_2\boldsymbol{e}_2 + m_3\boldsymbol{e}_3) + \epsilon\Delta\boldsymbol{m} + \boldsymbol{h}_{\mathrm{s}} + \boldsymbol{h}_{\mathrm{e}}$$

- Model problem:

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

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

Literature review

Well-posedness: [Alouges and Soyeur, 1992; Guo and Hong, 1993; Carbou and Fabrie, 2001]

Numerics:

1. FEM: [Bartels and Prohl, 2006] and FDM: [E and Wang, 2001];
2. Linearity: Explicit by [Jiang et al., 2001]; Fully implicit by [Prohl, 2001]; Semi-implicit by [E and Wang, 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;

Outline

Semi-implicit projection methods (SIPM) [Xie, García-Cervera, Wang, Zhou, and Chen (2020)]

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

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

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

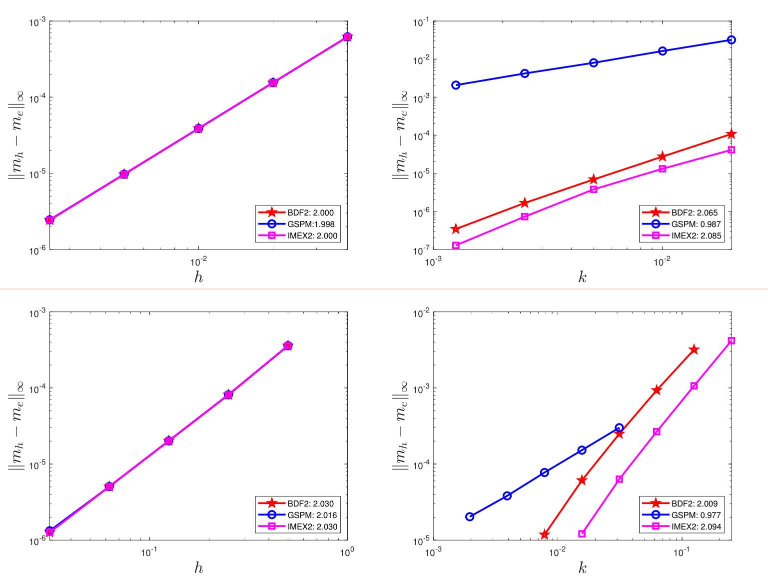
$$\frac{\frac{3}{2}\tilde{\boldsymbol{m}}_h^{n+2} - 2\boldsymbol{m}_h^{n+1} + \frac{1}{2}\boldsymbol{m}_h^n}{k} = -\hat{\boldsymbol{m}}_h^{n+2} \times \Delta_h \tilde{\boldsymbol{m}}_h^{n+2} - \alpha \hat{\boldsymbol{m}}_h^{n+2} \times \left(\hat{\boldsymbol{m}}_h^{n+2} \times \Delta_h \tilde{\boldsymbol{m}}_h^{n+2}\right);$$

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

Test: Accuracy

1D

3D



Test: Efficiency

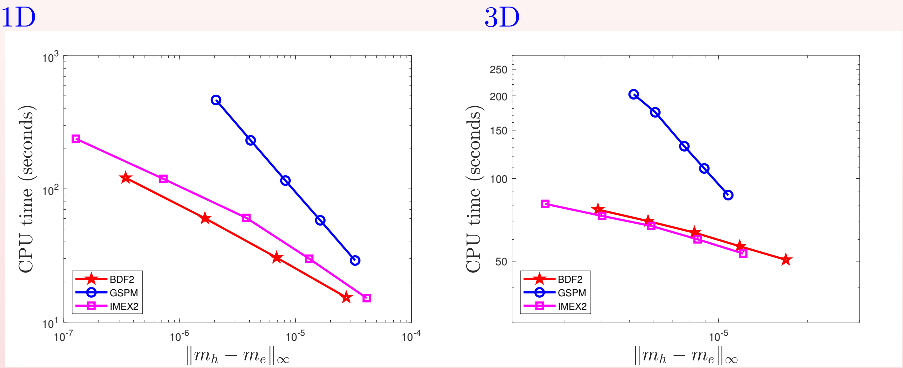


Figure 1: CPU time (in seconds) of BDF2, GSPM and IMEX2 versus error $\|\boldsymbol{m}_h - \boldsymbol{m}_e\|_\infty$. For a given tolerance of error, costs of: BDF2 $<$ IMEX2 $<$ GSPM in 1D (left); BDF2$\approx$ IMEX2$<$GSPM when $h_x = h_y = h_z = 1/16$ in 3D (right).

