Numerical Methods for the Landau-Lifshitz Equation

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Abstract

We discuss numerical schemes for various forms of the Landau-Lifshitz equation. A new simple projection method is introduced and is shown to be unconditionally stable. The advantage over other schemes are also demonstrated numerically.

1 Introduction

The Landau-Lifshitz equation which describes the evolution of magnetization n continuum ferromagnets plays an important role in the understanding of nonequilibrium magnetism. In this paper, we will discuss various numerical methods for the Landau-Lifshitz equation in the form:

$$m_t = m \times \Delta m - \gamma m \times (m \times \Delta m) \tag{1.1}$$

where $m: \Omega \subset \mathbf{R}^d \to S^2$, d=1,2,3, γ is a damping parameter. The boundary condition is taken to be

$$\frac{\partial m}{\partial n} = 0 \tag{1.2}$$

on $\Gamma = \partial \Omega$. (1.1) is the result of the Landau-Lifshitz equation

$$m_t = m \times h - \gamma m \times (m \times h) \tag{1.3}$$

after neglecting lower order terms [7] [8]. In (1.3), $h = -\frac{\delta F}{\delta m}$ where the free energy F is given by

$$F(m) = \int_{\Omega} \{ \frac{1}{2} |\nabla m|^2 + \Phi(m) + m \cdot \nabla u \} d^3 x$$
(1.4)

Here Φ is a function of m, and u solves

$$\nabla \cdot \left(\nabla u + m\chi_{\Omega}\right) = 0 \tag{1.5}$$

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on \mathbf{R}^3 , with χ_{Ω} being the indicator function of Ω .

Although the nonlocal term in (1.4) also presents very important computational issues, in this paper, we will concentrate on the questions raised by the leading order term in (1.4), thereby neglecting the last two terms at the right hand side of (1.4). In this case $h = \Delta m$ and (1.3) reduces to (1.1). The three terms in (1.4) are the exchange, anisotropy and magnetostatic energies respectively. A term of the form $\int_{\Omega} m \cdot H d^3 x$ should be added to the right hand side of (1.4) if there is an external field H. It is easy to see that (1.3) can also be written as

$$m_t + \gamma m \times m_t = (1 + \gamma^2)m \times h \tag{1.6}$$

or

$$\gamma m_t - m \times m_t = -(1 + \gamma^2)m \times (m \times h) \tag{1.7}$$

(1.6) is sometimes referred to as the Gilbert equation.

The following identities will be useful later:

$$-m \times (m \times h) = h - (m, h)m \tag{1.8}$$

$$-m \times (m \times \Delta m) = \Delta m + |\nabla m|^2 m \tag{1.9}$$

where we have used the fact that (m, m) = 1.

Two special cases of (1.1) are of particular interest. They correspond to $\gamma = 0$ and $\gamma = +\infty$.

$$m_t = m \times \Delta m \tag{1.10}$$

$$m_t = -m \times (m \times \Delta m) \tag{1.11}$$

or

$$m_t = \Delta m + |\nabla m|^2 m \tag{1.12}$$

(1.11) is the equation describing the heat flow of harmonic maps to S^2 [12]. It has been studied extensively in the geometry and geometric analysis literature. In contrast, (1.10) describes the Hamiltonian (or symplectic) flow of harmonic maps to S^2 . At this point, there is much less literature on (1.10). Although the two models (1.11) and (1.12) are mathematically equivalent [4], (1.11) gives much better numerically stable solutions than that of (1.12), as we show in section 2.

Even though it is generally expected, and for special situations of (1.11) rigorously proved [1], that the solutions of (1.1), (1.10), (1.11) develop finite time singularities, we will restrict our attention to smooth solutions of these equations, leaving the discussions on singular solutions to future publications.

In this paper, various numerical schemes will be discussed. In particular, a simple projection scheme is proposed to solve (1.11) which is implicit and unconditionally stable. Time step size is an important issue for the numerical solution of the Landau-Lifshitz since the fastest time scale in the application of (1.3) is on the order of picoseconds. This means that straightforward explicit time stepping procedures will suffer from very severe constraints on the size of the time step. On the other hand, implicit schemes will have to deal with the severe nonlinearity present in the equation in the form of the Lagrange multiplier for the constraint that the length of m is 1. Here we propose time stepping method in the form of a projection method that circument both problems.

The paper is organized as following. In section 2, we explain the differences between the performance of numerical schemes for equations (1.11) and (1.12). Convergence of the spatial discretizations is also proved. In section 3, an implicit projection scheme is proposed and its unconditional stability is proved. Numerical examples are give in section 4 to demonstrate that the performance of the projection scheme is better than most of the other numerical schemes.

2 Spatial discretizations

Most discussions in this section will be in the setting of semi-discrete schemes, i.e. time will be kept continuous. For simplicity of presentation, we will assume that we are working with a uniform grid Ω_h with size h. The numerical results we present in this section are computed with sufficiently small Δt that the numerical error from time discretization is basically negligible.

On a regular finite difference grid, there are two obvious ways to discretize (1.1). The first is

$$\frac{dm_h}{dt} = m_h \times \Delta_h m_h - \gamma m_h \times (m_h \times \Delta_h m_h)$$
(2.1)

The second is

$$\frac{dm_h}{dt} = m_j \times \Delta_h m_h + \gamma (\Delta_h m_h + |\nabla m_h|^2 m_h)$$
(2.2)

Here Δ_h and ∇_h are the standard discretization of Δ and ∇ respectively using centered differences. Other difference approximations can be used. But it suffices to discuss this simplest case.

