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

Don Porter

Mike Donahue

Mathematical & Computational Sciences Division

Information Technology Laboratory

National Institute of Standards and Technology

Gaithersburg, Maryland

Background

- For fixed H, the Landau-Lifshitz equation

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

  has analytical solution.

- In spherical coordinates based on H and initial m,

$$\phi(t) = |\gamma H| t \tag{2}$$

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

- 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.

Ben Van de Wiele, Femke Olyslager, and Luc Dupré, “Fast semianalytical time integration schemes for the Landau-Lifshitz equation”, *IEEE Trans. Magn.*, vol. 43, no. 6, pp. 2917–2919, June 2007.

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 $H \times m$

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

- 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

$$\tilde{H} = H + \lambda m \tag{5}$$

- Compute torque

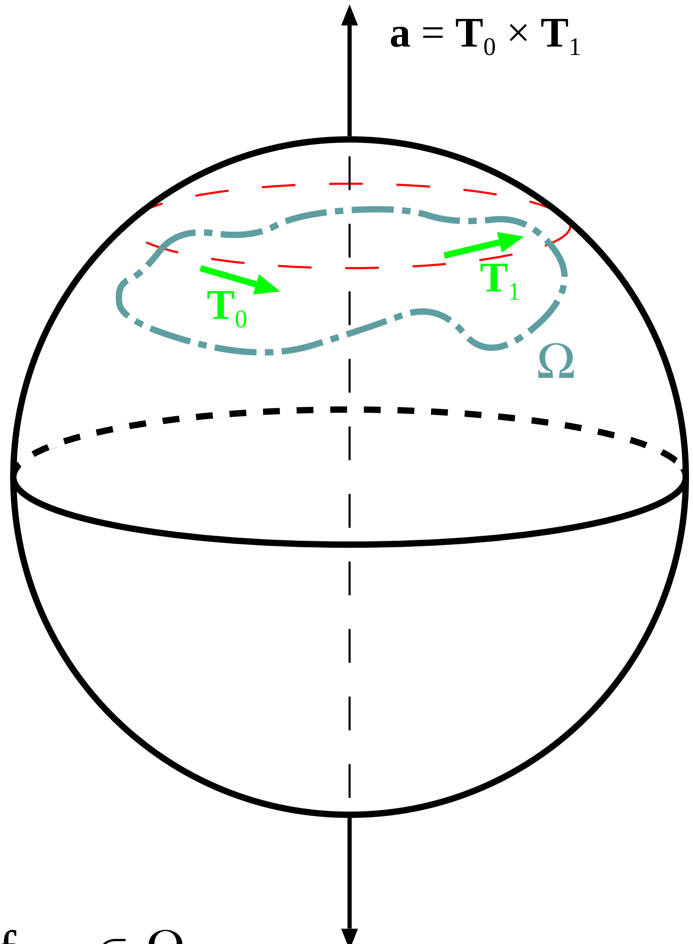
$$\tilde{T} = \tilde{H} \times m = H \times m + \lambda m \times m \tag{6}$$

$$= H \times m = T. \tag{7}$$

- Modified $\tilde{H}$ computes same torque; same LLG solutions.

