A practical guide to solving the stochastic Landau-Lifshitz-Gilbert-Slonczewski equation for macrospin dynamics

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Abstract

In this paper, we discuss the accuracy and complexity of various numerical techniques to solve the stochastic Landau-Lifshitz-Gilbert-Slonczewski (s-LLGS) equation. The s-LLGS equation is widely used by researchers to study the temporal evolution of the macrospin subject to spin torque and thermal noise. The numerical simulation of the s-LLGS equation requires an appropriate choice of stochastic calculus and the numerical integration scheme. In this paper, we focus on implicit midpoint, Heun, and Euler-Heun methods that converge to the Stratonovich solution of the s-LLGS equation. We also demonstrate a new method intended to solve stochastic differential equations (SDEs) with small noise, and test its capability to handle the s-LLGS equation. The choice of specific stochastic calculus while solving SDEs determines which numerical integration scheme to use. In this sense, methods, such as Euler and Gear, which are typically used by SPICE-based circuit simulators do not yield the expected outcome when solving the Stratonovich s-LLGS equation. While the trapezoidal method in SPICE does solve for the Stratonovich solution, its accuracy is limited by the minimum time-step of integration in SPICE. Through several numerical tests, including path-wise error, preservation of the magnetization norm, and 50\% magnetization reversal boundary of the macrospin, we clearly illustrate the accuracy of various numerical schemes for solving the s-LLGS equation. The results in this paper will serve as guidelines for researchers to understand the tradeoffs between accuracy and complexity of various numerical methods and the choice of appropriate calculus to handle SDEs.

1. Introduction

Within the macrospin approximation\textsuperscript{[1]}, the evolution of the magnetization vector, $M$, of a nanomagnet under the effects of spin-transfer torque (STT)\textsuperscript{[2]–[6]} and thermal noise is given by the s-LLGS equation

$$\frac{dM}{dt} = -\gamma \mu_0 (M \times H_{\text{eff}}) + \frac{\alpha}{M_s} (M \times \frac{dM}{dt}) - \frac{M \times (M \times I_s)}{q N_s M_s} - \beta \frac{M \times I_s}{q N_s},$$

(1)

where $H_{\text{eff}}$ is the effective field experienced by the nanomagnet, $\alpha$ is the dimensionless Gilbert damping constant, $M_s$ is the saturation magnetization, $I_s$ is the applied spin current, $q$ is the electron charge, $\beta$ is the field-like torque (FLT)\textsuperscript{[7]–[10]} factor, $N_s$ is the number of spins given as $N_s = \frac{2M_s V}{\gamma \hbar}$, and $V$ is the volume of the nanomagnet.

The first term on the right hand side (RHS) in (1) is the conservative precessional torque that governs the precession of the magnetization vector around the effective field acting on the nanomagnet. This effective field comprises the magnetocrystalline anisotropy field, the shape anisotropy field, and the external applied field. A Langevin field $h_r = h_x \hat{x} + h_y \hat{y} + h_z \hat{z}$, representing gaussian white noise, is added into the effective field in the s-LLGS equation to model thermal noise. The second term on the RHS in (1) is the Gilbert damping torque, which is responsible for damping the precessions of the magnetization vector, and eventually relaxing it to one of its stable states\textsuperscript{[11]}. The third term on the RHS in (1) is the Slonczewski spin torque arising from the deposition of spin angular momentum by the itinerant electrons of the spin-polarized current. The final term is the FLT resulting from the non-equilibrium spin accumulation in the nanomagnet, where the transverse component of spin current may persist with

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a characteristic length of a few angstroms or nanometers.

For analysis in this paper, we transform (1) into its dimensionless form expressed as

\[
\frac{dm}{dt} = -m \times h_{eff} + \alpha \left( m \times \frac{dm}{dt} \right) - m \times (m \times i_s) - \beta (m \times i_s), \tag{2}
\]

where we have the normalized quantities \( m = \frac{M}{M_s}, \) \( h_{eff} = \frac{H_{eff}}{H_c}, \) and \( i_s = \frac{I}{T}. \) Here, we define the current scale \( I = q \gamma \mu_0 M_s N_s. \) Also we consider a new time scale \((\gamma \mu_0 M_s)^{-1}. \) The advantages of the normalized equation (2) over (1) are (a) that it is easier to deal with normalized quantities and (b) normalized entities are mathematically well behaved under the application of a numerical scheme. The explicit decoupled form of (2) is given as (See Appendix A for derivations)

\[
\frac{dm}{dt} = -\frac{1}{1 + \alpha^2} \left[ m \times h_{eff} + (1 + \alpha \beta)(m \times (m \times i_s)) + (m \times (m \times h_{eff}) - \alpha m \times i_s) \right]. \tag{3}
\]

While we implement the FLT in our solver, the simulation results presented in this paper are reported for \( \beta = 0, \) unless otherwise stated. Our research leverages prior works [12–14], but presents a comprehensive treatment of the interplay of thermal noise and the deterministic macrospin dynamics. In this context, we clarify the differences in various numerical schemes and the impact of time-step to numerically integrate the s-LLGS equation.

