Exploiting Effective Field Time Derivative Information to ImproveAccuracy of <sup>a</sup> Norm-preservingLandau-Lifshitz Solver

> Donald G. PorterMichael J. Donahue

NIST, Gaithersburg, Maryland, USA

### Background

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

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

has analytical solution.

 $\bullet\,$  In spherical coordinates based on  $H$  and initial  $m,$ 

$$
(2) \qquad \phi(t) \quad = \quad |\gamma H|t \qquad \qquad \alpha
$$

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

<span id="page-1-1"></span><span id="page-1-0"></span>• 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 enoughthat fixed  $H$  assumption remains an acceptable approximation.
- •• Computed trajectories satisfy  $|m|=1$ .
- •No renormalization scheme required.
- • Naturally avoids errors in energy computations, dissipationrates, 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 timeintegration 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 demagnetizationdominates,  $H$  is expected to vary at same<br>rote as  $\infty$ rate as  $m_{\rm \scriptscriptstyle I}$
- • Semi-analytical technique only valid for small time steps

Predictor/corrector using  $dH/dt$ 

ldea: Use  $\dot{H}_0$  $_{\rm 0}$  to produce time-varying estimate  $H(t).$ 

**Step 1a:** Compute  $H_0$  and  $\dot{H}_0$  $_0$  at  $m_0.$ 

 ${\bf Step~1b:}$  Compute  $m_1$  along  ${\bf sph}$ estimate  $H(t)=H_0+t\dot{H}_0.$  $_{\rm 1}$  along sphere using linear

 $\operatorname{\mathbf{Step}}{}$  **1c:** Compute  $H_1$  $\frac{1}{1}$  at  $m_1$ .



Predictor/corrector using  $dH/dt$ 

**Step 2a:** Fit quadratic estimate $H(t)=H_0+t\dot{H}_0+ct^2$  where  $c=$  $\sqrt{ }$  $H_1-\,$  $\left(\begin{array}{c}\right)$  $H_0+t$  $t_1\dot H$  $\begin{bmatrix} 0 \end{bmatrix}$   $\begin{bmatrix} t \end{bmatrix}$ 21.

**Step 2b:** Compute  $m_{\text{final}}$  using quadratic  $H(t)$ estimate.

The resulting method is 3rd order in  $\Delta t.$ 



**Computation of** 
$$
dH/dt
$$

\n
$$
H_i^{\text{demag}} = -\sum_j N_{ij} m_j \qquad \dot{H}_i^{\text{demag}} = -\sum_j N_{ij} m_j
$$
\n
$$
H_i^{\text{exch}} = \frac{2A}{\mu_0 M_s \Delta^2} \sum_{j \in \mathcal{N}_i} m_j \qquad \dot{H}_i^{\text{exch}} = \frac{2A}{\mu_0 M_s \Delta^2} \sum_{j \in \mathcal{N}_i} m_j
$$
\n
$$
H_i^{\text{anis}} = \frac{2K_1}{\mu_0 M_s} (m_i \cdot u_i) u_i \qquad \dot{H}_i^{\text{anis}} = \frac{2K_1}{\mu_0 M_s} (m_i \cdot u_i) u_i
$$
\n
$$
H^{\text{Zeeman}} = ? \qquad \dot{H}^{\text{Zeeman}} = \dot{?} \text{ (often 0)}
$$
\n**Notes:**  $\dot{m}$  is given by (1). Computational cost for

\n
$$
dH/dt
$$
 similar to cost for  $H$ .

Coupled Two-spin System (Includes exchange, demag, Zeeman, $\mathbf{m}_{\scriptscriptstyle\rm a}$  $\mathbf{m}_{\text{b}}$ and cubic anisotropy energies)



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## Summary: Two spin system

- •• LLG has been integrated on the sphere using  $H_0$ ,  $\dot{H}_0$ , and  $H_1$ .
- •• Computing  $\dot{H}_0$  $\overline{\phantom{a}}_0$  costs similar to computing  $H_0.$
- • Proposed predictor/corrector method is 3rdorder in  $\Delta t.$
- • On 2-spin test, proposed method yields smaller errors than 4th order Runge-Kutta forreasonable  $\Delta t.$

# Summary: Multi-spin test

- •• Smaller cells require smaller  $\Delta t$  to reach stable regime.
- •• In stable regime, integration error depends on  $\Delta t$  but not cellsize.
- •• Stability critical  $\Delta t$  for 4th order RK is 4 times larger than for 2nd order RK.
- • The semi-analytic methods have goodstability characteristics.