Axis Modification

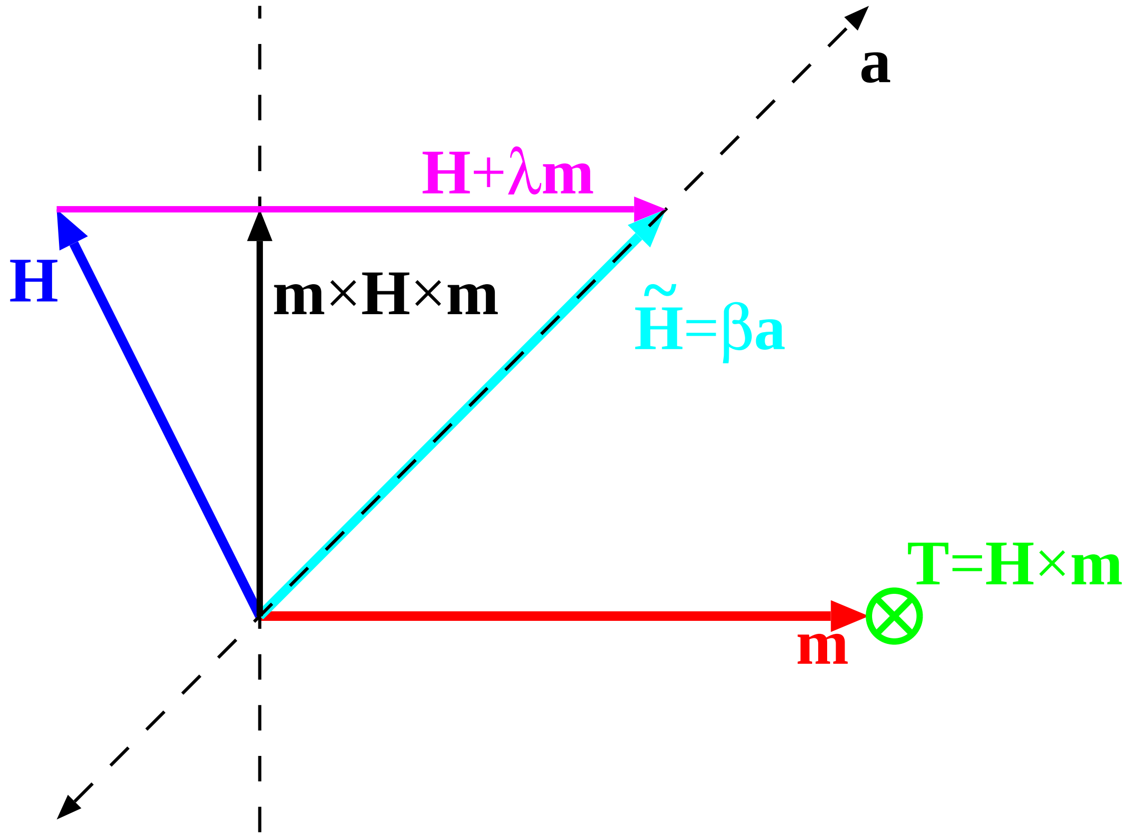
- Freedom to choose $\tilde{H}$
- What choice for $\tilde{H}$ best suits semi-analytical step?
- Value of λ determines direction of $\tilde{H}$.
- Select λ value equivalent to select axis direction, a.
- For long time steps, want single fixed $\tilde{H}$ suitable for all $m \in \Omega$, in a neighborhood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



- $\tilde{H}/\|\tilde{H}\|$ independent of $m \in \Omega$
- $\Longrightarrow \tilde{H} \parallel T_0 \times T_1$ for any m_1, m_2 in Ω.