Both (2.1) and (2.2) provide convergent and second order accurate approximations for smooth solutions of (1.1). This is relatively easy to establish for (2.1).

Theorem 1: Let $m(x,t) \in L^{\infty}([0,T], H^3)$ be a smooth solution of (1.1) with initial data

$$m(x,0) = m_0(x)$$

and let m_h be the solution of (2.1) with the same initial data on a uniform grid Ω_h . Then we have

$$\max_{x \in \Omega_h} |m(x,t) - m_h(x,t)| \le c(t)h^2$$
(2.3)

where c(t) depends only on m.

The proof of this result will be given at the end of this section.

Even though both (2.1) and (2.2) give second order approximations to (1.11), their actual performance is very different. Note that (2.1) preserves the normalization exactly:

$$\frac{d}{dt}(m_h, m_h) = 0$$

and (2.2) does not. Let us examine the numerical solutions for the heat flow of harmonic maps, by comparing the results of the following two schemes:

$$\frac{dm_h}{dt} = -m_h \times (m_h \times \Delta_h m_h) \tag{2.4}$$

or

$$\frac{dm_h}{dt} = \Delta_h m_h + |\nabla_h m_h|^2 m_h \tag{2.5}$$

In Figures 1 and 2, we plot the time history of the error computed by these two methods, for the exact solution

$$m_e(x,t) = (\sin x \cos t, \sin x \sin t, \cos x) \tag{2.6}$$

on $[0, \pi]$ with Dirichlet boundary condition. For (2.6) to be an exact solution of (1.11), a forcing term $f = \frac{\partial m_e}{\partial t} + m_e \times (m_e \times \frac{\partial^2 m_e}{\partial x^2})$ has to be added to the right hand side of (1.11). We can see that while the error for (2.4) remains small, the error for (2.5) grows exponentially fast with time.

The origin of the exponential growth of the error for (2.5) can be understood from the following argument.

Consider the equation

$$m_t = \Delta m + |\nabla m|^2 m \tag{2.7}$$

Let e = (m, m) - 1. It is easy to see that e satisfies

$$e_t = \Delta e + 2|\nabla m|^2 e \tag{2.8}$$

This shows that if e is not identically zero, then e grows exponentially fast. Since the solutions of (2.5) does not preserve the normalization exactly, We expect $(m_h, m_h) - 1$ to grow exponentially fast. This means that the error $|m - m_h|$ will exhibit exponential growth.

A simple fix of this problem is to consider instead the following equivalent form of (2.7)

$$m_t = (m, m)\Delta m + |\nabla m|^2 m \tag{2.9}$$

and replace (2.5) by

$$\frac{dm_h}{dt} = (m_h, m_h)\Delta_h m + |\nabla_h m|^2 m_h \tag{2.10}$$

For (2.9), (2.8) changes to

$$e_t = (m, m)\Delta e \tag{2.11}$$

The term that was responsible for the exponential growth of e in (2.8) is now eliminated.

In Figure 3, we plot the error for the same exact solution as in (2.6) with (2.5) replaced by (2.10). We can see that the exponential growth of the error is now replaced by linear growth.

Proof of Theorem 1:

$$\frac{\partial m}{\partial t} = m \times \Delta m - \gamma m \times (m \times \Delta m)$$

$$\frac{dm_j}{dt} = m_j \times \Delta_h m_j - \gamma m_j \times (m_j \times \Delta_h m_j)$$

Let $\tilde{m}_j(t) = m(x_j, t)$. We have

$$\frac{d\tilde{m}_j}{dt} = \tilde{m}_j \times \Delta_h \tilde{m}_j - \gamma \tilde{m}_j \times (\tilde{m}_j \times \Delta_h \tilde{m}_j) + O(h^2)$$

Denote $e_j = m_j - \tilde{m}_j$, then

$$\frac{de_j}{dt} = m_j \times \Delta_h e_j + e_j \times \Delta_h \tilde{m}_j
- \gamma [m_j \times (m_j \times \Delta_h e_j) + m_j \times (e_j \times \Delta_h \tilde{m}_j)
+ e_j \times (\tilde{m}_j \times \Delta_h \tilde{m}_j)] + O(h^2)$$
(2.12)

 and

$$\sum_{j} \left(\frac{de_{j}}{dt}, \Delta_{h} e_{j} \right) = \sum_{j} \left(e_{j} \times \Delta_{h} \tilde{m}_{j}, \Delta_{h} e_{j} \right)$$

+ $\gamma \sum_{j} |m_{j} \times \Delta_{h} e_{j}|^{2} - \gamma \sum_{j} \left(m_{j} \times (e_{j} \times \Delta_{h} \tilde{m}_{j}), \Delta_{h} e_{j} \right)$
- $\gamma \sum_{j} \left(e_{j} \times (\tilde{m}_{j} \times \Delta_{h} \tilde{m}_{j}), \Delta_{h} e_{j} \right) + \sum_{j} \left(O(h^{2}), \Delta_{h} e_{j} \right)$
= $I_{1} + I_{2} + I_{3} + I_{4}$