The remainder of this paper is organized as follows. Section 2 describes the formulation of the effective field. The details underlying the midpoint method are presented in Section 3. In Section 4, the accuracy of various numerical methods, including a method for small noise, is validated. The accuracy analysis of the implicit midpoint method to the results from SPICE solvers and the NIST-standard micromagnetic tool OOMMF. Section 5 concludes the paper by comparing the results of the treatment of the interplay of thermal noise and the deterministic macrospin dynamics.

2. Effective Field

2.1. Model of the effective field

To arrive at the expression for the effective field in the s-LLGS equation, we consider the following energies, per unit volume, in the energy landscape of the macrospin: \([15–18]\):

1. Zeeman energy due to an externally applied field, \( E_{\text{zeeman}} = -\mu_0 (H_{\text{app}} \cdot M), \)
2. Uniaxial anisotropy energy, \( E_{\text{uniaxial}} = -K_u \cos^2 \theta, \)
3. Shape anisotropy energy, \( E_{\text{shape}} = \frac{1}{2} \mu_0 (N_s M_s^2 + N_y M_y^2 + N_z M_z^2), \)
4. Thermal energy, \( E_T. \)

In the above set of equations, \( H_{\text{app}} \) is the external magnetic field, \( K_u \) is the uniaxial energy density, \( \theta \) is the angle between the easy axis and the magnetization \((\cos \theta = \hat{n} \cdot m = \hat{n} \cdot \frac{M}{M_s}), \) and \( N_s, N_y, \) and \( N_z \) are the geometry-dependent demagnetization coefficients of the nanomagnet. In this treatment, we will consider the (normalized) thermal field \( h_T \) due to the thermal energy \( E_T \) separately at the the end.

The total energy of the macrospin (excluding the thermal energy) is

\[
E_{\text{total}} = V \left[ E_{\text{zeeman}} + E_{\text{uniaxial}} + E_{\text{shape}} \right] = V \left[ -\mu_0 (H_{\text{app}} \cdot M) - K_u \cos^2 \theta + \frac{1}{2} \mu_0 (N_s M_s^2 + N_y M_y^2 + N_z M_z^2) \right]. \tag{4}
\]

The normalized effective field (excluding the thermal field) is then given as

\[
h_{eff}' = \frac{H_{eff}'}{M_s} = -\frac{1}{\mu_0 M_s V} \nabla_M E_{\text{total}}(M)
= h_{app} + \frac{2K_u}{\mu_0 M_s^2} (\hat{n} \cdot m) \hat{n} - \sum_i N_i m_i, \tag{5}
\]
where we have normalized as \( h_{\text{app}} = \frac{H_{\text{app}}}{M_s}, m_i = \frac{M_i}{M_s} \), and \( \nabla_M \) is the gradient with respect to the magnetization \( M \).

Substituting \( K_u = \frac{1}{2} \mu_0 M_s H_k \) (\( H_k \) is the anisotropy field) in (5),

\[
\begin{align*}
\hat{h}_e' &= h_{\text{app}} + \frac{H_k}{M_s} (\hat{n} \cdot m) \hat{n} - \sum_i N_i m_i. \\
\hat{h}_e &= h_{\text{app}} + \frac{H_k}{M_s} (\hat{n} \cdot m) \hat{n} - \sum_i N_i m_i + h_T.
\end{align*}
\]

The total normalized effective field including the thermal field is then

\[
\hat{h}_e = h_{\text{app}} + \frac{H_k}{M_s} (\hat{n} \cdot m) \hat{n} - \sum_i N_i m_i + h_T.
\]

2.2. Thermal field modeling

The thermal field \( H_T(t) \) can be expressed in terms of the Wiener process as \( H_T(t)dt = \nu dW(t) \) [19], where \( W(t) \) is the Wiener process, and \( \nu = \sqrt{\frac{2\alpha K_b T}{\mu_0 M_s^2 V}} \) [20, 21]. Here, \( K_b T \) is the thermal energy.

The statistical properties of this thermal field discussed by Brown and Kubo [22, 23] are given as

1. The mean \( \langle H_{T,i}(t) \rangle = 0 \),
2. The correlation between the components of \( H_T \) defined over a time interval \( \tau \),

\[
\begin{align*}
\langle H_{T,i}(t) H_{T,j}(t+\tau) \rangle &= \frac{2K_b T \alpha}{\gamma \mu_0^2 M_s V} \delta_{ij} \delta(\tau),
\end{align*}
\]

where \( \delta_{ij} \) is the Kronecker delta function.