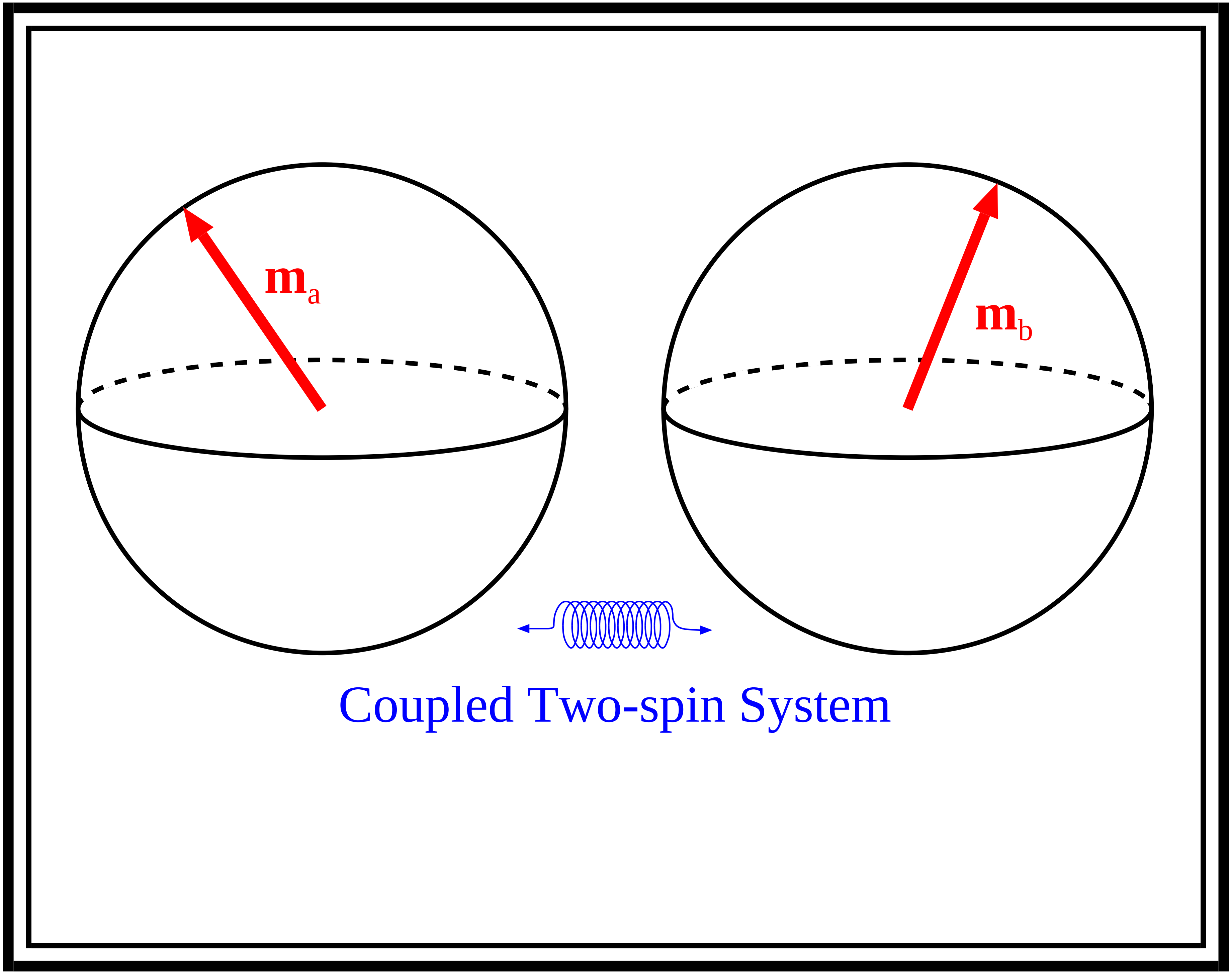
Modified Axis Semi-analytical Algorithm

- From current value of m, compute current H.
- Use current and past torque values (T and T_{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.



$$\mathbf{H} \cdot (\mathbf{m} x \mathbf{H} x \mathbf{m}) = \beta \mathbf{a} \cdot (\mathbf{m} x \mathbf{H} x \mathbf{m})$$