Outline

SIPM for micromagnetics

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

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

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

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

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

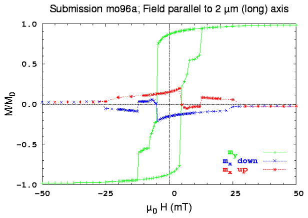
- $\boldsymbol{m}_t = -\boldsymbol{m} \times \boldsymbol{h} - \alpha \boldsymbol{m} \times (\boldsymbol{m} \times \boldsymbol{h})$:

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

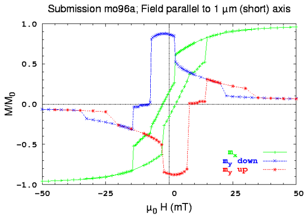
- A projection step: $\boldsymbol{m}_h^{n+2} = \frac{\tilde{\boldsymbol{m}}_h^{n+2}}{|\tilde{\boldsymbol{m}}_h^{n+2}|}$.

Hysteresis loop (Benchmark from NIST[8])

mo96a:

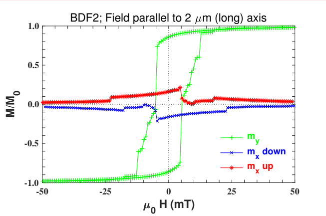


(a) $H_0//y\text{-}axis$

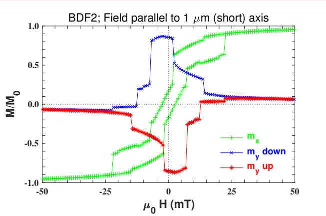


(b) $H_0//x\text{-}axis$

BDF2:



(c) $H_0//y\text{-}axis$



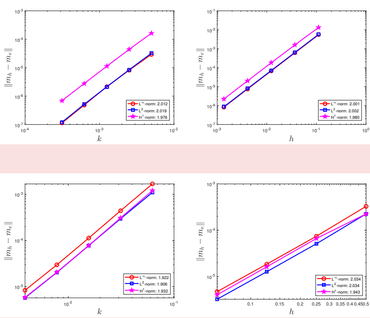
(d) $H_0//x\text{-}axis$

[8] https://www.ctcms.nist.gov/∼rdm/mumag.org.html

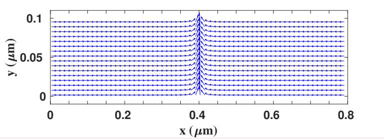
SIPM revisited

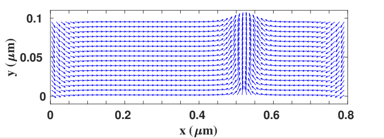
- Lack of numerical stability of Lax-Richtmyer type;
- Two sets of approximations $\tilde{\boldsymbol{m}}_h^n$ and $\boldsymbol{m}_h^n$;
- Separation of the time-marching step and the projection step:

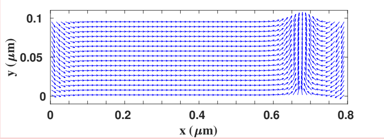
$$
\begin{aligned}
\frac{\frac{3}{2}\tilde{m}_h^{n+2} - 2\tilde{m}_h^{n+1} + \frac{1}{2}\tilde{m}_h^n}{k} &= -\hat{\boldsymbol{m}}_h^{n+2} \times \Delta_h \tilde{m}_h^{n+2} \\
&\quad - \alpha \hat{\boldsymbol{m}}_h^{n+2} \times (\hat{\boldsymbol{m}}_h^{n+2} \times \Delta_h \tilde{m}_h^{n+2}), \\
\hat{\boldsymbol{m}}_h^{n+2}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



Domain wall dynamics







Outline

1. Semi-implicit projection methods
2. Applications for micromagnetics simulations
3. Main theoretical results
   - Unconditional unique solvability
   - Optimal rate convergence analysis

Outline

Unconditional unique solvability

Theorem

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

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

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

are uniquely solvable.

Proof

Observe that

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

- 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;
- $|\lambda I - MS| = |\lambda I - MC^T C| = |\lambda I - CMC^T|$;
- $(CMC^T)^T = -CMC^T$;
- $\det(\frac{3}{2} I_h - A) \neq 0$.

Cont'd ...

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

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

and

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

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

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

Cont'd ...

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

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

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

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.

Outline

Optimal rate convergence analysis [Chen, Wang and Xie (2021)]

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

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

- $\tilde{\boldsymbol{e}}_h^n = \underline{\boldsymbol{m}}_h^n - \tilde{\boldsymbol{m}}_h^n, \quad \boldsymbol{e}_h^n = \underline{\boldsymbol{m}}_h^n - \boldsymbol{m}_h^n$, $k \le \mathcal{C}h$;
- $(*)$ $\|\boldsymbol{e}_h\|_2 \le 2\|\tilde{\boldsymbol{e}}_h\|_2 + \mathcal{O}(h^2), \ \|\nabla_h \boldsymbol{e}_h\|_2 \le \mathcal{C}(\|\nabla_h \tilde{\boldsymbol{e}}_h\|_2 + \|\tilde{\boldsymbol{e}}_h\|_2) + \mathcal{O}(h^2)$;