To simulate the thermal effects numerically, we have to discretize the model,

\[
H_T(t) \Delta t = \nu \Delta W(t),
\]

where \( \Delta W(t) = W(t + \Delta t) - W(t) \). Accordingly, the standard deviation of either side of (9) is

\[
\sigma = \sqrt{\frac{2\alpha K_b T \Delta t}{\gamma \mu_0^2 M_s V}},
\]

where \( \Delta t \) is the time step of the numerical method used. The normalized expression for (10) is then given by

\[
\sigma' = \sqrt{\frac{2\alpha K_b T}{\mu_0 M_s^2 V}} \sqrt{\frac{\Delta t'}{\gamma \mu_0 M_s}},
\]

where \( t' = (\gamma \mu_0 M_s) t \). Then we have

\[
h_T(t) \Delta t' = \sigma' \xi_t,
\]

where the normalized thermal field \( h_T = H_T/M_s \) and \( \xi_t \sim N(0, 1) \) is a standard Gaussian vector.

3. The Implicit Midpoint method

Using a numerical scheme based on the midpoint rule ensures that (2) converges to the Stratonovich solution in the limit of \( \Delta t \to 0 \). In this section, we define the implicit midpoint method, discretize the deterministic LLGS equation, and derive the Jacobian for use in the Gauss-Newton algorithm.

3.1. The deterministic case

For simplicity, we start the discussion with a one-dimensional (1D) deterministic ordinary differential equations (ODE) of the form

\[
y'(t) = f(t, y(t)),
\]

with initial condition \( y(0) = y_0 \). The implicit midpoint update is given as

\[
y_{n+1} = y_n + \Delta t \cdot f \left( t_n + \frac{\Delta t}{2}, \frac{y_n + y_{n+1}}{2} \right),
\]

3
3.2. Discretizing the deterministic Landau-Lifshitz-Gilbert-Slonczewski equation

The s-LLGS equation is

\[ S(y) = y - y_n - \Delta t \cdot f \left( t_n + \frac{\Delta t}{2}, \frac{y_n + y}{2} \right). \]  

In order to solve a non-linear system \( S: \mathbb{C}^n \rightarrow \mathbb{C}^m \), we can use a generalized version of Newton’s method, the Gauss-Newton algorithm. Analogous to the 1D case, we can Taylor expand a differentiable system \( S \)

\[ S(x) = S(x_0) + J[S](x_0) \cdot (x - x_0) + \epsilon, \]  

where \( J[S](x_0) \) is the Jacobian of \( S \) at \( x_0 \). Note that \( x, x_0 \in \mathbb{C}^n, S(x) \in \mathbb{C}^m, \) and \( J[S](x_0) \in \mathbb{C}^{m \times n} \), and \( \epsilon = o(||x - x_0||^2) \). The \( ij^{th} \) entry of the Jacobian of \( S \) is defined by

\[ J[S](x)_{ij} = \frac{\partial S_i(x)}{\partial x_j}, \]  

where \( S_i \) is the \( i^{th} \) component of \( S \), and \( x_j \) is the \( j^{th} \) component of \( x \). Setting \( S(x) = 0 \), dropping the higher-order terms, and setting \( x_{n+1} = x, x_n = x_0 \), we can write

\[ x_{n+1} = x_n - J[S](x_n)^{-1} \cdot S(x_n), \]  

if \( J[S] \) is invertible. As a result, we can use implicit methods on multi-dimensional ODE’s, including the s-LLGS equation.

3.3. Derivation of the Jacobian

Having set up the system \( S \), it remains to derive its Jacobian with respect to \( m \).

3.3.1. Derivation of the Jacobian

First, we state that for \( a, b \in \mathbb{C}^3 \), the cross product of \( a \) and \( b \) can be restated in terms of matrix-vector multiplication

\[ a \times b = (a^\times)b, \]  

where

\[ a^\times = \begin{bmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{bmatrix}. \]  

The Jacobian of a cross product of two functions \( f, g : \mathbb{C}^n \rightarrow \mathbb{C}^3 \) is given by

\[ J[f \times g] = f^\times J[g] - g^\times J[f]. \]  

Using the above relation, one can derive the Jacobian as
To summarize, we will use the Jacobian in (23) to solve \( S \) is a stochastic process \( W \) RK4-Heun. The accuracy of the methods is tested on an SDE with a known analytical solution.

4. Methods to solve the s-LLGS equation

The focus of this section is on the accuracy of various numerical techniques to solve the s-LLGS equation. Specifically, we focus on implicit midpoint, Heun, Euler-Heun, and a new method, namely the RK4-Heun. The accuracy of the methods is tested on an SDE with a known analytical solution.

4.1. Primitives of stochastic calculus

We begin by reviewing the definition of a stochastic integral over a Wiener process. A Wiener process is a stochastic process \( W(t) : \mathbb{R}^+ \rightarrow \mathbb{R} \) that satisfies

1. \( W(0) = w_0 \in \mathbb{R} \) a.s.
2. Independent increments: \( W(t_2) - W(t_1) \) and \( W(t_1) - W(t_0) \) are independent for \( 0 \leq t_0 < t_1 < t_2 \).
3. \( W(t + s) - W(t) \sim \mathcal{N}(0, s) \).
4. \( W(t) \) is almost surely continuous.