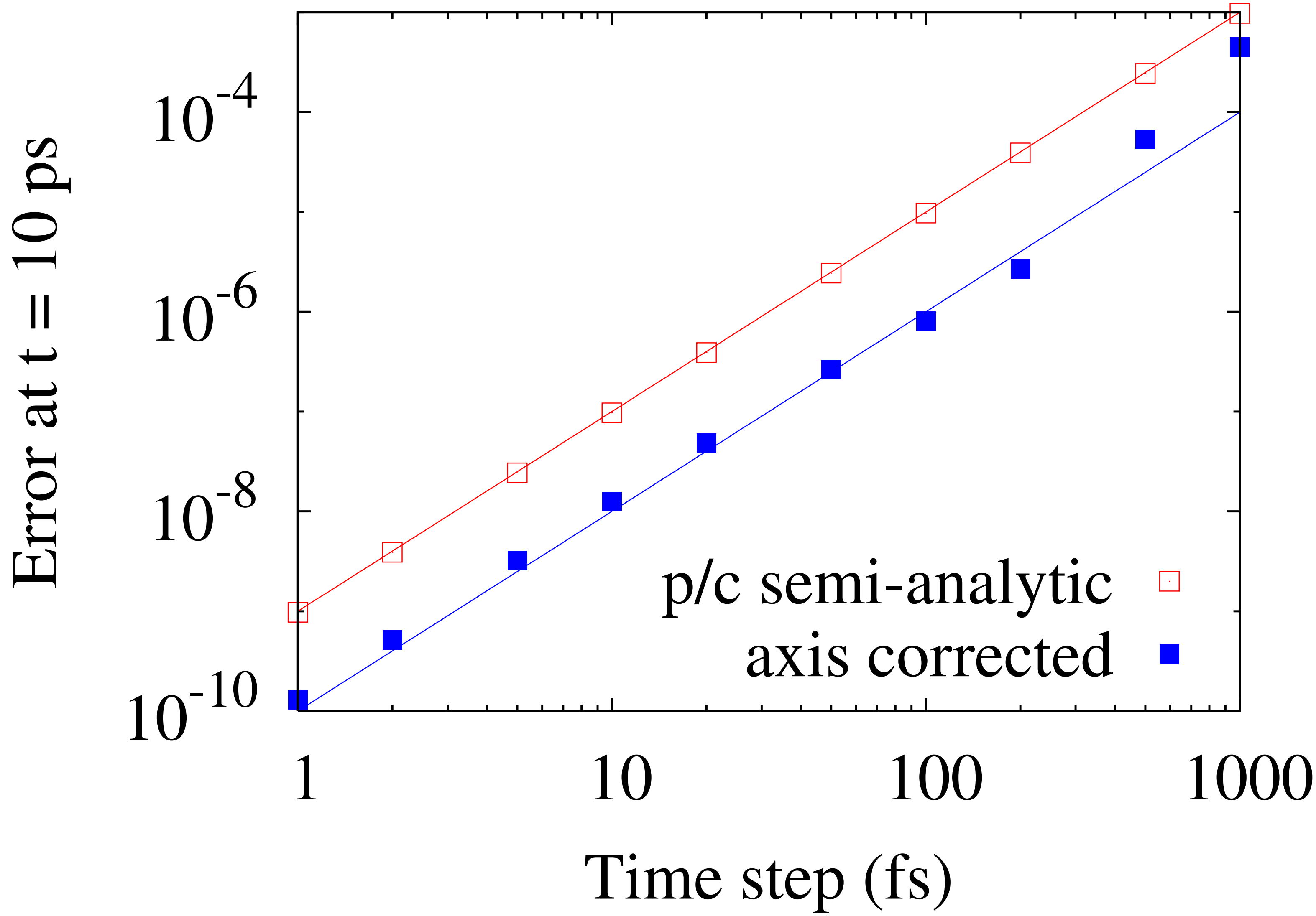
$$\longrightarrow \quad \beta = \mathbf{H} \cdot (\mathbf{m} x \mathbf{H} x \mathbf{m}) \,/\, \mathbf{a} \cdot (\mathbf{m} x \mathbf{H} x \mathbf{m})$$