and

$$\frac{1}{2} \frac{d}{dt} \sum_{j} (\nabla_{h} e_{j}, \nabla_{h} e_{j}) h^{d} + \gamma \sum_{j} |m_{j} \times \Delta_{h} e_{j}|^{2} h^{d} = -\sum_{j} \left(e_{j} \times \Delta_{h} \tilde{m}_{j}, \Delta_{h} e_{j} \right) h^{d} \\
+ \gamma \sum_{j} \left(m_{j} \times (e_{j} \times \Delta_{h} \tilde{m}_{j}), \Delta_{h} e_{j} \right) h^{d} \\
+ \gamma \sum_{j} \left(e_{j} \times (\tilde{m}_{j} \times \Delta_{h} \tilde{m}_{j}), \Delta_{h} e_{j} \right) h^{d} - \sum_{j} \left(O(h^{2}), \Delta_{h} e_{j} \right) h^{d} \\
= I_{1} + I_{2} + I_{3} + I_{4}$$

$$\frac{1}{2}\frac{d}{dt}\sum_{j} (\nabla_{h}e_{j}, \nabla_{h}e_{j})h^{d} \le |I_{1}| + |I_{2}| + |I_{3}| + |I_{4}|$$
(2.13)

Let us assume for the time being that there exists a $T^* < T$, s.t.

$$\max_{j} |\nabla_h m_j| \le 2C_0 \tag{2.14}$$

for $0 \leq t \leq T^*$, where C_0 is chosen so that

$$C_0 > \max_{0 \le t \le T} |\nabla m|.$$

Then

where $d \leq 3$ is the dimension. Notice that the $O(h^2)$ term is smooth. Summation by parts in I_4 leads to

$$I_4| \leq \sum_j O(h^2) |\nabla_h e_j| h^d \leq O(h^4) + \sum_j |\nabla_h e_j|^2 h^d$$
$$h^d \sum_j |\nabla_h e_j|^2 \leq Ch^2$$
(2.15)

(2.13) implies that

where C depends on C_0 and m only.

The assumption (2.14) can be dealt with using Strang's trick. Namely, we construct a correction to the exact solution in the form

$$\bar{m}(x,t) = m(x,t) + h^2 m_1(x,t)$$

such that \bar{m} satisfies the difference equation with higher order accuracy:

$$\frac{d\bar{m}_j}{dt} = \bar{m}_j \times \Delta_h \bar{m}_j - \gamma \bar{m}_j \times (\bar{m}_j \times \Delta_h \bar{m}_j) + O(h^4)$$

where $\bar{m}_j(t) = \bar{m}(x_j, t)$. For this purpose, it is necessary and sufficient that m_1 satisfy

$$m_{1t} = \frac{1}{12}m \times D^4m + m \times \Delta m_1 + m_1 \times \Delta m + \gamma \Big[\frac{1}{12}m \times (m \times D^4m) + m \times (m \times \Delta m_1)\Big].$$
(2.16)

where

$$D^4 = \sum_i \partial_{x_i}^4$$

The initial condition is $m_1(x,0) = 0$ and boundary condition is $\frac{\partial m_1}{\partial n}|_{\Gamma} = 0$. Equation (2.16) is a second order linear parabolic system in m_1 . The existence and uniqueness follows from the general theory in [5].

We have, for h small enough

$$\max_{j} |\nabla \bar{m}_{j}(t)| \le C_{0} \tag{2.17}$$

for $0 \leq t \leq T$. From continuity, there exist δ small enough, such that

$$\max_{j} |\nabla_h m_j(t)| \le 2C_0 \tag{2.18}$$

for $0 \leq t \leq \delta$. This means that $T^* > \delta$.

Now proceed as in (2.12)-(2.15), we get

$$h^d \sum_j |\nabla_h(\bar{m} - m_j)|^2 \le Ch^4$$

for $0 \leq t \leq \delta$ for some C depending on C_0 and \bar{m} only. Therefore

$$|\nabla(\bar{m}_j - m_j)|^2 \le Ch^{4-d} \le Ch$$
$$|\nabla m_j|^2 \le 2(|\nabla \bar{m}_j|^2 + Ch) \le 3C_0^2$$

when h is small enough. This shows that the condition (2.18) will never be violated and T^* can be any preset positive value T if h is small enough, depending only on T. This completes the proof.

3 Temporal discretization

Again we will look first at the equation for the heat flow of harmonic map, (1.12), and then extend our results to the Landau-Lifshitz equation (1.1).

The main purpose of this section is to construct time discretization procedures that have good stability property. Since we are mainly concerned with temporal discretizations, we will keep the spatial variables continuous.

3.1 Projection method for the heat flow of harmonic maps

The main idea is to rewrite (1.11) as

$$m_t = \Delta m + \lambda m \tag{3.1}$$

and view $\lambda = |\nabla m|^2$, or $\lambda = -(m, \Delta m)$ as the Lagrange multiplier for the pointwise constraint (m, m) = 1.

Projection method is a fractional step procedure in which an intermediate magnetization field, called m^* , is first computed by disregarding the constraint and the Lagrange multiplier. The intermediate field m^* is then projected to S^2 to obtain the numerical solution at the next time step. The simplest example of such a projection method is the following algorithm:

Knowing $\{m^n\}$, $\{m^{n+1}\}$ is computed by: Step 1: Solve

$$\frac{m^* - m^n}{\Delta t} = \Delta m^* \tag{3.2}$$

with the boundary condition

$$\frac{\partial m^*}{\partial n}|_{\Gamma} = 0 \tag{3.3}$$

Step 2:

$$m^{n+1} = \frac{m^*}{|m^*|} \tag{3.4}$$

The simplicity of such a scheme is obvious.