Then a stochastic integral over a Wiener process is defined as

\[
\int_a^b g(t) dW(t) = \lim_{\Delta t \to 0} \sum_k g(\tau_k)(W(t_{k+1}) - W(t_k)),
\]

where \( \{t_k\}_k \) forms a partition of \( [a, b] \). Contrary to the Riemann integral, different choices of \( \tau_k \) yield different results of the integral. This is the case if \( g \) is a function of both \( t \) and the Wiener process \( W(t) \). The most common choices are \( \tau_k = t_k \) and \( \tau_k = (t_{k+1} + t_k)/2 \). The former yields the Ito calculus, while the latter results in the Stratonovich calculus. A widely used notation for the Stratonovich integral, to distinguish it from the Ito integral, is

\[
\int_a^b g(t) \circ dW(t),
\]

which we will use in the following. Numerical schemes that attempt to approximate a stochastic differential equation’s (SDE) solution have to be constructed for a specific calculus. In our case, this is the Stratonovich interpretation [20].

In a somewhat general form, we can write a Stratonovich SDE as

\[
dX_t = f(X_t, t)dt + g(X_t, t) \circ dW_t.
\]

The s-LLGS equation in (3) can be restated in the general SDE form given in (27). To this end, let \( X(t) = m_t \), and define

\[
f(m_t, t) = -\alpha' |m_t \times h| + (1 + \alpha \beta) m_t \times (m_t \times i_s)
+ \alpha (m_t \times (m_t \times h) - m_t \times i_s),
\]

(28a)
Further, we will deal with two modes of convergence of numerical approximations to solutions of SDEs, introduced in [27]. Given a solution \( X_t \) of (27), an approximation \( \tilde{X}_t \) is said to converge to \( X_t \) in the *strong sense with order* \( \gamma > 0 \) if there is a \( C \in \mathbb{R} \) such that

\[
\mathbb{E} \left( |\tilde{X}_t - X_t| \right) < C(\Delta t)^\gamma,
\]

holds for any discrete approximation \( \tilde{X}_t \) with maximum step-size \( \Delta t \) [27]. On the other hand, an approximation \( \tilde{X}_t \) is said to converge to \( X_t \) in the *weak sense with order* \( \gamma > 0 \) if there is a \( C \in \mathbb{R} \) such that

\[
\mathbb{E}(p(\tilde{X}_t)) - \mathbb{E}(p(X_t)) < C(\Delta t)^\gamma,
\]

holds for any polynomial \( p \) and any discretization with maximum step size \( \Delta t \). Note that convergence in the strong sense is equivalent to convergence for each realization of \( W_t \) (i.e. path), while convergence in the weak sense merely implies that the statistical properties of the approximation converge to those of the solution.

### 4.2. Numerical schemes for Stratonovich SDEs

In order to numerically solve (27), the following must be computed:

\[
X_t = \int_0^t f(X_s, t) dt + \int_0^t g(X_s, t) \circ dW(t) + X_0,
\]

where the first integral is a regular Riemann integral, and the second integral is a stochastic integral interpreted in the Stratonovich sense. In our case, we are dealing with three-dimensional (3D) vector integrals, and \( W(t) \) is a 3D Wiener process. Below, we briefly outline the methods that we focus on in this work.

1. **Euler-Heun**

   Arguably the simplest method which converges to the Stratonovich solution is the Euler-Heun method which is defined by

   \[
   X_{n+1} = X_n + f(X_n, t_n) \Delta t + \frac{1}{2} \left( g(\tilde{X}_{n+1}, t_{n+1}) + g(X_n, t_n) \right) \eta_n,
   \]

   \[
   \tilde{X}_{n+1} = X_n + f(X_n, t_n) \eta_n,
   \]

   where \( \eta_n = \sqrt{\Delta t} \xi_n, \Delta t \in \mathbb{R}^+, \) and \( \xi_n \sim \mathcal{N}(0, 1) \).

2. **Heun**

   The Heun method is given by

   \[
   X_{n+1} = X_n + \frac{1}{2} \left( f(\tilde{X}_{n+1}, t_{n+1}) + f(X_n, t_n) \right) \Delta t + \frac{1}{2} \left( g(\tilde{X}_{n+1}, t_{n+1}) + g(X_n, t_n) \right) \eta_n,
   \]

   where

   \[
   \tilde{X}_{n+1} = X_n + f(X_n, t_n) \Delta t + g(X_n, t_n) \eta_n.
   \]

3. **Implicit midpoint**

   The implicit midpoint rule is defined by

   \[
   X_{n+1} = X_n + f(X_{n+1/2}, t_n + \Delta t/2) \Delta t + g(X_{n+1/2}, t_n + \Delta t/2) \eta_n,
   \]

   where \( X_{n+1/2} = (X_{n+1} + X_n)/2 \). Note that this defines an implicit system just as in the deterministic case, and we can use the methods derived for the deterministic case to solve it. We use the Euler step

   \[
   X^* = X_n + f(X_n, t_n) \Delta t + g(X_n, t_n) \eta_n,
   \]

   as the initial guess for the Gauss-Newton algorithm, to find \( X_{n+1} \).
All of the above methods are known to converge to the Stratonovich solution with a strong order 1/2, and a weak order 1 \cite{27,28}. Compared to numerical methods for deterministic DEs, this order of convergence is low. However, stochastic higher-order methods generally require the approximation of iterated stochastic integrals, which is a detailed and time-intensive procedure \cite{29}. If an SDE has a special structure, like an additive or commutative noise term, this calculation can be simplified. Unfortunately, the noise term of the s-LLGS equation is multiplicative and non-commutative.

