A GPU simulation of skyrmion

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I. LLG

The Landau-Lifshitz-Gilbert-Equation (LLG) can be written as (Eq. (13) of Ref. [1] and Eq. (7) of Ref. [2], NOTE that the sign of the last term is '+' in Eq. (7) of Ref. [2])

$$\dot{\mathbf{n}} = \gamma \mathbf{B}_{\text{eff}} \times \mathbf{n} - \frac{\alpha\gamma}{|n|}\mathbf{n} \times \dot{\mathbf{n}} - \frac{\hbar\gamma}{2e}\left(\mathbf{j}\cdot\nabla\right)\mathbf{n} \tag{1}$$

where $\mathbf{n}$ is the magnetic momentum, $\gamma(\gamma > 0)$ is the gyromagnetic ratio, α represents Gilbert damping, $\mathbf{B}_{\text{eff}}$ is the effective field arising from the spin Hamiltonian, and can be written as (H_S is from Ref. [2], before Eq. (1), also Eq. (4) in Ref. [3])

$$\begin{aligned} &\mathbf{B}_{\text{eff}} \equiv \frac{\delta H_S}{\delta \mathbf{n}} \\ &H_S = \int d^D x \frac{J}{2a}(\nabla \mathbf{n})^2 + \frac{D}{a^2}\mathbf{n}\cdot(\nabla\times\mathbf{n}) - \frac{\mu}{a^3}\mathbf{B}\cdot\mathbf{n} \end{aligned} \tag{2}$$

II. LLG IN 2D LATTICE

In the following, for simplicity, we use $\delta = a(\mathbf{e}_x, \mathbf{e}_y)$, $\delta_x = a\mathbf{e}_x, \delta_y = a\mathbf{e}_y$, where a is the distance between two lattice.

A. Spin torque

Written in lattice, so that

$$\left(\mathbf{j}\cdot\nabla\right)\mathbf{n} = \sum_i j_i \partial_i n_x \mathbf{e}_x + \sum_i j_i \partial_i n_y \mathbf{e}_y + \sum_i j_i \partial_i n_z \mathbf{e}_z \tag{3}$$

In 2D, it is

$$\begin{aligned} &\left(\mathbf{j}\cdot\nabla\right)\mathbf{n} = \sum_{i=x,y} j_i(\partial_i n_x \mathbf{e}_x + \partial_i n_y \mathbf{e}_y + \partial_i n_z \mathbf{e}_z) \\ &= \frac{1}{a}\sum_{i=x,y} j_i(\frac{n_x(\mathbf{r}+\delta_i) - n_x(\mathbf{r}-\delta_i)}{2}\mathbf{e}_x + \frac{n_y(\mathbf{r}+\delta_i) - n_y(\mathbf{r}-\delta_i)}{2}\mathbf{e}_y + \frac{n_z(\mathbf{r}+\delta_i) - n_z(\mathbf{r}-\delta_i)}{2}\mathbf{e}_z) \\ &= \frac{1}{a}\sum_{i=x,y} j_i \frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} \end{aligned} \tag{4}$$

Sometimes, it is also written as (see last term in Eq. (8) in Ref. [4], it also says this is the discrete version of the continuous term $(\mathbf{j}\cdot\nabla)\mathbf{n}$ before Eq. (10))

$$\left(\mathbf{j}\cdot\nabla\right)\mathbf{n} = \frac{1}{a}\sum_{i=x,y} j_i \mathbf{n}(\mathbf{r}) \times \left(\frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} \times \mathbf{n}(\mathbf{r})\right) \tag{5}$$

that is because, for a unit vector, one have

$$\mathbf{n}\cdot\partial_i \mathbf{n} = 0 \tag{6}$$

the discrete version is

$$\mathbf{n}(\mathbf{r}) \cdot \frac{\mathbf{n}(\mathbf{r}+\delta_{\mathbf{i}}) - \mathbf{n}(\mathbf{r}-\delta_{\mathbf{i}})}{\mathbf{2a}} = \mathbf{0} \tag{7}$$

so that

$$
\begin{aligned}
&\mathbf{n}(\mathbf{r}) \times \left(\frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} \times \mathbf{n}(\mathbf{r}) \right) \\
&= \frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} (\mathbf{n}(\mathbf{r}) \cdot \mathbf{n}(\mathbf{r})) - \mathbf{n}(\mathbf{r}) \left(\mathbf{n}(\mathbf{r}) \cdot \frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} \right) \\
&= \frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2}
\end{aligned} \tag{8}
$$

to be consist with the references, we use

$$
(\mathbf{j} \cdot \nabla) \, \mathbf{n} = \frac{1}{a} \sum_{i=x,y} j_i \mathbf{n}(\mathbf{r}) \times \left(\frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} \times \mathbf{n}(\mathbf{r}) \right) \tag{9}
$$

