Precession Axis Modification to a Semi-analytical Landau-Lifshitz Solution Technique

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Background

- For fixed $H$, the Landau-Lifshitz equation

$$\frac{dm}{dt} = \frac{|\gamma|}{1 + \alpha^2} H \times m + \frac{\alpha |\gamma|}{1 + \alpha^2} m \times H \times m$$ (1)

has analytical solution.

- In spherical coordinates based on $H$ and initial $m$,

$$\phi(t) = |\gamma H| t$$ (2)

$$\theta(t) = 2 \tan^{-1}(\tan(\frac{\theta(0)}{2}) \exp(-|\alpha \gamma H| t))$$ (3)

- While $H$ remains fixed, exact trajectory $m(t)$ can be computed for any time step.
Semi-analytical Solution Technique

- Apply analytical solution only over time steps small enough that fixed $H$ assumption remains an acceptable approximation.
- Computed trajectories satisfy $|m| = 1$.
- No renormalization scheme required.
- Naturally avoids errors in energy computations, dissipation rates, etc. that renormalization schemes can introduce.
- Semi-analytical step extends to predictor-corrector scheme.

Limitations

- $H$ is a function of $m$; varies over simulation time scales.
- When exchange or demagnetization dominates, $H$ is expected to vary at same rate as $m$.
- Semi-analytical technique only valid for small time steps
Landau-Lifshitz Analysis

• In LLG, $H$ appears only as part of $H \times m$

$$\frac{dm}{dt} = \frac{|\gamma|}{1 + \alpha^2} H \times m + \frac{\alpha|\gamma|}{1 + \alpha^2} m \times H \times m.$$  \hspace{1cm} (4)

• Torque $T = H \times m$ drives the equation, not field.

• Changes to field that preserve torque, preserve LLG solution.

• Consider adding any scalar multiple of $m$ to $H$

$$\tilde{H} = H + \lambda m$$  \hspace{1cm} (5)

• Compute torque

$$\tilde{T} = \tilde{H} \times m = H \times m + \lambda m \times m$$  \hspace{1cm} (6)

$$= H \times m = T.$$  \hspace{1cm} (7)

• Modified $\tilde{H}$ computes same torque; same LLG solutions.
Axis Modification

- Freedom to choose $\tilde{H}$
- What choice for $\tilde{H}$ best suits semi-analytical step?
- Value of $\lambda$ determines direction of $\tilde{H}$.
- Select $\lambda$ value equivalent to select axis direction, $a$.
- For long time steps, want single fixed $\tilde{H}$ suitable for all $m \in \Omega$, in a neighborhood of a long trajectory segment.
\[ a = T_0 \times T_1 \]

- \( \tilde{H} / \| \tilde{H} \| \) independent of \( m \in \Omega \)
- \( \implies \tilde{H} \parallel T_0 \times T_1 \) for any \( m_1, m_2 \) in \( \Omega \).
Modified Axis Semi-analytical Algorithm

• From current value of \( m \), compute current \( H \).

• Use current and past torque values (\( T \) and \( T_{\text{past}} \)) to determine axis \( a \).

• From \( m \) and \( H \), compute \( (m \times H \times m) \).

• Solve \( \tilde{H} = \beta a = H + \lambda m \); see figure below.

• Take semi-analytical step based on \( \tilde{H} \).

• Extend this semi-analytical foundation to predictor-corrector scheme.
\[ H \cdot (m \times H \times m) = \beta a \cdot (m \times H \times m) \]

\[ \beta = \frac{H \cdot (m \times H \times m)}{a \cdot (m \times H \times m)} \]
Coupled Two-spin System
Comparison Results

- Simulate two-spin system with several energy terms.
  - Exchange ($A = 13 \text{nJ/m}; \Delta = 5 \text{ nm}$)
  - Demag ($M = 800 \text{kA/m}$)
  - Cubic Anisotropy ($K = 57 \text{ kJ/m}^3$)
- Compute trajectories for $\alpha = 0.01$ over $10 \text{ ps}$ interval.
- Compute with three solvers
  - Baseline solution via 5/4 Runge-Kutta-Fehlberg
    - Time steps reduced to achieve converged solution
  - Original semi-analytical predictor corrector
  - Modified axis semi-analytical predictor corrector
- Plot error at $t = 10 \text{ ps}$ against time step.
Error at $t = 10$ ps

Time step (fs)
Comparison Results

- Axis corrected solver achieves...
  - ...order of magnitude less error at the same time step.
  - ...same error magnitude with three times longer time steps.
- Both semi-analytical solvers exhibit second order convergence.
  - Suitable for adjustable time step algorithms
Adjustable Time Step Comparison

- Another two-spin system.
- Zeeman energy added.
- Simulation over 5 ns duration.
- Baseline solution computed by the Runge-Kutta-Fehlberg solver with 1 fs time step.
- Both semi-analytical solvers compute solutions within $2 \times 10^{-6}$ relative error.
- Original semi-analytical solver time steps all $< 2$ fs.
- Axis corrected solver reaches time step $> 200$ fs.
- Overall thirty times less computation.
Exchange-only Analysis

- Consider two-spin system with only exchange energy.
- Effective field:
  \[ H_1 = \frac{2A}{\mu_0 M \Delta^2} m_2. \]  
  \[ (8) \]
- Axis-corrected field:
  \[ \tilde{H} = \tilde{H}_1 = \tilde{H}_2 = \frac{2A}{\mu_0 M \Delta^2} (m_1 + m_2). \]  
  \[ (9) \]
- Time-evolution of axis-corrected field:
  \[ \frac{d\tilde{H}}{dt} = \frac{2A}{\mu_0 M \Delta^2} \left( \frac{dm_1}{dt} + \frac{dm_2}{dt} \right) \]  
  \[ = \frac{4A^2 \alpha \gamma}{(\mu_0 M \Delta^2)^2} \sin(\theta) \tan(\frac{\theta}{2}) \frac{m_1 + m_2}{2}, \]  
  \[ (11) \]
Exchange-only Analysis

- Both $\tilde{H}$ and $d\tilde{H}/dt$ in fixed direction $(m_1 + m_2)$.
- Two spins precess around common, fixed axis, synchronized opposite each other.
- For $\alpha > 0$, $|\tilde{H}|$ increases to a limit.
- Thus precession frequency also increases to a limit:

$$f_{\text{max}} = \frac{2A|\gamma|}{\pi \mu_0 M \Delta^2}.$$  \hspace{1cm} (12)

- For smaller $\Delta$
  - Precession frequency increases.
  - Precession period decreases.
  - Small time steps to represent precession.
Summary

- LLG driven by torque, not field.
- Field axis may be chosen to serve computing needs.
- Axis corrected version of semi-analytical solver more efficiently solves LLG when strong coupling undermines fixed $H$ assumption.
- Semi-analytical solvers have second order convergence.
- Semi-analytical solvers support adjustable time step algorithm.
- Analysis of exchange-only two-spin system suggests finer spatial resolution may force smaller time steps.