Further, it is important to note that semi-implicit numerical methods based on extrapolation, which are used to handle deterministic DEs, generally do not converge to solutions of SDEs. The reason for this is that extrapolations from the past destroy the Markov property (independent increments) of the Wiener process over which we integrate. As seen in Figure 1, a semi-implicit midpoint scheme using Adam’s extrapolation \cite{30}, where \( X_{n+1/2} = \frac{1}{2}(3X_n - X_{n-1}) \), does not converge to the solution of the SDE, \( dX_t = X_t dt + X_t \circ dW_t \), with solution \( X_t = e^{t+W_t} \).

4.3. A method for small noise

In many stochastic models corresponding to physical systems, the noise term is usually much smaller than the drift term. Indeed, while the stochastic term plays a critical role in the s-LLGS equation, it is frequently one to two orders of magnitude smaller than the deterministic term, if \( T \) is close to room temperature. This means a higher order approximation of the drift term alone could improve the accuracy of the entire approximating process, when the absolute error is dominated by the error in the deterministic term. This idea has been investigated for Ito SDEs in \cite{31,32}. Here, we propose a scheme for Stratonovich SDEs, which we are going to refer to as RK4-Heun. It is defined by

\[
X_{n+1} = X_n + D\Delta t + S\eta_n, \\
D = (d_1 + 2d_2 + 2d_3 + d_4)/6, \\
S = (s_1 + s_2)/2, \\
s_1 = g(X_n, t_n), \\
s_2 = g(X_n + f(X_n, t_n)\Delta t + s_1\eta_n), \\
d_1 = f(X_n, t_n), \\
d_2 = f(X_n + (d_1 + s_1)/2, t_n + \Delta t/2), \\
d_3 = f(X_n + (d_2 + s_1)/2, t_n + \Delta t/2), \\
d_4 = f(X_n + d_3 + s_1, t_n + \Delta t).
\]

Importantly, the RK4 stages are only used to approximate the deterministic part of the equation. Therefore, convergence to the Stratonovich solution is maintained. Further, we made the observation that
making the additional update
\[
X'_{n+1} = X_n + D\Delta t + S'\eta_n,
\]
\[
S' = (s_1 + s'_2)/2,
\]
\[
s'_2 = g(X_{n+1}, t_{n+1}),
\]
(40)

after computing the above, leads to a significant increase in accuracy for the test equation (37). The additional update includes the higher order approximation of the deterministic term in the Heun step of the stochastic term. As a consequence, it is not surprising that this leads to a better approximation. However, we have not yet investigated analytical justifications of this update. Future work will look into that, and the possible limitations of this effect.

4.4. Numerical tests

To compare the accuracy of the various methods discussed above, we consider a modified version of the SDE (37),
\[
dX_t = aX_t dt + bX_t \circ dW_t,
\]
where \(a, b \in \mathbb{R}\). A Stratonovich solution to (41) is given by
\[
X_t = X_0 + \int_0^t X_s ds + \int_0^t X_s \circ dW_s = e^{at+bW_t},
\]
(42)

where \(X_0 = 1\). We can now compare the results of different numerical schemes to this analytical solution. The implicit midpoint method for (37) is defined by
\[
X_{t+1} = X_t + \frac{1}{2}(X_{t+1} + X_t)\Delta t + \frac{1}{2}(X_{t+1} + X_t)\eta_t.
\]
(43)

This can be solved for \(X_{t+1}\) analytically, according to
\[
X_{t+1} = X_t \left(\frac{2 + c}{2 - c}\right),
\]
\[
c = a\Delta t + b\eta_t.
\]
(44)

The experimental results for the path-wise error to the analytical solution, \(X_1\), are shown in Figure 2a and 2b for two different choices of \(b\) in (41). The data shows that the RK4-Heun scheme is more accurate than all other methods for all step sizes considered. Interestingly, the empirical order of convergence, which is the slope of the error function in Figure 2, is only constant for the Euler-Heun method. All other methods start out with a faster order (steeper slope) for larger step sizes. This is due to the fact that the deterministic part of the equation, and hence the error in its approximation, dominates the stochastic part. Therefore, the slope for big step sizes is more like the deterministic second order of convergence for the Heun and implicit midpoint schemes. We see this effect for smaller step sizes as the size \(b\) of the stochastic part is decreased in Figure 2b.