In simulation, to simplify, we always take the direction of $\mathbf{j}$ as $\mathbf{x}$-axis, so we only have

$$
\frac{1}{a} j_x \mathbf{n}(\mathbf{r}) \times \left(\frac{\mathbf{n}(\mathbf{r}+\delta_x) - \mathbf{n}(\mathbf{r}-\delta_x)}{2} \times \mathbf{n}(\mathbf{r}) \right) \tag{10}
$$

B. J term

$(\nabla \mathbf{n})^2$ is confusing, in 2D, it is in fact $\sum_{i=x,y} (\partial_i \mathbf{n}) \cdot (\partial_i \mathbf{n})$ Consider in 1-dimension, we have

$$
\begin{aligned}
&\mathbf{n}(x) \cdot \partial_i \mathbf{n}(x) = 0 \\
&0 = \sum_{i=x,y} \partial_i \left(\mathbf{n}(x) \cdot \partial_i \mathbf{n}(x) \right) = \sum_{i=x,y} (\partial_i \mathbf{n}) \cdot (\partial_i \mathbf{n}) + \mathbf{n} \cdot (\sum_{i=x,y} (\partial_i)^2) \mathbf{n}
\end{aligned} \tag{11}
$$

In lattice, the derivate can be written as

$$
\frac{d^2}{dx^2} \mathbf{n}(\mathbf{r}) = \frac{1}{a} \left(\mathbf{n}'(\mathbf{r} + \frac{a}{2} \mathbf{e}_x) - \mathbf{n}'(\mathbf{r} - \frac{a}{2} \mathbf{e}_x) \right) \tag{12}
$$

with

$$
\begin{aligned}
\mathbf{n}'(\mathbf{r} + \frac{a}{2} \mathbf{e}_x) &= \frac{1}{a} \left(\mathbf{n}(\mathbf{r} + a\mathbf{e}_x) - \mathbf{n}(\mathbf{r}) \right) \\
\mathbf{n}'(\mathbf{r} - \frac{a}{2} \mathbf{e}_x) &= \frac{1}{a} \left(\mathbf{n}(\mathbf{r}) - \mathbf{n}(\mathbf{r} - a\mathbf{e}_x) \right)
\end{aligned} \tag{13}
$$

so that

$$
(\sum_{i=x,y} (\partial_i)^2) \mathbf{n} = \frac{1}{a^2} \sum_{i=x,y,-x,-y} \mathbf{n}(\mathbf{r}+\delta_i) - 4\mathbf{n}(\mathbf{r}) \tag{14}
$$

and

$$
\mathbf{n} \cdot (\sum_{i=x,y} (\partial_i)^2) \mathbf{n} = \frac{1}{a^2} \sum_{\langle i \rangle} \mathbf{n} \cdot \mathbf{n}_i - 4 \tag{15}
$$

Throw away the constant term

$$
\int d^D x \frac{J}{2a} (\nabla \mathbf{n})^2 = -\frac{J}{2a^3} \sum_{\langle i,j \rangle} \mathbf{n}_i \cdot \mathbf{n}_j \tag{16}
$$

where j are all neighbours of i, $j = i + \delta_x, i - \delta_x, i + \delta_y, i - \delta_y$.

When J is constant, it can also been written as

$$
\int d^D x \frac{J}{2a} (\nabla \mathbf{n})^2 = -\frac{J}{a^3} \sum_{\mathbf{r}} \mathbf{n}(\mathbf{r}) \cdot (\mathbf{n}(\mathbf{r}+\delta_x) + \mathbf{n}(\mathbf{r}+\delta_y)) \tag{17}
$$