Direct calculation of local truncation error shows that the scheme is of first order accuracy. More generally, consider the equation

$$m_t = h - (m, h)m = -m \times (m \times h) \tag{3.5}$$

The analog of the projection method (3.2)-(3.4) for this equation is

$$\frac{m^* - m^n}{\Delta t} = h(t^{n+1}) \tag{3.6}$$

$$m^{n+1} = \frac{m^*}{|m^*|} \tag{3.7}$$

It is easy to check that this method is first order accurate.

To verify the first order convergence of the projection method, we again use the exact solution (2.6) for (1.11) with a forcing term. The following table gives $\frac{e_{max}}{\Delta t}$ where e_{max} is the maximum error.

	$e_{max}/\Delta t$						
T	$\Delta t = 0.01$	$\Delta t = 0.005$	$\Delta t = 0.0025$				
0.2000	0.1100	0.0878	0.0679				
0.4000	0.1172	0.0907	0.0684				
0.6000	0.1197	0.0915	0.0684				
0.8000	0.1207	0.0918	0.0684				
1.0000	0.1211	0.0919	0.0684				

For this particular example, the scheme provides an accuracy slightly higher than first order.

Next, we prove that (3.2)-(3.4) is unconditionally stable and convergent with first order accuracy.

Theorem 2: Let $m(x,t) \in L^{\infty}([0,T], H^3)$ be a smooth solution of (1.12) with initial data $m(x,0) = m_0(x)$. Let $m_{\Delta t}$ be the numerical solution of (3.2)-(3.4) with the same initial data. Then we have

$$\max_{x \in \Omega} |m(x, t^n) - m_{\Delta t}(x, t^n)| \le C(t^n) \Delta t$$
(3.8)

where $t^n = n\Delta t, n = 1, 2, 3, ...$ and C(t) depends only on m.

Proof: We begin by rewriting (3.2)-(3.4) as

$$m^{n+1} = \frac{(I - \Delta t \Delta)^{-1} m^n}{|(I - \Delta t \Delta)^{-1} m^n|}$$
(3.9)

It is understood in (3.9) that the Neumann boundary condition is imposed when inverting $I - \Delta t \Delta$. Standard local truncation error analysis gives

$$m(x,t^{n+1}) = \frac{(I - \Delta t \Delta)^{-1} m(x,t^n)}{|(I - \Delta t \Delta)^{-1} m(x,t^n)|} + O(\Delta t^2)$$
(3.10)

if m satisfies (1.12).

In order to deal with the nonlinear recursion relation that arises in the analysis of the error, we will need an adaptation of Strang's trick [11] by constructing a correction of the exact solution of (1.12) which satisfies (3.10) to higher order accuracy. To do this, let

$$\tilde{m}(x,t) = m(x,t) + \Delta t m_1(x,t) + \Delta t^2 m_2(x,t)$$
(3.11)

We will choose m_1 and m_2 such that

$$\tilde{m}(x,t^{n+1}) = \frac{(I - \Delta t \Delta)^{-1} \tilde{m}(x,t^n)}{|(I - \Delta t \Delta)^{-1} \tilde{m}(x,t^n)|} + O(\Delta t^3)$$
(3.12)

This is a tedious, but straightforward calculation. The key steps of this calculation are summarized below.

$$|(I - \Delta t \Delta)^{-1} \tilde{m}|^2 = 1 + 2\Delta t (m, m_1 + \Delta m) + \Delta t^2 (2(m, m_2 + \Delta^2 m + \Delta m_1) + |m_1 + \Delta m|^2) + O(\Delta t^3)$$
(3.13)

$$|(I - \Delta t \Delta)^{-1} \tilde{m}|^{-1} = 1 - \Delta t (m, m_1 + \Delta m) - \Delta t^2 (m, m_2 + \Delta^2 m + \Delta m_1) - \frac{\Delta t^2}{2} |m_1 + \Delta m|^2 + \frac{3}{2} \Delta t^2 (m, m_1 + \Delta m)^2 + O(\Delta t^3)$$
(3.14)

$$\frac{(I - \Delta t \Delta)^{-1} \tilde{m}}{|(I - \Delta t \Delta)^{-1} \tilde{m}|} = m + \Delta t m_1 + \Delta t^2 m_2 + \Delta t \Delta m + \Delta t^2 \Delta m_1 + \Delta t^2 \Delta^2 m$$

$$- \Delta t (m, m_1 + \Delta m) m - \Delta t^2 (m, \Delta m_1) m$$

$$- \Delta t^2 (m, m_1 + \Delta m) m_1 - \Delta t^2 (m, m_1 + \Delta m) \Delta m$$

$$- \Delta t^2 [(m, m_2 + \Delta^2 m) + \frac{1}{2} |m_1 + \Delta m|^2$$

$$- \frac{3}{2} (m, m_1 + \Delta m)^2]m + O(\Delta t^3)$$
(3.15)

From (3.15), we see that in order to satisfy (3.12), m_1 and m_2 must obey

$$(m_1, m) = 0 \tag{3.16}$$

$$\frac{\partial m_1}{\partial t} + \frac{1}{2} \frac{\partial^2 m}{\partial t^2} = \Delta \tilde{m}_1 - (m, \Delta m) \tilde{m}_1
- \left\{ (m, \Delta \tilde{m}_1) + \frac{1}{2} |\tilde{m}_1|^2
- \frac{3}{2} (m, \Delta m)^2 + (m, m_2) \right\} m$$
(3.17)

where $\tilde{m}_1 = m_1 + \Delta m$. We can rewrite (3.17) as

$$\frac{\partial m_1}{\partial t} = \Delta m_1 + a(x,t)m_1 + b(x,t) - \mu m \tag{3.18}$$

where $a(x,t) = |\nabla m|^2$, $b(x,t) = \Delta^2 m + |\nabla m|^2 \Delta m - \frac{1}{2}m_{tt}$ are known functions depending on m(x,t). $\mu(x,t)$ can be viewed as the Lagrangian multiplier for the constraint (3.16). In Appendix A, we show that with initial and boundary conditions

$$m_1(x,0) = 0, \quad \frac{\partial m_1}{\partial n}\Big|_{\Gamma} = 0$$
 (3.19)

there exists an unique $\mu(x,t)$ such that the solution $m_1(x,t)$ of the linear equation (3.18) satisfies (3.16). Once m_1 is determined, m_2 is chosen so that (3.17) and (3.18) are consistant. This completes the construction of \tilde{m} .