![Graph](image1.png)

![Graph](image2.png)

Figure 2: Average path-wise error of the numerical approximations corresponding to equation (41) with two different choices of \(a\) and \(b\).
Now, we are going to test the properties of these methods on the s-LLGS equation, defined by (28a) and (28b). It is important to note that the norm of the magnetization vector $m$ is preserved if the equation is interpreted in the Stratonovich sense. This follows from the fact that in the Stratonovich calculus,

$$d(\|m_t\|^2) = 2m_t \cdot dm_t = 0,$$

whereas in the Ito calculus, Ito’s Lemma gives

$$d(\|m_t\|^2) = 2m_t \cdot dm_t + \sum_{i,j=1}^{3} \frac{\partial^2 \|m_t\|^2}{\partial m_i \partial m_j}(m_t) \ (dm_{i,t} \cdot dm_{j,t}),$$

which is, in general, not zero. Explicit schemes like Euler-Heun or Heun, while solving the Stratonovich equation, do not preserve the norm. Indeed, one has to take a very small step size $\Delta t$ so that the norm of the magnetization does not blow up. On the other hand, the implicit midpoint method preserves the norm. The contrasting behavior of the magnetization norm obtained using different stochastic calculi is highlighted in Figures 3a and 3b. Indeed the midpoint method that converges to the Stratonovich solution preserves the norm while the Ito solution does not.

![Figure 3: Time evolution of magnetization with (a) implicit midpoint converging to the Stratonovich solution and (b) Heun-Euler converging to the Ito solution. Conditions are zero spin current (only noise) and energy barrier $U = 10K_B T$. The magnetization norm is preserved with the former, but blows up with the latter.](image)

The deviation of the magnetization norm from unity for different numerical techniques is depicted in Figure 4a. The error tolerance for the Gauss-Newton algorithm in the implicit midpoint method was $10^{-12}$. For this reason, the norm is only preserved up to this order of magnitude. In practice, decreasing the error tolerance further only slows down the algorithm without significant benefit. In Figure 4b, we show the maximum norm of the difference of the magnetization vectors, calculated by the Heun, implicit midpoint, and RK4-Heun methods. The difference is quite pronounced at larger time steps as expected, and diminishes as the time step is reduced. We see that the explicit methods converge to the same path quickly, while the difference to the implicit scheme decreases at a slower rate.

It would be interesting to see the discrepancy in the switching boundaries obtained from the Heun and implicit midpoint schemes. The 50% switching boundary is a useful metric since it is commonly used to benchmark solvers. To this end, we construct a contour plot (Figure 5) by sweeping over spin current durations and amplitudes to ascertain the 50% and 90% switching boundaries from the two methods. The maximum discrepancy in the switching boundaries is observed at the 50% switching probability. However, the difference in the switching probability between the two methods diminishes in the high current, long time-scale regimes for the chosen time-step of numerical integration.
5. Comparison with SPICE solvers and benchmarking with OOMMF

5.1. Comparison with SPICE

Circuit-level simulations using nanomagnets are often conducted using SPICE-based models, which represent the nanomagnet using basic circuital elements such as resistors, capacitors, and current sources. It is, therefore, important to benchmark the accuracy of SPICE numerical solvers with respect to the implicit midpoint method to solve the s-LLGS equation. SPICE uses methods such as Euler, Gear, trapezoidal, or a combination of these, to numerically integrate DEs. While the trapezoidal method is compatible with the Stratonovich stochastic calculus, other numerical methods in SPICE require that the s-LLGS equation be transformed into the equivalent Ito representation. While there are many versions of SPICE available [33–35], possibly with varying minimum time-steps and specific algorithms to solve equations, we use Cadence SPICE for our simulations in this paper.

Figure 6a shows the SPICE circuit implementation of a nanomagnet subject to thermal effects and spin torque, in one particular direction (x, y or z). The other two magnetization directions are implemented similarly. Detailed circuit derivations can be found in prior works [21] and [36]. Large-scale Monte Carlo
Simulations were conducted using the circuit representation in Figure 6a to generate the probability density function (PDF) plots of the magnetization reversal of an in-plane nanomagnet. The time-step of integration is taken to be 1 ps, reducing which leads to convergence issues in the SPICE nodal analysis. From the results shown in Figure 6b we find that SPICE solvers overestimate the mean delay of magnetization reversal as compared to the implicit midpoint method. In addition, unlike the implicit midpoint method, SPICE solvers are unable to preserve the magnetization norm as shown in Fig. 7. We also highlight the differences in the initial angle distribution obtained from various numerical schemes in Fig. 8. In this figure, the macrospin is subject to thermal noise for a period of 1 ns and no external magnetic field or spin torque is applied. As expected, the discrepancy in results is exacerbated for Euler method due to the fact that it does not solve for the correct Stratonovich SDE equation and will require an alternative Ito representation of the s-LLGS equation. Whereas the trapezoidal method does converge to the Stratonovich solution for $\Delta t \to 0$, but it is limited by the minimum time-step of the DE solver in SPICE. Hence we see a 200 ps difference in the mean reversal delay obtained with implicit midpoint and the trapezoidal solver of SPICE. It must be noted that these significant errors in magnetization reversal computed from SPICE will ultimately lead to inaccurate estimates of circuit-level performance metrics such as error-rate, latency, and energy dissipation of complex magneto-logic networks.