C. D term

In 2D, we find

$$
\begin{aligned}
&\mathbf{n}\cdot(\nabla\times\mathbf{n}) = n_x\partial_y n_z - n_y\partial_x n_z + n_z\partial_x n_y - n_z\partial_y n_x \\
&= \frac{1}{2a}\left[(n_x(\mathbf{r})(n_z(\mathbf{r}+\delta_y) - n_z(\mathbf{r}-\delta_y)) - n_z(\mathbf{r})(n_x(\mathbf{r}+\delta_y) - n_x(\mathbf{r}-\delta_y)))\right. \\
&\left.+ (n_z(\mathbf{r})(n_y(\mathbf{r}+\delta_x) - n_y(\mathbf{r}-\delta_x)) - n_y(\mathbf{r})(n_z(\mathbf{r}+\delta_x) - n_z(\mathbf{r}-\delta_x)))\right] \\
&= \frac{1}{2a}\left[(n_x(\mathbf{r})n_z(\mathbf{r}+\delta_y) - n_z(\mathbf{r})n_x(\mathbf{r}+\delta_y)) - (n_x(\mathbf{r})n_z(\mathbf{r}-\delta_y) - n_z(\mathbf{r})n_x(\mathbf{r}-\delta_y))\right. \\
&\left.+ (n_z(\mathbf{r})n_y(\mathbf{r}+\delta_x) - n_y(\mathbf{r})n_z(\mathbf{r}+\delta_x)) - (n_z(\mathbf{r})n_y(\mathbf{r}-\delta_x) - n_y(\mathbf{r})n_z(\mathbf{r}-\delta_x))\right] \\
&= -\frac{1}{2a}\left[\mathbf{n}(\mathbf{r})\cdot(\mathbf{n}(\mathbf{r}+\delta_y)\times\mathbf{e}_y) - \mathbf{n}(\mathbf{r})\cdot(\mathbf{n}(\mathbf{r}-\delta_y)\times\mathbf{e}_y)\right. \\
&\left.+\mathbf{n}(\mathbf{r})\cdot(\mathbf{n}(\mathbf{r}+\delta_x)\times\mathbf{e}_x) - \mathbf{n}(\mathbf{r})\cdot(\mathbf{n}(\mathbf{r}-\delta_x)\times\mathbf{e}_x)\right] \\
&= -\frac{1}{2a^2}\left[\mathbf{n}(\mathbf{r})\times\mathbf{n}(\mathbf{r}+\delta_y)\cdot\delta_y - \mathbf{n}(\mathbf{r})\times\mathbf{n}(\mathbf{r}-\delta_y)\cdot\delta_y\right. \\
&\left.+\mathbf{n}(\mathbf{r})\times\mathbf{n}(\mathbf{r}+\delta_x)\cdot\delta_x - \mathbf{n}(\mathbf{r})\times\mathbf{n}(\mathbf{r}-\delta_x)\cdot\delta_x\right]
\end{aligned} \tag{18}
$$

so, one have

$$
\int d^D x \frac{D}{a^2}\mathbf{n}\cdot(\nabla\times\mathbf{n}) = -\frac{D}{a^4}\sum_{\mathbf{r}}\left(\mathbf{n}(\mathbf{r})\times\mathbf{n}(\mathbf{r}+\delta_x)\cdot\delta_x + \mathbf{n}(\mathbf{r})\times\mathbf{n}(\mathbf{r}+\delta_y)\cdot\delta_y\right) \tag{19}
$$

It is also

$$
\int d^D x \frac{D}{a^2}\mathbf{n}\cdot(\nabla\times\mathbf{n}) = -\frac{D}{a^4}\sum_{\mathbf{r}}\left(\mathbf{n}(\mathbf{r}+\delta_x)\times\delta_x + \mathbf{n}(\mathbf{r}+\delta_y)\times\delta_y\right)\cdot\mathbf{n}(\mathbf{r}) \tag{20}
$$

D. Effective magnetic field

Using the results, we can write the discrete version of H_s as

$$
H_S = \sum_{\mathbf{r}}\left[-\frac{J}{a^3}(\mathbf{n}(\mathbf{r}+\delta_x) + \mathbf{n}(\mathbf{r}+\delta_y)) - \frac{D}{a^3}(\mathbf{n}(\mathbf{r}+\delta_x)\times\mathbf{e}_x + \mathbf{n}(\mathbf{r}+\delta_y)\times\mathbf{e}_y) - \frac{\mu}{a^3}\mathbf{B}\right]\cdot\mathbf{n}(\mathbf{r}) \tag{21}
$$

which leads to

$$
\begin{aligned}
\mathbf{B}_{\text{eff}}(\mathbf{r}) = \frac{\delta H_S}{\delta\mathbf{n}} &= -\frac{1}{a^3}\sum_{i=x,y}\left[J(\mathbf{r})\mathbf{n}(\mathbf{r}+\delta_i) + J(\mathbf{r}-\delta_i)\mathbf{n}(\mathbf{r}-\delta_i)\right] \\
&- \frac{1}{a^3}\sum_{i=x,y}\left[D(\mathbf{r})\mathbf{n}(\mathbf{r}+\delta_i)\times\mathbf{e}_i - D(\mathbf{r}-\delta_i)\mathbf{n}(\mathbf{r}-\delta_i)\times\mathbf{e}_i\right] - \frac{\mu}{a^3}\mathbf{B}(\mathbf{r})
\end{aligned} \tag{22}
$$

