# TECHNICAL RESEARCH REPORT

Cayley Transforms in Micromagnetics

*by P. S. Krishnaprasad, Xiaobo Tan*

CDCSS TR 2001-6
(ISR TR 2001-34)

**CENTER FOR DYNAMICS
AND CONTROL OF
SMART STRUCTURES**

# Cayley transforms in micromagnetics

P. S. Krishnaprasad, Xiaobo Tan

Department of Electrical and Computer Engineering

and Institute for Systems Research

University of Maryland, College Park, MD 20742

{krishna, xbtan}@isr.umd.edu

**Abstract**

Methods of numerical integration of ordinary differential equations exploiting the Cayley transform arise in a variety of contexts, ranging from the classical mid-point rule to symplectic and (almost) Poisson integrators, to numerical methods on Lie Groups. In earlier work, the first author investigated the interplay between the Cayley transform and the Jacobi identity in establishing certain error formulas for the mid-point rule (with applications to coupled rigid bodies). In this paper, we use the Cayley transform to lift the Landau-Lifshitz-Gilbert equation of micromagnetics to the Lie algebra of the group of currents (on a compact magnetic body) with values in the 3-dimensional rotation group. This follows an idea of Arieh Iserles and, we use the lift to numerically integrate the Landau-Lifshitz-Gilbert equation conserving automatically the norm of the magnetization everywhere.

Keywords: Geometric integration; Cayley transform; Landau-Lifshitz-Gilbert equation

Further correspondence: P. S. Krishnaprasad, same address as above. Fax: (301)314-9920.

# 1 Introduction

Numerical integration of the Landau-Lifshitz-Gilbert (LLG) equation is widely practised by researchers in the field of magnetic recording media. The present authors came to the subject through an interest in exploring magnetostriction (a phenomenon which will be ignored in the rest of this paper). A key question of interest is to ask if there are suitable numerical methods that are sufficiently accurate and at the same time (possibly independently) preserve a key conserved quantity associated to the LLG equation, namely, the magnitude of the magnetization everywhere in the body. It is clear that off-the-shelf schemes such as a Runge-Kutta solver applied to a standard space discretization of the dynamics will fail to conserve the magnitude of magnetization. In [1] the authors propose a scheme that is second order accurate, conserves the magnitude of magnetization, and yields easy-to-solve algebraic equations by choice of a special temporal mesh. The mid-point rule enters here in an essential way.

In the present paper, we seek methods that in effect decouple the accuracy of an integrator from the property of conservation of magnitude of magnetization. While it is well-known that for linear ordinary differential equations (o.d.e.'s) the mid-point rule defines a Cayley transform[2], here we use the Cayley transform in a different way. The roots of this go back to classical results on representing an element of the 3-dimensional rotation group[3]. A main result of this paper is that there is a 'lifting' of the LLG equation to a space of fields with values in skew symmetric matrices. Required numerical methods follow from this.

## 2 Model

The Landau-Lifshitz-Gilbert equation takes the form

$$(1 + \alpha^2)\frac{\partial \mathbf{M}}{\partial t} = \gamma_0 \mathbf{M} \times \mathbf{H}_{eff} + \frac{\gamma_0 \alpha}{M_s} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{eff}), \tag{1}$$

where $\mathbf{M} = \mathbf{M}(t, \mathbf{x})$ denotes the time dependent magnetization at a point $\mathbf{x} \in \mathcal{B}$, the ferromagnetic body (viewed as a compact subset of $\mathbb{R}^3$). The effective field $\mathbf{H}_{eff}$ is the sum of the external field, the exchange field, the anisotropy field and the demagnetizing field. From the structure of (1), it follows that $\| \mathbf{M}(t, \mathbf{x}) \|^2 = M_s^2$ for all time $t > 0$, if it is true at $t = 0$. Further in terms of the free energy functional $\mathcal{E}$, one finds $\mathbf{H}_{eff} = -\frac{\delta \mathcal{E}}{\delta \mathbf{M}}$, negative of the variational derivative[4]. Throughout this paper we treat the external field as time-independent. The system (1) evolves on the space of maps from $\mathcal{B}$ to $S^2$, the 2-dimensional sphere. Any spatial discretization of (1) yields a system of o.d.e.'s of the form

$$\dot{\mathbf{M}}^i = a\mathbf{M}^i \times \mathbf{H}^i_{eff} + b\mathbf{M}^i \times (\mathbf{M}^i \times \mathbf{H}^i_{eff}), \tag{2}$$

where $i = 1, 2, \cdots, N$ denotes the site of magnetization, and $a$ and $b$ are constants, with $b$ proportional to $\alpha$, the damping factor. The o.d.e.'s (2) are coupled through the effective field.