Now we can proceed with the error estimates. Let $e^n(x) = m^n(x) - \tilde{m}(x, t^n)$, $\bar{m} = (I - \Delta t \Delta)^{-1} \tilde{m}(t^n)$, $\tilde{e} = m^* - \bar{m}$. Then from (3.12), we have

$$e^{n+1} = m^{n+1} - \tilde{m}(x, t^{n+1}) = \frac{m^*}{|m^*|} - \frac{\bar{m}}{|\bar{m}|} + O(\Delta t^3)$$
(3.20)

Using the elementary inequality:

$$\left|\frac{m^{\star}}{|m^{\star}|} - \frac{\bar{m}}{|\bar{m}|}\right| \le \max\left(\frac{1}{|m^{\star}|, |\bar{m}|}\right)|m^{\star} - \bar{m}|, \tag{3.21}$$

we obtain

$$|e^{n+1}| \le \max\left(\frac{1}{|m^*|}, \frac{1}{|\bar{m}|}\right)|\tilde{e}| + O(\Delta t^3)$$
 (3.22)

Lemma 1: Assume that

$$(I - \Delta)u = f \tag{3.23}$$

$$\frac{\partial u}{\partial n}\Big|_{\Gamma} = 0 \tag{3.24}$$

where $u = (u_1, u_2, u_3)$, $f = (f_1, f_2, f_3)$. Then

$$\max_{x} |u| \le \max_{x} |f| \tag{3.25}$$

Proof: A direct computation gives

$$\Delta |u| = \frac{1}{|u|} \Big[(u, \Delta u) + |\nabla u|^2 - \frac{|(u, \nabla u)|^2}{|u|^2} \Big]$$
(3.26)

Therefore

$$(I - \Delta)|u| = |u| - \Delta|u|$$

= $\frac{1}{|u|}(u, f) - \frac{1}{|u|} \left(|\nabla u|^2 - \frac{|(u, \nabla u)|^2}{|u|^2} \right)$
 $\leq \frac{1}{|u|}(u, f) \leq |f|$ (3.27)

We also have $\frac{\partial}{\partial n}|u| = 0$ at the boundary. Now (3.25) follows directly from the strong maximum principle.

Continue now with the proof of the theorem. We have from (3.22) and the previous lemma, that

$$|e^{n+1}| \le \max\left(\frac{1}{|m^{\star}|, |\bar{m}|}\right)|e^{n}| + O(\Delta t^{3})$$
(3.28)

Let T^{\star} be a time (which may depend on Δt) such that

$$\frac{1}{|m^*|} \le \frac{1}{|\bar{m}|} + \Delta t \tag{3.29}$$

for $0 \le t \le T^{\star}$. Since $\frac{1}{|m|} \le 1 + C\Delta t$ for some constant C which depends only on t and m, we get

$$|e^{n+1}| \le (1 + C\Delta t)|e^n| + O(\Delta t^3)$$
(3.30)

for a different C. Therefore

$$e^{n+1}| \le C_0 \Delta t^2 \tag{3.31}$$

if $n\Delta t \leq T^*$. Here C_0 does not depend on Δt .

Now let us estimate T^* . Assume that (3.29) holds for $0 \le t \le n\Delta t$. Then for $t = (n+1)\Delta t$,

$$\frac{1}{|m^{\star}|} - \frac{1}{|\bar{m}|} \le \frac{|m^{\star} - \bar{m}|}{|m^{\star}||\bar{m}|} \le \frac{C_o \Delta t^2}{|m^{\star}||\bar{m}|} \le \frac{C \Delta t^2}{|m^{\star}|}$$
(3.32)

Hence

$$\frac{1}{|m^{\star}|} \leq \frac{1}{1 - C\Delta t^2} \frac{1}{|\bar{m}|} \\
\leq \frac{1}{|\bar{m}|} + C_1 \Delta t^2$$
(3.33)

where C_1 does not depend on Δt . If Δt is small enough such that $C_1\Delta t < 1$, we see that (3.29) is still satisfied at $(n+1)\Delta t$. This argument shows that T^* can be any preset positive value T by choosing Δt small enough, depending only on T. This completes the proof.

3.2 The second order scheme

Our next task is to look for the second order versions of the projection method. It is easy to check that the two-step method

$$\frac{m^{\star} - m^{n}}{\Delta t} = \Delta \frac{m^{\star} + m^{n}}{2}$$

$$m^{n+1} = \frac{m^{\star}}{|m^{\star}|}$$
(3.34)

gives only a first order accurate approximation. However, we can add correction terms to (3.34) to achieve the second order accuracy.

