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Weak stochastic Runge–Kutta Munthe-Kaas methods for finite spin ensembles

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ABSTRACT

In this article we construct weak Runge–Kutta Munthe-Kaas methods for a finite-dimensional version of the stochastic Landau–Lifshitz equation (LL-equation). We formulate a Lie group framework for the stochastic LL-equation and derive regularity conditions for the corresponding SDE system on the Lie algebra. Using this formulation we define weak Munthe-Kaas methods based on weak stochastic Runge–Kutta methods (SRK methods) and provide sufficient conditions such that the Munthe-Kaas methods inherit the convergence order of the underlying SRK method. The constructed methods are fully explicit and preserve the norm constraint of the LL-equation exactly. Numerical simulations are provided to illustrate the convergence order as well as the long time behaviour of the proposed methods.

1. Introduction and general framework

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space together with a filtration $\mathcal{F}_{t\in[0,T]}$ which satisfies the usual conditions. We consider a finite ensemble of N magnetic nanoparticles occupying a domain $D \subset \mathbb{R}^3$. Let $\mathbb{S}^2$ denote the unit sphere of $\mathbb{R}^3$. The time evolution of the magnetisation

$$m(t) = (m_1(t), \dots, m_N(t)), m_i \in \mathbb{S}^2$$

of the particles can be described by the finite-dimensional Landau–Lifshitz equation (see [4,9,26])

$$\begin{aligned} dm_i(t) &= -m_i(t) \times V_i(m)dt + \eta m_i(t) \times dW_i(t) \\ m_i(0) &= m_i^0 \in \mathbb{S}^2, \qquad 1 \le i \le N. \end{aligned} \tag{1}$$

Here, $W = (W_1, \dots, W_N)$ is an $\mathcal{F}_t$-adapted $3N$-dimensional Wiener process representing thermal fluctuations acting on the magnetisation m; the strength of the fluctuations is scaled via the temperature dependent constant $\eta \in \mathbb{R}$. To ensure the correct thermodynamical behaviour the stochastic integrals have to be interpreted in the Stratonovich sense (see the discussion in [9,26]). Note that we use dW_i for denoting the Stratonovich integral in contrast to the more common notation

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$\circ dW_i$ to avoid confusion with the "$\circ$" operators in our vector field notation later on. $V = (V_1, \dots, V_N)$ is a collection of smooth vectorfields $V_i : \mathbb{R}^{3N} \to \mathbb{R}^3$, such that

$$V_i(m) = \nabla_{m_i}\mathcal{E}(m) - \alpha m_i \times \nabla_{m_i}\mathcal{E}(m). \tag{2}$$

Here, $\alpha \in \mathbb{R}^+$ denotes a dimensionless damping parameter, ∇_{m_i} denotes the gradient with respect to m_i and $\mathcal{E} : \mathbb{R}^{3N} \to \mathbb{R}$ describes the free energy of the system. A typical model for $\mathcal{E}$ (as e.g. used in [2]) incorporating exchange energy, uniaxial anisotropy energy and exterior energy is given by

$$\mathcal{E}(m) = \underbrace{\frac{A}{2}\langle J_{\text{exch}} m, m\rangle_{\mathbb{R}^{3N}}}_{\text{exchange}} + \underbrace{\frac{K}{2}\sum_{i=1}^{N}\left(1 - \langle m_i, e_{\text{ani}}\rangle^2_{\mathbb{R}^3}\right)}_{\text{anisotropy}} - \underbrace{\sum_{i=1}^{N}\langle m_i, h_{\text{ext}}\rangle_{\mathbb{R}^3}}_{\text{exterior}}, \tag{3}$$

where $J_{\text{exch}} \in \mathbb{R}^{3N\times 3N}$, symmetric, positive definite, $h_{\text{ext}}, e_{\text{ani}} \in \mathbb{R}^3$ and $A, K \in \mathbb{R}^+$.