Letting $\mathcal{E}^d$ denote a discrete approximation to the free energy, one can write

$$\mathbf{H}^i_{eff} = -\frac{\delta \mathcal{E}^d}{\delta \mathbf{M}^i}, \tag{3}$$

and rewrite system (2) in the form

$$\dot{\mathbf{M}}^i = a\mathbf{M}^i \times (-\frac{\delta \mathcal{E}^d}{\delta \mathbf{M}^i}) + b\mathbf{M}^\mathbf{i} \times (\mathbf{M}^i \times (-\frac{\delta \mathcal{E}^d}{\delta \mathbf{M}^i})), \tag{4}$$

$$i = 1, 2, \cdots, N.$$

The discrete dynamical system has interesting mathematical/physical structure that applies over all possible discrete free energy functions. If $b = 0$, the system is a (reduced) hamiltonian

system in the Lie-Poisson form ([2, 5]) with conserved hamiltonian $-\mathcal{E}^d$. Even if $b \neq 0$ (i.e. in the presence of the so-called double-bracket dissipation [6]) there are $N$ conserved quantities $\| \mathbf{M}^i \|$, $i = 1, 2, \cdots, N$, the magnitudes of the magnetization at each site. This last remark follows by differentiating $\mathbf{M}^i \cdot \mathbf{M}^i$ and invoking (4).

Consider the standard isomorphism between vectors in $\mathbb{R}^3$ and $3 \times 3$ skew symmetric matrices,

$$\hat{} : \mathbb{R}^3 \quad \longrightarrow \quad so(3) = \text{ Lie algebra of}$$

$$3 \times 3 \text{ skew symmetric matrices}$$

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \longmapsto \hat{\mathbf{x}} = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}. \tag{5}$$

Observe the elementary identities $\mathbf{x} \times \mathbf{y} = \hat{\mathbf{x}}\mathbf{y}$ and $\widehat{\mathbf{x} \times \mathbf{y}} = \hat{\mathbf{x}}\hat{\mathbf{y}} - \hat{\mathbf{y}}\hat{\mathbf{x}}$, a matrix commutator (=Lie bracket $[\hat{\mathbf{x}}, \hat{\mathbf{y}}]$).

It is now possible to write the discrete dynamics (2) and (4) in the form

$$\dot{\mathbf{M}}^i = \mathbf{F}^i(\mathbf{M})\mathbf{M}^i, \ i = 1, 2, \cdots, N, \tag{6}$$

where, using (5), we have defined

$$\begin{aligned} \mathbf{F}^i(\mathbf{M}) &= -a\widehat{\frac{-\delta\mathcal{E}^d}{\delta\mathbf{M}^i}} - b[\widehat{\mathbf{M}}^i, \widehat{\frac{-\delta\mathcal{E}^d}{\delta\mathbf{M}^i}}] \\ &= -a\widehat{\mathbf{H}}^i_{eff} - b[\widehat{\mathbf{M}}^i, \widehat{\mathbf{H}}^i_{eff}], \ \ i = 1, 2, \cdots, N. \end{aligned}$$

In (6), $\mathbf{M}$ stands for the stacked vector of all magnetizations $\mathbf{M}^i$ at all sites. Thus $\mathbf{M}$ defines a point in the Cartesian product of spheres $(S^2)^N$. See also [7]. The system (6) is analogous to the dynamics of an assembly of linked rigid bodies (with strong material symmetries)[8]. In their

4

work[7], Lewis and Nigam develop a lifting approach inspired by the method of moving frames due to Cartan (further elaborated by Olver and others). They are clearly aware of the work of the Cambridge-Norway school on integration on manifolds. But their work involves use of free actions on tangent bundles on spheres and schemes involving acceleration updates. Here we are led to a rather simple approach to lifting suggested in the following section.