$\mathbf{m}_a$
$\mathbf{m}_b$
Coupled Two-spin System

Comparison Results

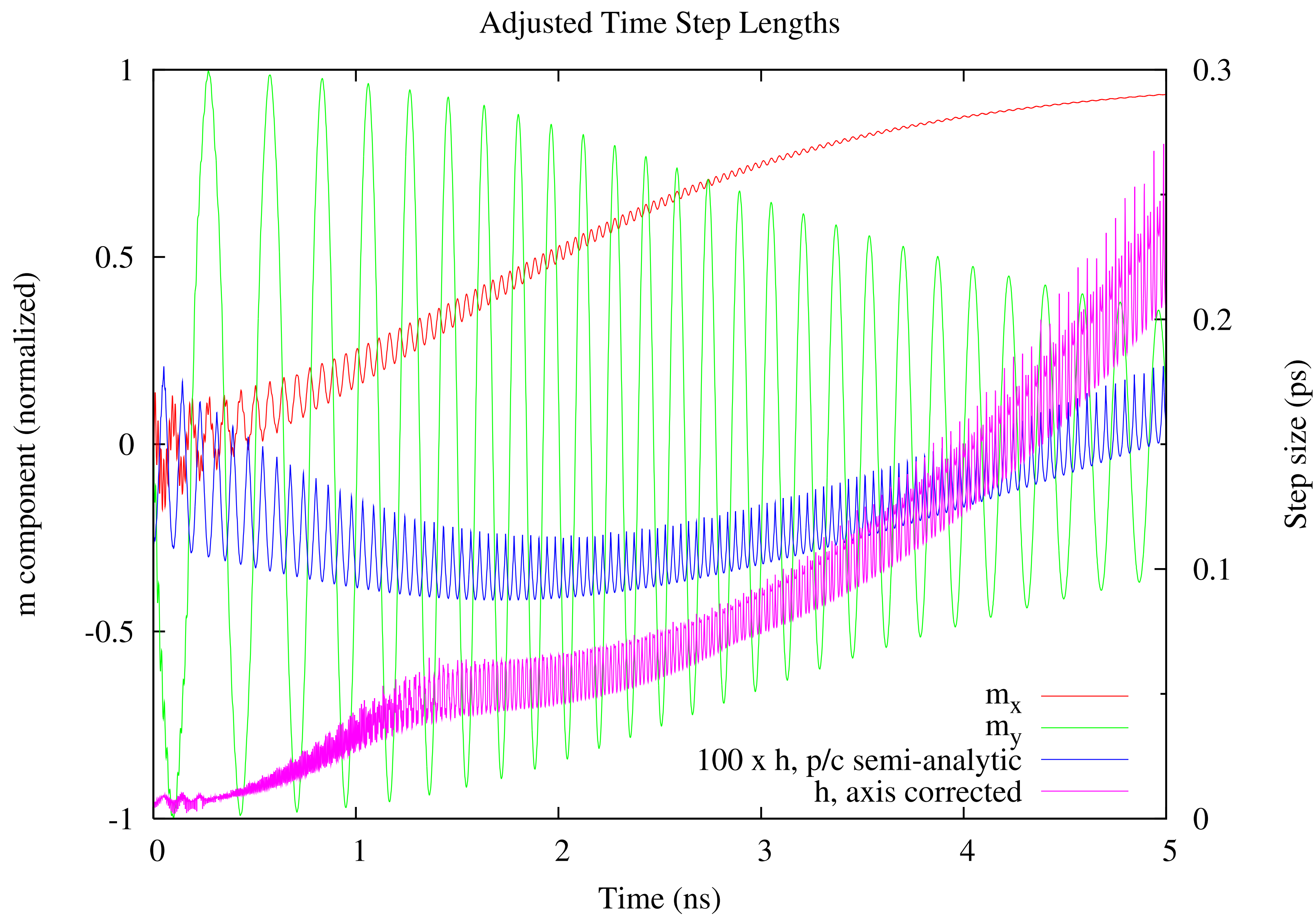
- Simulate two-spin system with several energy terms.
  - Exchange ($A = 13$ nJ/m; $\Delta = 5$ nm)
  - Demag ($M = 800$ kA/m)
  - Cubic Anisotropy ($K = 57$ kJ/m^3)
- Compute trajectories for $\alpha = 0.01$ over 10 ps interval.
- Compute with three solvers
  - Baseline solution via 5/4 Runge-Kutta-Fehlberg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



Error at t = 10 ps
10^{-4}
10^{-6}
10^{-8}
10^{-10}
1
10
100
1000
Time step (fs)
p/c semi-analytic
axis corrected

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



Adjusted Time Step Lengths
m component (normalized)
Step size (ps)
Time (ns)
1
0.5
0
-0.5
-1
0.3
0.2
0.1
0
1
2
3
4
5
m_x
m_y
100 x h, p/c semi-analytic
h, axis corrected

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 2×10^{-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:

$$H_1 = \frac{2A}{\mu_0 M \Delta^2} m_2. \tag{8}$$

- Axis-corrected field:

$$\tilde{H} = \tilde{H}_1 = \tilde{H}_2 = \frac{2A}{\mu_0 M \Delta^2}(m_1 + m_2). \tag{9}$$

- Time-evolution of axis-corrected field:

$$\frac{d\tilde{H}}{dt} = \frac{2A}{\mu_0 M \Delta^2}(\frac{dm_1}{dt} + \frac{dm_2}{dt}) \tag{10}$$

$$= \frac{4A^2\alpha|\gamma|}{(\mu_0 M \Delta^2)^2} \sin(\theta)\tan(\frac{\theta}{2})\frac{m_1 + m_2}{2}, \tag{11}$$

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:

$$f_{\max} = \frac{2A|\gamma|}{\pi \mu_0 M \Delta^2}. \tag{12}$$

- For smaller Δ
  - 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.