E. anisotropy

In some material, the effective Hamiltonian can be written with anisotropy terms as (ignore a, this is as same as Eq. (10) in Ref. spintransfer)

$$
\begin{aligned}
H_S = \sum_{\mathbf{r}}&\left[-\frac{J}{a^3}(\mathbf{n}(\mathbf{r}+\delta_x) + \mathbf{n}(\mathbf{r}+\delta_y)) - \frac{D}{a^3}(\mathbf{n}(\mathbf{r}+\delta_x)\times\mathbf{e}_x + \mathbf{n}(\mathbf{r}+\delta_y)\times\mathbf{e}_y) - \frac{\mu}{a^3}\mathbf{B}\right. \\
&\left.-\mathbf{h}\right]\cdot\mathbf{n}(\mathbf{r}) - K\left(\mathbf{e}_z\cdot\mathbf{n}(\mathbf{r})\right)^2
\end{aligned} \tag{23}
$$

The contribution of $\mathbf{h}$ can be just put into the applied magnetic field $\mathbf{B}$, we also include the contribution of K.

F. dimensionless LLG

Using dimensionless parameters, the LLG can be written as

$$\begin{aligned} \dot{\mathbf{n}} &= \mathbf{B}_{\text{eff}} \times \mathbf{n} - \alpha \mathbf{n} \times \dot{\mathbf{n}} - \sum_{i=x,y} j_i \mathbf{n}(\mathbf{r}) \times \left(\frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} \times \mathbf{n}(\mathbf{r}) \right) \\ \mathbf{B}_{\text{eff}}(\mathbf{r}) &= \frac{\delta H_S}{\delta \mathbf{n}} = -\sum_{i=x,y} \left[J(\mathbf{r})\mathbf{n}(\mathbf{r}+\delta_i) + J(\mathbf{r}-\delta_i)\mathbf{n}(\mathbf{r}-\delta_i) \right] \\ &- \sum_{i=x,y} \left[D(\mathbf{r})\mathbf{n}(\mathbf{r}+\delta_i) \times \mathbf{e}_i - D(\mathbf{r}-\delta_i)\mathbf{n}(\mathbf{r}-\delta_i) \times \mathbf{e}_i \right] - \mathbf{B}(\mathbf{r}) - 2K \left(\mathbf{e}_z \cdot \mathbf{n}(\mathbf{r}) \right) \mathbf{e}_z \end{aligned} \tag{24}$$

Ignoring the anisotropy term, this is as same as Eq. (9) in Ref. [4].

III. EVALUATION

Let $\mathbf{N} = \mathbf{B}_{\text{eff}} \times \mathbf{n} - \sum_{i=x,y} j_i \mathbf{n}(\mathbf{r}) \times \left(\frac{\mathbf{n}(\mathbf{r}+\delta_i) - \mathbf{n}(\mathbf{r}-\delta_i)}{2} \times \mathbf{n}(\mathbf{r}) \right)$, we have

$$\dot{\mathbf{n}} = \mathbf{N} - \alpha \mathbf{n} \times \dot{\mathbf{n}} \tag{25}$$

This is in fact a combine of 3 equations which can be written as

$$\frac{dn_x}{dt} = \frac{1}{1+\alpha^2} \left(\alpha^2 n_x^2 N_x + \alpha(\alpha n_x(n_y N_y + n_z N_z) - n_y N_z + N_y n_z) + N_x \right), \ldots \tag{26}$$

Assuming $\alpha \ll 1$, it can be written as

$$\frac{d\mathbf{n}}{dt} = \mathbf{N} + \alpha \mathbf{N} \times \mathbf{n} + \mathcal{O}(\alpha^2) \tag{27}$$