## 3  Lifting construction

Since each $\mathbf{M}^i(t)$ evolves on a sphere $S^2$, given $\parallel \mathbf{M}^i(0) \parallel = M_s, \ i = 1, 2, \cdots, N$, there is a curve $\mathbf{\Phi}^i(t)$ evolving on $SO(3)$, the Lie group of $3 \times 3$ rotation matrices such that

$$\mathbf{M}^i(t) = \mathbf{\Phi}^i(t)\mathbf{M}^i(0), \tag{7}$$

and $\mathbf{\Phi}^i(0) = \mathbb{I}$, the $3 \times 3$ identity matrix. The curves in each copy of $SO(3)$ define a curve $\mathbf{\Phi}(t)$ in the Cartesian product group $(SO(3))^N$. Each $\mathbf{\Phi}^i(t)$ satisfies the o.d.e.

$$\dot{\mathbf{\Phi}}^i(t) = \mathbf{F}^i(\mathbf{\Phi}(t)\mathbf{M}(0))\mathbf{\Phi}^i(t), \ i = 1, 2, \cdots, N, \tag{8}$$

where $\mathbf{\Phi}(t)$ should be understood as a block diagonal matrix with $\mathbf{\Phi}^i(t)$ as its $i$th block.

Solving (8) in $SO(3)$, numerically, and substituting in (7) is tantamount to solving the discrete magnetization dynamics. It is unfortunately no easier than trying to conserve $\parallel \mathbf{M}^i \parallel$ numerically.

However the Cayley transform comes to our rescue. Given any element $\mathbf{\Phi}$ of $SO(3)$ not within the set of measure zero $\{P \in SO(3) : -1 \in \text{spectrum} (P)\}$, one can write

$$\mathbf{\Phi} = (\mathbb{I} - \frac{1}{2}\mathbf{\Omega})^{-1}(\mathbb{I} + \frac{1}{2}\mathbf{\Omega}), \tag{9}$$

where the unique $\mathbf{\Omega} \in so(3)$, the Lie algebra of $3 \times 3$ skew symmetric matrices. This classical representation[3] is useful in covering the manifold $SO(3)$ by local coordinate charts and for a

5

variety of practical purposes in kinematics of mechanisms, spacecraft attitude control etc. The idea of lifting (suggested in the setting of numerical integration on Lie groups by Arieh Iserles of Cambridge University [9]) is very straightforward: derive a differential equation for $\mathbf{\Omega}^i$ in (9) where $\mathbf{\Phi}^i$ satisfies (8).

First we define $Cay(\mathbf{\Omega})$ to be the right hand side of (9). Then one can show

$$\dot{\mathbf{\Omega}}^i = \mathbf{F}^i - \frac{1}{2}[\mathbf{\Omega}^i, \mathbf{F}^i] - \frac{1}{4}\mathbf{\Omega}^i\mathbf{F}^i\mathbf{\Omega}^i, \tag{10}$$

$i = 1, 2, \cdots, N$, where

$$\mathbf{F}^i = \mathbf{F}^i(\mathbf{M}(t)), \tag{11}$$

$$\mathbf{M}^i(t) = Cay(\mathbf{\Omega}^i(t))\mathbf{M}^i(0). \tag{12}$$

Each of the o.d.e.'s in (10) evolves in a flat space of $3 \times 3$ skew symmetric matrices. We refer to (10)-(12) as the Cayley lift of the space discretized Landau-Lifshitz-Gilbert dynamics.

Formally one can construct a lift of the Landau-Lifshitz-Gilbert partial differential equation too. Let $\mathbf{\Omega}(t, \mathbf{x})$ take value in $so(3)$, the Lie algebra of the rotation group. Then the Cayley lift of the LLG equation is

$$\frac{\partial \mathbf{\Omega}}{\partial t} = F - \frac{1}{2}[\mathbf{\Omega}, \mathbf{F}] - \frac{1}{4}\mathbf{\Omega}\mathbf{F}\mathbf{\Omega}, \tag{13}$$

where

$$\mathbf{F} = \mathbf{F}(t, \mathbf{x}) = -a\widehat{\mathbf{H}}_{eff} - b[\widehat{\mathbf{M}}, \widehat{\mathbf{H}}_{eff}],$$

$$\mathbf{M} = \mathbf{M}(t, \mathbf{x}) = Cay(\mathbf{\Omega}(t, \mathbf{x}))\mathbf{M}(0, \mathbf{x}).$$

The system (13) evolves on the space of maps from $\mathcal{B}$ to $so(3)$. This space is easily viewed (formally) as the infinite dimensional Lie algebra of the infinite dimensional Lie group of currents (= space of maps from $\mathcal{B}$ to $SO(3)$). See [10] for another perspective on the underlying geometry. Under the

assumption of a compact body $\mathcal{B}$, the relevant functional analytic details (which we omit here) can be worked out to make the formal construction rigorous.