We solve the heat flow of harmonic map

$$m_t = \Delta m + |\nabla m|^2 m \tag{3.35}$$

with the following scheme

$$\frac{m^* - m^n}{\Delta t} = \alpha \Delta m^* + f(m^n) + \Delta t g(m^n)$$
(3.36)

$$m^{n+1} = \frac{m^*}{|m^*|} \tag{3.37}$$

where α , f and g are to be determined so that the scheme is second order, i.e.

$$m|_{t=t^{n+1}} = \frac{(I - \alpha \Delta t \Delta)^{-1} (m + \Delta t f + (\Delta t)^2 g)}{|(I - \alpha \Delta t \Delta)^{-1} (m + \Delta t f + (\Delta t)^2 g)|} |_{t=t^n} + O((\Delta t)^3)$$

$$= \frac{H(t)}{|H(t)|} |_{t=t^n} + O((\Delta t)^3)$$
(3.38)

where

$$H(t) = (I - \alpha \Delta t \Delta)^{-1} (m(t) + \Delta t f(m(t)) + (\Delta t)^2 g(m(t)))$$
(3.39)

$$\approx m + \Delta t (f + \alpha \Delta m) + (\Delta t)^2 (g + \alpha \Delta f + \alpha^2 \Delta^2 m).$$
(3.40)

Simple calculations (in Appendix) show that we shall take

$$f = \frac{1}{2}\Delta m$$

and

$$g = \nabla(|\nabla m|^2) \cdot \nabla m.$$

i.e. $g_j = \nabla(|\nabla m|^2) \cdot \nabla m_j$ for j = 1, 2 and 3. Therefore, we have a second order scheme

$$\frac{m^* - m^n}{\Delta t} = \frac{1}{2} (\Delta m^* + \Delta m^n) + \Delta t \nabla (|\nabla m^n|^2) \cdot \nabla m^n$$
(3.41)

$$m^{n+1} = \frac{m^*}{|m^*|} \tag{3.42}$$

Note that (3.41) is no longer unconditionally stable due to the the form of the correction term. However, it is easy to see that the CFL condition is $\frac{dt}{dx} \leq C$. For the example S6 in Section 4, C is calculated numerically to be 0.509.

3.3 Extension to the Landau-Lifshitz equation

To extend the projection method to the Landau-Lifshitz equation, we will use (1.7). To simplify writing we will omit the coefficients γ and $\frac{1+\gamma^2}{\gamma}$ and consider

$$m_t - m \times m_t = -m \times (m \times \Delta m) = \Delta m + |\nabla m|^2 m$$
(3.43)

The simplest projection scheme for (3.43) is given by the following two step procedure

$$\frac{m^* - m^n}{\Delta t} - m^n \times \frac{m^* - m^n}{\Delta t} = \Delta m^* \tag{3.44}$$

with the boundary condition $\frac{\partial m^*}{\partial n}|_{\Gamma} = 0$, and

$$m^{n+1} = \frac{m^*}{|m^*|} \tag{3.45}$$

We can formally write (3.44)-(3.45) as

$$m^{n+1} = \frac{(I - m^n \times -\Delta t\Delta)^{-1}m^n}{|(I - m^n \times -\Delta t\Delta)^{-1}m^n|}$$
(3.46)

It is easy to see that the scheme is first order accurate. Similar calculations give a second order scheme as following

$$\begin{cases} \frac{m^* - m^n}{\Delta t} - m^n \times \frac{m^* - m^n}{\Delta t} = \frac{1}{2} (\Delta m^* + \Delta m^n) \\ + (\Delta t)^2 \{ \nabla (|\nabla m^n|^2) \cdot \nabla m^n + \frac{1}{2} |\nabla m^n|^2 B \Delta m^n \} \\ m^{n+1} = \frac{m^*}{|m^*|} \end{cases}$$
(3.47)

where

$$B = (I - m^n \times)^{-1} - I$$

Again, convergence of the scheme (3.44) and (3.45) is verified by computing the exact solution (2.6) for equation (3.43) with a forcing term. The following table shows the ratio of the maximum error to Δt for different Δt . A slightly better than first order accuracy is obtained in this case.

	$e_{max}/\Delta t$							
T	$\Delta t = 0.01$	$\Delta t = 0.005$	$\Delta t = 0.0025$					
0.200000	3.831069	3.179168	2.555914					
0.400000	4.015820	3.355095	2.747515					
0.600000	4.230660	3.535197	2.950982					
0.800000	4.399771	3.680398	3.126004					
1.000000	4.558102	3.825170	3.287008					

4 Comparison of the performances of various numerical schemes

In this section, we present numerical results for equations (1.11), (1.12) and (2.9) in one dimension. We will compare the results for various schemes. The equations are solved on interval $[0, \pi]$ with initial conditions

$$m(x,0) = \begin{pmatrix} \cos(x/2)\sin(x)\\ \sin(x/2)\sin(x)\\ \cos(x) \end{pmatrix}$$

The "exact" solution is calculated by the fourth order Runge-Kutta scheme in time and the second order center difference with 800 grid points and $\Delta t = 10^{-6}$.