$$
\begin{aligned}
\frac{\frac{3}{2}\tilde{\boldsymbol{e}}_h^{\ell+2} - 2\tilde{\boldsymbol{e}}_h^{\ell+1} + \frac{1}{2}\tilde{\boldsymbol{e}}_h^{\ell}}{k} = & -\left(2\boldsymbol{m}_h^{\ell+1} - \boldsymbol{m}_h^{\ell}\right) \times \Delta_h \tilde{\boldsymbol{e}}_h^{\ell+2} - \left(2\boldsymbol{e}_h^{\ell+1} - \boldsymbol{e}_h^{\ell}\right) \times \Delta_h \underline{\boldsymbol{m}}_h^{\ell+2} \\
& - \alpha\left(2\boldsymbol{m}_h^{\ell+1} - \boldsymbol{m}_h^{\ell}\right) \times \left((2\boldsymbol{m}_h^{\ell+1} - \boldsymbol{m}_h^{\ell}) \times \Delta_h \tilde{\boldsymbol{e}}_h^{\ell+2}\right) \\
& - \alpha\left(2\boldsymbol{m}_h^{\ell+1} - \boldsymbol{m}_h^{\ell}\right) \times \left((2\boldsymbol{e}_h^{\ell+1} - \boldsymbol{e}_h^{\ell}) \times \Delta_h \underline{\boldsymbol{m}}_h^{\ell+2}\right) \\
& - \alpha\left(2\boldsymbol{e}_h^{\ell+1} - \boldsymbol{e}_h^{\ell}\right) \times \left((2\underline{\boldsymbol{m}}_h^{\ell+1} - \underline{\boldsymbol{m}}_h^{\ell}) \times \Delta_h \underline{\boldsymbol{m}}_h^{\ell+2}\right) + \tau^{\ell+2}
\end{aligned}
$$

- Inner product $\tilde{\boldsymbol{e}}_h^{\ell+2}$, $-\Delta_h \tilde{\boldsymbol{e}}_h^{\ell+2}$, using $(*)$ and discrete Gronwall ineq.;
- $\|\tilde{\boldsymbol{e}}_h^n\|_2 + \|\nabla_h \tilde{\boldsymbol{e}}_h^n\|_2 \le \mathcal{C}(k^2 + h^2) \xrightarrow{(*)} \|\boldsymbol{e}_h^n\|_2 + \|\nabla_h \boldsymbol{e}_h^n\|_2 \le \mathcal{C}(k^2 + h^2)$;
- To guarantee the assumptions in the recursive demonstration.

Sketch of the proof

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

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

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

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

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

Then

$$\boldsymbol{m}_e(\hat{x}_i, \hat{y}_j, \hat{z}_0) = \boldsymbol{m}_e(\hat{x}_i, \hat{y}_j, \hat{z}_1) - \frac{h^3}{24} \partial_z^3 \boldsymbol{m}_e(\hat{x}_i, \hat{y}_j, 0) + \mathcal{O}(h^5),$$

$$\boldsymbol{m}^{(1)}(\hat{x}_i, \hat{y}_j, \hat{z}_0) = \boldsymbol{m}^{(1)}(\hat{x}_i, \hat{y}_j, \hat{z}_1) + \frac{h}{24} \partial_z^3 \boldsymbol{m}_e(\hat{x}_i, \hat{y}_j, 0) + \mathcal{O}(h^3),$$

$$\underline{\boldsymbol{m}}(\hat{x}_i, \hat{y}_j, \hat{z}_0) = \underline{\boldsymbol{m}}(\hat{x}_i, \hat{y}_j, \hat{z}_1) + \mathcal{O}(h^5),$$

$$\Delta_h \underline{\boldsymbol{m}}_{i,j,k} = \Delta \boldsymbol{m}_e(\hat{x}_i, \hat{y}_j, \hat{z}_k) + \mathcal{O}(h^2), \quad \forall 1 \le i, j, k \le N.$$

Step 2: Error function evolution system for

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

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

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

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

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

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

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

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

- Combination of both

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

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*

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

- Using the Lemma

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

- Discrete Gronwall inequality

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

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

Lemma

Assume the numerical error function:

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

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

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

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

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

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

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

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

- Convergence estimate for e_h^n:

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

Verification of assumptions.

$$|\tilde{m}_h| \ge \frac{1}{2}, \quad \text{at a point-wise level},$$
$$\|m_h\|_\infty + \|\nabla_h m_h\|_\infty \le M, \quad \|\tilde{m}_h\|_\infty + \|\nabla_h \tilde{m}_h\|_\infty \le M,$$
$$\|e_h^n\|_\infty \le \frac{1}{6}, \quad \|\nabla_h e_h^n\|_\infty \le \frac{1}{6},$$
$$\|\tilde{e}_h^n\|_\infty \le \frac{1}{6}, \quad \|\nabla_h \tilde{e}_h^n\|_\infty \le \frac{1}{6}.$$

□

Summary

What we have done

1. Two second-order semi-implicit schemes for LL equation;
2. Application to 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