# 4   Lifting and integration

The discrete dynamics of the Cayley lift (10) can be integrated using methods of required accuracy. Unconditional stability will be achieved by suitable implicit schemes (with concomitant computational costs). The function evaluations (12) automatically conserve magnitude of magnetization to machine precision. We have effectively decoupled the conservation property from the question of accuracy.

It should be pointed out that integrating (6) by the mid-point rule (for a regular temporal mesh of resolution $h$) yields,

$$
\frac{\mathbf{M}^i(k+1) - \mathbf{M}^i(k)}{h} = \quad \mathbf{F}^i(\frac{\mathbf{M}(k+1) + \mathbf{M}(k)}{2})
$$
$$
\frac{\mathbf{M}^i(k+1) + \mathbf{M}^i(k)}{2}, \tag{14}
$$

or equivalently, the Cayley transform implicit scheme

$$
\mathbf{M}^i(k+1) = \quad (\mathbb{I} - \frac{h}{2}\mathbf{F}^i(\frac{\mathbf{M}(k+1) + \mathbf{M}(k)}{2}))^{-1}
$$
$$
(\mathbb{I} + \frac{h}{2}\mathbf{F}^i(\frac{\mathbf{M}(k+1) + \mathbf{M}(k)}{2}))\mathbf{M}^i(k). \tag{15}
$$

In this case accuracy is of order 2, and the scheme is implicit (with significant computational burden arising from the coupling in $\mathbf{H}_{eff}$). We refer to similar considerations in the computational mechanics literature [11].

Numerical experiments with the Cayley lift of the spatially discretized LLG equation have been

7

made together with comparisons with alternate schemes. The results are encouraging. Fig. 1 shows hysteresis computation on a small spatial grid. Table 1 gives some comparative computational loads. In this, RK4 refers to the explicit fourth order Runge-Kutta scheme, Cay_RK4 refers to the integration of (10) using RK4, and MP refers to the mid-point rule (14). Further studies based on the approach here are warranted to obtain additional speed-up and accuracy.

# 5    Acknowledgement

# References

[1]   C. Serpico, I.D. Mayergoyz, G. Bertotti, J. Appl. Phys. 89 (2001) 6991.

[2]   M. A. Austin, P. S. Krishnaprasad, L-S. Wang, J. Comp. Phys. 107 (1993) 105.

[3]   O. Bottema, B. Roth, Theoretical Kinematics, North-Holland Publ., Amsterdam, 1979.

[4]   A. Aharoni, Introduction to the Theory of Ferromagnetism, (2nd edition), Oxford University Press, Oxford, 2000.

[5]   J. E. Marsden, T. S. Ratiu, Introduction to Mechanics and Symmetry: A Basic Exposition of Classical Mechanical Systems, (2nd edition), Springer, New York, 1999.

[6]   A. M. Bloch, P. S. Krishnaprasad, J. E. Marsden, T. S. Ratiu, Commun. Math. Phys. 175 (1996).

[7]   D. Lewis and N. Nigam, A geometric integration algorithm with application to micromagnetics, Institute for Mathematics and its Applications Technical Report, (9 pages), University of Minnesota, September 2000.

[8]   J. E. Marsden, P. S. Krishnaprasad, J. C. Simo (eds), Dynamics and Control of Multibody Systems, in Contemporary Mathematics Series, V. 97, American Mathematical Society, Providence, 1989.

[9]   A. Iserles, Numerical Analysis Group Report NA 1999-04, (29 pages), Cambridge University, 1999.

[10]  V. A. Aleksovskii, M. Lukatskii, Theoret. Math. Phys. 85 (1990) 1090.

[11]  D. Lewis and J. C. Simo, J. Nonlin. Sci. 4 (1994) 253.

Table 1: Computation time needed for calculation of the hysteresis loop (simulation done on Sun Ultra 10 workstation).

| Algorithm | Stepsize (sec.) | Time (sec.) |
|---|---|---|
| RK4 | $2 \times 10^{-13}$ | 1656 |
| RK4 | $6 \times 10^{-13}$ | 953 |
| MP | $6 \times 10^{-13}$ | 789 |
| Cay_RK4 | $6 \times 10^{-13}$ | 367 |

**List of Figures:**