(a) Schematic of nanomagnet used in the circuit simulations.

(b) PDFs of reversal delays of a nanomagnet using implicit midpoint, SPICE trapezoidal-gear2 solver, and SPICE backward-Euler solver.

Figure 6: The simulations were performed for an in-plane magnet using identical dimensions $40 \times 40 \times 1$ nm$^3$, parameters $M_s = 1.11e6$ A/m, $H_k = 1.11e5$ A/m, $\alpha = 0.01$, time step 1 ps, and spin current 0.16 mA.

Figure 7: Norm of the magnetization vector in the course of a simulation, calculated with SPICE and implicit mid-point solvers. The parameters used are the same as for Figure 6b.

Figure 8: Initial angle distribution of the nanomagnet after it has been subjected to only thermal noise for 1 ns, from SPICE and our implicit midpoint solver.
5.2. Benchmarking with OOMMF

The Object Oriented MicroMagnetic Framework (OOMMF) by NIST is a widely used open source, portable, public domain tool for micromagnetics. The Oxs (OOMMF eXtensible Solver) is an extensible micromagnetic computation engine capable of solving problems defined on three-dimensional grids of rectangular cells holding three-dimensional spins [37]. We use OOMMF’s Oxs with evolver class “SpinXferEvolve” to simulate a single magnet whose magnetization evolves under the application of a spin current. Unfortunately there are no default evolver classes from OOMMF that include the effects of thermal noise. Hence, in this section we compare the magnetization vectors in the deterministic case with the corresponding vectors obtained from our implementation of the implicit midpoint method, as shown in Figure 9. This exercise substantiates the claim that our implicit midpoint realization is very close to the NIST standard.

![Figure 9: The evolution of the magnetization vector under STT (without thermal effects) using our implicit midpoint implementation and the OOMMF solver.](image)

While OOMMF does not have a default implementation of a thermal noise model in its evolvers, there are third-party extensions capable of performing thermal simulations in OOMMF. While the extension “XL_ThermSpinXferEvolve” [38] implements the solution of the s-LLGS equation using the Heun method, it naively renormalizes the magnetization norm in every iteration. The numerical accuracy and stability of this operation are questionable and there appears to be no physical reason for this.

6. Outlook

While a discussion of strong higher-order methods was not the goal of this paper, there are notable developments, whose applicability in solving the s-LLGS equation will be investigated in the future. Namely, the efficient strong order stochastic Runge-Kutta schemes which were proposed in [39]. These schemes have the advantage that the number of evaluations of the drift term of an SDE only increases linearly with the dimension of the driving Wiener process. This is in contrast to previous methods, which relied on a quadratically increasing number of evaluations of the drift term. For the approximation of the general multiple stochastic integrals, a method introduced in [40, 41] can be used.

Further, is important to note that many properties of magnets that are of interest to engineers can be solved for using weakly convergent schemes. For example, the switching probability of a magnet at an
arbitrary time is such a property. Importantly, there are known schemes which converge in the weak sense with orders up to 4 \[27\]. Recently, a very efficient explicit scheme with weak convergence order 2 has been introduced in \[12\] \[13\]. Many of these schemes can be simplified so that no iterated stochastic integrals have to be computed. This is a time-intensive process because many random variables have to be computed at each time step, and it is one of the reasons why efficient high strong-order schemes are currently only available for equations with special structure. In order to take advantage of these higher order approximations, the authors are currently investigating weakly convergent higher-order schemes for the s-LLGS equation.

7. Conclusion

In this paper, we examine the accuracy of (i) implicit midpoint, (ii) Heun, (iii) Euler-Heun, and (iv) RK4-Heun numerical methods to solve the s-LLGS equation of macrospin dynamics. We compare the performance of these methods in terms of the average path-wise error, preservation of the magnetization norm, and 50% switching boundary of macrospin reversal. We clearly show the higher accuracy of the implicit midpoint method as compared to other methods. However, the RK4-Heun method offers significant benefits in precision when the stochastic term in the s-LLGS equation is 2-3 orders of magnitude lower than the deterministic term. We also demonstrate that SPICE-based numerical integration schemes, such as trapezoidal, Gear, and Euler, perform poorly and lead to significant errors in the results when compared with the implicit midpoint method at the same time step. Through an exhaustive study, we provide guidelines that will help researchers analyze macrospin dynamics more accurately in the context of appropriate stochastic calculus and the use of numerical integration method.