An important qualitative property of Eq. (1) is that the modulus of m_i is conserved over time, i.e.

$$\|m_i(t)\|^2_{\mathbb{R}^3} = 1, \qquad \forall t \in [0, T], \quad 1 \le i \le N, \quad \mathbb{P}\text{-a.s.} \tag{4}$$

Equivalently, we can say that the solution trajectories of Eq. (1) evolve $\mathbb{P}$-a.s. on the N-times product of the unit sphere $\mathbb{S}^{2\otimes N} := \bigotimes_{i=1}^{N}\mathbb{S}^2$. In fact, let $\mathrm{T}\mathbb{S}^2|_y$ denote the tangent space of $\mathbb{S}^2$ at $y \in \mathbb{S}^2$, then for all $y \in \mathbb{S}^2$ the term $y \times z \in \mathrm{T}\mathbb{S}^2|_y$ for any vector z. As both drift and diffusion of Eq. (1) have this structure the solution m evolves on $\mathbb{S}^{2\otimes N}$ (see [17, Lemma 8.1]).

Computational micromagnetism (and in particular the Landau–Lifshitz equation) is an active field of research and plays an essential role in the development of magnetic materials used in e.g. magnetic storage technologies. Equation (1) has been treated extensively in the literature both from an analytical point of view (see [4,9,19,26]) as well as from a numerical point of view in the sense of mean-square approximations (see [1,2,20] and the references therein). In contrast to the pathwise perspective we focus here on the weak approximation of Eq. (1). In particular, we are interested in the time evolution of $\mathbb{E}[\mathcal{E}(m(T))]$ on large time horizons which corresponds to the average magnetisation relaxation of the magnetic ensemble.

Of course, any mean-square convergent method is also weak convergent with at least the same order of convergence and can be used for the approximation of $\mathbb{E}[\mathcal{E}(m(T))]$ (see e.g. the numerical experiments in [1,2]). Nevertheless, we want to emphasise that it is not necessarily a computationally efficient solution to use mean-square convergent methods. The classical way to approximate expectations is via Monte Carlo estimation; due to the nature of Monte Carlo estimation a large number of realisations is needed to keep the Monte Carlo error small. Thus, a computationally cheap weak convergent method can be preferable to a more expensive mean-square convergent method for Eq. (1). A perfect example for this is the linear implicit method proposed in [26] which is essentially a "less" implicit version of the mean-square convergent method proposed in the same article. To the best of our knowledge, this is the only method which is constructed as a weak method for Eq. (1) proposed in the literature.

A second aspect which makes weak convergent methods preferable is the order of convergence. In the mean-square case one has to simulate iterated Wiener integrals to obtain high convergence orders; however, the simulation of these integrals is a computationally demanding task (we refer to the discussion in [1, Section 4.3]). For weak convergent methods it suffices to approximate higher moments of iterated Wiener integrals and this can efficiently be achieved by using discrete random variables (see e.g. [21, Lemma 3.6] and the example in the Appendix). Following these considerations we propose that the weak convergent methods should combine the following desirable properties:

(i) The numerical method should be fast and accurate.
(ii) The numerical method should reproduce the qualitative properties of Eq. (1), i.e. the numerical trajectories should evolve on $\mathbb{S}^{2\otimes N}$.

The first property is at least partially fulfilled in the class of stochastic Runge–Kutta methods (SRK methods). SRK methods are flexible and there exists a theory for order conditions (we refer to [5–8,14,21,28–30] and the references therein). In particular, it is possible to construct SRK methods of weak order two which have reasonable computational cost (see [29]). However, a direct application of SRK methods to Eq. (1) is difficult as the numerical trajectories of these methods typically do not stay on the manifold $\mathbb{S}^{2\otimes N}$. This behaviour is highly problematic both from a physics point of view as well as from a numerical point of view:

- A weak approximation of the solution m of Eq. (1) is essentially an approximation of the distribution of m which is supported on $\mathbb{S}^{2\otimes N}$. Approximating this distribution with a distribution supported on $\mathbb{R}^{3N}$ assigns positive probability to states of the system which are impossible from a thermodynamical point of view.
- Even for small time steps the numerical trajectories of standard explicit SRK methods (e.g. the Heun method or modifications of the Euler–Maruyama method) do not only leave the manifold $\mathbb{S}^{2\otimes N}$ but rapidly explode on short time horizons (see the discussion in [20,3]). Note that there are SRK methods which automatically stay on $\mathbb{S}^{2\otimes N}$ and we will provide corresponding algebraic conditions on the entries of the Butcher tableau in the Appendix. These conditions are