We will give numerical results for the following schemes:

(1) Forward Euler for (1.11)

$$\frac{m^{n+1} - m^n}{\Delta t} = -m^n \times (m^n \times \Delta_h m^n) \tag{S1}$$

(2) Forward Euler for (1.12)

$$\frac{m^{n+1} - m^n}{\Delta t} = \Delta_h m^n + |\nabla_h m^n|^2 m^n \tag{S2}$$

(3) Forward Euler for (2.9)

$$\frac{m^{n+1} - m^n}{\Delta t} = (m^n, m^n)\Delta_h m^n + |\nabla_h m^n|^2 m^n$$
(S3)

(4) Backward Euler for (1.12)

$$\frac{m^{n+1} - m^n}{\Delta t} = \Delta_h m^{n+1} + |\nabla_h m^n|^2 m^n \tag{S4}$$

(5) The first order projection method for (1.12)

$$\begin{cases} \frac{m^* - m^n}{\Delta t} = \Delta_h m^* \\ m^{n+1} = \frac{m^*}{|m^*|} \end{cases}$$
(S5)

(6) The second order projection method for (1.12)

$$\begin{cases} \frac{m^* - m^n}{\Delta t} = \Delta_h \frac{m^* + m^n}{2} + \Delta t \nabla_h (|\nabla_h m^n|^2) \nabla_h m^n \\ m^{n+1} = \frac{m^*}{|m^*|} \end{cases}$$
(S6)

The following table shows the error for these schemes with $\Delta t = 0.0001$, $\Delta x = \pi/200$. For S2, the error grows too fast. Stable results for S3, S4, S5 can also be obtained with Δt as large as 0.1 for the Δx given above. For S6, Δt is slightly restrictive to 0.08. However, S1 can only be run for $\Delta t = 0.0001$ due to CFL condition.

The results show that for the first order schmes, the accuracy for S1 and S5 are comparable and both are much better than S2, S3, and S4. However S5 is unconditionally stable (although more expensive) while S1 is restricted by the CFL condition. Therefore the projection scheme is a better scheme not only for its simplicity but also for its stability and accuracy.

Т	S1	S2	S3	S4	S5	$\mathbf{S6}$
0.5	0.75291 E-05		0.60626E-01	0.48056 E-04	0.34438E-04	0.93681E-05
1.0	0.63458E-05		0.80183E-01	0.11777E-03	0.14998 E-04	0.41371E-05
1.5	0.59942 E-05		$0.11340 \mathrm{E}{+00}$	0.24742 E-03	0.51972 E-05	0.14723 E-05
2.0	0.59510 E-05		0.12362E + 00	0.46078 E-03	0.24537 E-05	0.67426 E-06
2.5	0.59471 E-05		0.12292E + 00	0.81217 E-03	0.24376 E-05	0.55257 E-06
3.0	0.59468E-05		$0.12275E{+}00$	0.13906E-02	0.24354 E-05	0.54592 E-06
3.5	0.59468E-05		0.12273E + 00	0.23421 E-02	0.24350 E-05	0.54819E-06
4.0	0.59468E-05		0.12273E + 00	0.39047 E-02	0.24350 E-05	0.55060 E-06
4.5	0.59468E-05		0.12273E + 00	0.64647 E-02	0.24350 E-05	0.55304 E-06
5.0	0.59468E-05		$0.12273E{+}00$	0.10642 E-01	0.24350 E-05	0.55573 E-06
CPU(seconds)	22.64		28.66	44.45	40.60	56.21

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5 Appendix A: A proof of existence of Lagrangian multiplier

Let G(x, y, t) be the Green's function for the equation

$$u_t = \Delta u + a(x, t)u$$

with boundary condition

$$\frac{\partial u}{\partial n}\Big|_{\Gamma} = 0,$$

the solution of (3.18) is given by

$$m_1(x,t) = \int_0^t \int_{\Omega} G(x,y,t-s)(b(y,s) - \mu(y,s)m(y,s))dyds.$$

If we require

$$(m_1,m)=0,$$

then we have

$$\int_{0}^{t} \int_{\Omega} G(x, y, t - s) \mu(y, s)(m(y, s), m(x, t)) dy ds$$

=
$$\int_{0}^{t} \int_{\Omega} G(x, y, t - s)(b(y, s), m(x, t)) dy ds = f(x, t)$$
(5.1)

Differentiate with respect to t, we have

$$\mu(x,t) + \int_{0}^{t} \int_{\Omega} G_{t}(x,y,t-s)\mu(y,s)(m(y,s),m(x,t))dyds + \int_{0}^{t} \int_{\Omega} G(x,y,t-s)\mu(y,s)(m(y,s),m_{t}(x,t))dyds = f_{t}(x,t)$$
(5.2)

Apply the Laplacian to (5.1), we have

$$\int_{0}^{t} \int_{\Omega} \Delta G(x, y, t - s) \mu(y, s)(m(y, s), m(x, t)) dy ds + 2 \sum_{k} \int_{0}^{t} \int_{\Omega} G_{x_{k}}(x, y, t - s) \mu(y, s)(m(y, s), m_{x_{k}}(x, t)) dy ds + \int_{0}^{t} \int_{\Omega} G(x, y, t - s) \mu(y, s)(m(y, s), \Delta m_{t}(x, t)) dy ds = \Delta f(x, t)$$
(5.3)

(5.2)-(5.3) gives

$$\mu(x,t) + \int_0^t \int_{\Omega} G(x,y,t-s)\mu(y,s)(m(y,s),m_t(x,t))dyds$$

$$- 2\sum_{k} \int_{0}^{t} \int_{\Omega} G_{x_{k}}(x, y, t - s) \mu(y, s)(m(y, s), m_{x_{k}}(x, t)) dy ds - \int_{0}^{t} \int_{\Omega} G(x, y, t - s) \mu(y, s)(m(y, s), \Delta m(x, t)) dy ds - \int_{0}^{t} \int_{\Omega} G(x, y, t - s) a(x, t - s) \mu(y, s)(m(y, s), m(x, t)) dy ds = f_{t} - \Delta f = f^{*}(x, t)$$
(5.4)

We are going to prove the existence of solution $\mu(x, t)$ for (5.4) by a fixed point argument.