Appendix A. Derivation of dimensionless LLGS

Beginning with \[1\], we divide both sides by \(\gamma_0 M^2\),

\[
\frac{1}{\gamma_0 M^2} \frac{dM}{dt} = -\frac{1}{M^2}(M \times H_{eff}) + \frac{\alpha}{\gamma_0 M^2} \left(M \times \frac{dM}{dt}\right) - \frac{M \times (M \times I_s)}{q \gamma_0 M^2 N_s} - \beta \frac{M \times I_s}{q \gamma_0 M^2 N_s}. \tag{A.1}
\]

Let the scale for magnetization and effective field be \(M_s\). Then normalizing as \(m = \frac{M}{M_s}\) and \(h_{eff} = \frac{H_{eff}}{M_s}\),

\[
\frac{1}{\gamma_0 M_s} \frac{dm}{dt} = -m \times h_{eff} + \frac{\alpha}{\gamma_0 M_s} \left(m \times \frac{dm}{dt}\right) - \frac{m \times (m \times I_s)}{q \gamma_0 M_s N_s} - \beta \frac{m \times I_s}{q \gamma_0 M_s N_s}. \tag{A.2}
\]

Taking the current scale as \(I = q \gamma_0 M_s N_s\), we obtain the normalized spin current \(i_s = \frac{I}{L}\). Also we consider a new time scale \((\gamma_0 M_s)^{-1}\) such that \(t' = (\gamma_0 M_s) t\) and \(dt' = (\gamma_0 M_s) dt\).

\[
\frac{dm}{dt'} = -m \times h_{eff} + \alpha \left(m \times \frac{dm}{dt'}\right) - m \times (m \times i_s) - \beta (m \times i_s). \tag{A.3}
\]

Changing variables \(t := t'\) without loss of generality, we get

\[
\frac{dm}{dt} = -m \times h_{eff} + \alpha \left(m \times \frac{dm}{dt}\right) - m \times (m \times i_s) - \beta (m \times i_s). \tag{A.4}
\]

This is the implicit form of the dimensionless s-LLGS equation.

To further transform this and decouple \(\frac{dm}{dt}\) from the right hand side of \[A.4\], we take the cross product with \(m\) on both sides,

\[
m \times \frac{dm}{dt} = -m \times (m \times h_{eff}) + \alpha m \times \left(m \times \frac{dm}{dt}\right) - m \times (m \times (m \times i_s)) - \beta m \times (m \times i_s). \tag{A.5}
\]

Now,

\[
m \times \left(m \times \frac{dm}{dt}\right) = m \left(m \cdot \frac{dm}{dt}\right) - \frac{dm}{dt} (m \cdot m) = -|m|^2 \frac{dm}{dt}. \tag{A.6}
\]
And,
\[ m \times (m \times (m \times i_s)) = m(m \cdot (m \times i_s)) - (m \times i_s)(m \cdot m), \]
\[ = m(i_s \cdot (m \times m)) - |m|^2(m \times i_s), \]
\[ = -|m|^2(m \times i_s). \]  
(A.7)

Substituting (A.6) and (A.7) back in equation (A.5),
\[ m \times \frac{dm}{dt} = -m \times (m \times h_{eff}) - \alpha|m|^2\frac{dm}{dt} + |m|^2(m \times i_s) - \beta m \times (m \times i_s). \]  
(A.8)

Replacing \( m \times \frac{dm}{dt} \) from (A.8) in (A.5),
\[ \frac{dm}{dt} = -m \times h_{eff} + \alpha \left( -m \times (m \times h_{eff}) - \alpha|m|^2\frac{dm}{dt} + |m|^2(m \times i_s) - \beta m \times (m \times i_s) \right) - m \times (m \times i_s) \]
\[ = -m \times h_{eff} - \alpha m \times (m \times h_{eff}) - \alpha^2|m|^2\frac{dm}{dt} + \alpha|m|^2(m \times i_s) - (1 + \alpha\beta)(m \times (m \times i_s)), \]
which gives
\[ (1 + \alpha^2|m|^2)\frac{dm}{dt} = -m \times h_{eff} - \alpha m \times (m \times h_{eff}) + \alpha|m|^2(m \times i_s) - (1 + \alpha\beta)(m \times (m \times i_s)). \]  
(A.9)

Now \( |m|^2 = m_x^2 + m_y^2 + m_z^2 = 1 \), so that
\[ \frac{dm}{dt} = -\frac{1}{1 + \alpha^2}[m \times h_{eff} + (1 + \alpha\beta)(m \times (m \times i_s)) + \alpha(m \times (m \times h_{eff}) - m \times i_s)]. \]  
(A.10)

This is the explicit form of the dimensionless s-LLGS equation.

**Appendix B. Newton’s method**

Given a differentiable function \( S : \mathbb{C} \to \mathbb{C} \), we can write
\[ S(x) = S(x_0) + (x - x_0)S'(x_0) + o(x - x_0)^2, \]  
(B.1)
as \( x \to x_0 \). To find a zero of \( S \), we can approximate \( S \) linearly using (B.1). Setting \( S(x) = 0 \) and dropping the higher-order terms, we get
\[ x = x_0 - S(x_0)/S'(x_0). \]  
(B.2)

Newton’s method for zero-finding consists of calculating the step (B.2) iteratively, using
\[ x_{n+1} = x_n - S(x_n)/S'(x_n). \]  
(B.3)

This method has a quadratic rate of convergence if the initial guess \( x_0 \) is close to the actual zero and the function is “well behaved”.

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