Since m(x, t) is given, we may assume that

$$\sup_{x,y\in\Omega;s\leq t\leq T} \left\{ \left| (m(y,s), \nabla m(x,t)) \right|, \left| (m(y,s), \Delta m(x,t)) \right|, \\ \left| (m(y,s), m_t(x,t)) \right|, \left| a(x,t-s)(m(y,s), m(x,t)) \right| \right\} \leq M$$

where M is a constant. The Green's function G(x, y, t) satisfies the following properties (see e.g. [3])

$$\int_{\Omega} |G(x, y, t)| dy \le C_1 \quad 0 < t < T$$
(5.5)

$$\int_{\Omega} |\nabla_x G(x, y, t)| dy \le \frac{C_2}{\sqrt{t}} \quad 0 < t < T$$
(5.6)

Here C_1, C_2 are constants. It is easy to see that (5.5) (5.6) are true for the heat kernel

$$K(x, y, t) = \frac{1}{2^n (\pi t)^{\frac{n}{2}}} exp[-\frac{\sum (x_i - y_i)^2}{4t}]$$

and K(x, y, t) is the leading approximation to G(x, y, t) near the singularity [3].

The fixed point argument is formulated as following

$$\mu^{n+1}(x,t) + \int_{0}^{t} \int_{\Omega} G(x,y,t-s)\mu^{n}(y,s)(m(y,s),m_{t}(x,t))dyds - 2\sum_{k} \int_{0}^{t} \int_{\Omega} G_{x_{k}}(x,y,t-s)\mu^{n}(y,s)(m(y,s),m_{x_{k}}(x,t))dyds - \int_{0}^{t} \int_{\Omega} G(x,y,t-s)\mu^{n}(y,s)(m(y,s),\Delta m(x,t))dyds - \int_{0}^{t} \int_{\Omega} G(x,y,t-s)a(x,t-s)\mu^{n}(y,s)(m(y,s),m(x,t))dyds = f_{t} - \Delta f = f^{*}(x,t)$$
(5.7)

Let

$$A^{n}(t) = \sup \left\{ |\mu^{n}(x,s) - \mu^{n-1}(x,s)| \mid x \in \Omega, 0 < s < t \right\},$$

then we have the following estimate from (5.7)

$$A^{n+1}(t) \le C \int_0^t \frac{1}{\sqrt{t-s}} A^n(s) ds + C \int_0^t A^n(s) ds.$$

for some constant C. A standard fixed point argument will then show that $\mu^n(x, t)$ converges uniformly and therefore we have a unique solution for (5.4).

6 Appendix B: Derivation of the second order scheme

The right hand side of (3.39)

$$\begin{aligned} \frac{H}{|H|} + O((\Delta t)^3) &= m + \Delta t (f + \alpha \Delta m - (m, f + \alpha \Delta m)m) \\ &+ (\Delta t)^2 (g + \alpha \Delta f + \alpha^2 \Delta^2 m - (m, f + \alpha \Delta m)(f + \alpha \Delta m)) \\ &- (m, g + \alpha \Delta f + \alpha^2 \Delta^2 m)m - \frac{1}{2} |f + \alpha \Delta m|^2 m \\ &+ \frac{3}{2} (m, f + \alpha \Delta m)^2 m) + O((\Delta t)^3) \end{aligned}$$

The left hand side of (3.39) can be expended to

$$m_{t=t^{n+1}} = m + m_t \Delta t + \frac{1}{2} m_{tt} (\Delta t)^2 |_{t=t^n} + O(\Delta t)^3)$$

In order that (3.38) is satisfied, we need

$$m_t = f + \alpha \Delta m - (m, f + \alpha \Delta m)m \tag{6.1}$$

and

$$\frac{1}{2}m_{tt} = g + \alpha\Delta f + \alpha^{2}\Delta^{2}m - (m, f + \alpha\Delta m)(f + \alpha\Delta m)$$

- $(m, g + \alpha\Delta f + \alpha^{2}\Delta^{2}m)m - \frac{1}{2}|f + \alpha\Delta m|^{2}m$
+ $\frac{3}{2}(m, f + \alpha\Delta m)^{2}m$ (6.2)

From (3.35), we have that

$$\frac{1}{2}m_{tt} = \frac{1}{2}(\Delta m + |\nabla m|^2 m)_t$$

$$= \frac{1}{2}\Delta^2 m + \frac{1}{2}\Delta(|\nabla m|^2)m + \nabla(|\nabla m|^2)\nabla m$$

$$+ |\nabla m|^2\Delta m + (\nabla m \cdot \Delta \nabla m)m + \frac{3}{2}|\nabla m|^4 m$$
(6.3)

(3.35) and (6.1) imply that

 $f = (1 - \alpha)\Delta m.$

We will take $\alpha = \frac{1}{2}$, $f = \frac{1}{2}\Delta m$. Assuming (g, m) = 0 and equating right handside of (6.2) and (6.3), we have

$$g = \nabla(|\nabla m|^2)\nabla m$$

Therefore, we have a second order scheme

$$\frac{m^* - m^n}{\Delta t} = \frac{1}{2} (\Delta m^* + \Delta m^n) + \Delta t \nabla (|\nabla m^n|^2) \nabla m^n$$
(6.4)

$$m^{n+1} = \frac{m^*}{|m^*|} \tag{6.5}$$