One can use this to evaluate

$$\mathbf{n}(t+\Delta t) = \mathbf{n}(t) + \Delta t \left(\mathbf{N}(t) + \alpha \mathbf{N}(t) \times \mathbf{n}(t) \right) \tag{28}$$

IV. SIMULATION

The simulation is running on GPU using the compute shader in Unity3D. The implementation of LLG is the LLG_c.compute, the content is

```
// Each #kernel tells which function to compile; you can have many kernels
#pragma kernel CSMain

// Create a RenderTexture with enableRandomWrite flag and set it
// with cs.SetTexture
//RWStructuredBuffer<float3> magneticMomentum;
RWTexture2D<float4> magneticMomentum;
Texture2D<float4> boundaryCondition;
Texture2D<float4> exchangeStrength;

uint2 size;
float K;
float D;
float B;
float jx;
float alpha;
float timestep;

[numthreads(8, 8, 1)]
void CSMain (uint3 id : SV_DispatchThreadID)
{
```

```
    float4 zero4 = float4(0.5f, 0.5f, 0.5f, 1.0f);
    float3 s = magneticMomentum[id.xy].xyz;
    float3 sleft = id.x > 1 ? magneticMomentum[id.xy - uint2(1, 0)].xyz : zero4.xyz;
    float3 sright = id.x < (size.x - 1) ? magneticMomentum[id.xy + uint2(1, 0)].xyz : zero4.xyz;
    float3 sup = id.y > 1 ? magneticMomentum[id.xy - uint2(0, 1)].xyz : zero4.xyz;
    float3 sdown = id.y < (size.y - 1) ? magneticMomentum[id.xy + uint2(0, 1)].xyz : zero4.xyz;
    s = 2.0f * (s - 0.5f);
    sleft = 2.0f * (sleft - 0.5f);
    sright = 2.0f * (sright - 0.5f);
    sup = 2.0f * (sup - 0.5f);
    sdown = 2.0f * (sdown - 0.5f);

    float edge = boundaryCondition[id.xy].r > 0.5f ? 1.0f : 0.0f;

    float j_s = exchangeStrength[id.xy].x;
    float j_left = id.x > 1 ? exchangeStrength[id.xy - uint2(1, 0)].x : 0.0f;
    float j_up = id.y > 1 ? exchangeStrength[id.xy - uint2(0, 1)].x : 0.0f;

    float3 vright = float3(1.0, 0.0, 0.0);
    float3 vdown = float3(0.0, 1.0, 0.0);

    float3 beff = (j_left * sleft + j_s * sright + j_up * sup + j_s * sdown)
        + D * (cross(sright, vright) - cross(sleft, vright) + cross(sdown, vdown) - cross(sup, vdown))
        + float3(0.0f, 0.0f, B) + 2 K * float3(0.0f, 0.0f, s.z);

    float3 stt = -jx * cross(s, cross((sright - sleft) * 0.5f, s));

    float3 newS = cross(s, beff) + stt;
    newS = newS - alpha * cross(s, newS);

    float3 retColor = normalize(s + timestep * newS) * 0.5f + 0.5f;
    magneticMomentum[id.xy] = float4(retColor.r, retColor.g, retColor.b, 1.0f) * edge + (1.0f - edge) * zero4;
}
```

The magnetic momentum is a 512×512 64-bit ARGB texture, only R, G, B channel used. $\mathbf{n} = (2 \times r - 1, 2 \times g - 1, 2 \times b - 1)$.

The boundary condition is a 512×512 alpha 8-bit texture, only R channel used, when $R < 0.5$, it is a defect.

The exchange strength is a 32-bit RFloat texture, generated from a Lua script. For example, a constant exchange strength can be generated from a lua file as

```
-- Exchange Strength is constant
function GetJValueByLatticeIndex(x, y)
    return 2.0
end

-- Need to register the function
return {
    GetJValueByLatticeIndex = GetJValueByLatticeIndex,
}
```

While a pin with $J = 1 + \exp\left(-0.001\rho^2\right)$ at lattice index $(255, 255)$ can be written as

```
-- Exchange Strength is pin
function GetJValueByLatticeIndex(x, y)
    local j0 = 1
    local j1 = 1
    local j2 = 0.001
    local rho = (x - 255) * (x - 255) + (y - 255) * (y - 255)

    return j0 + j1 * math.exp(-1.0 * j2 * rho)
end

-- Need to register the function
return {
    GetJValueByLatticeIndex = GetJValueByLatticeIndex,
}
```

Manual.pdf is a document introduce how to use the pre-built software.

[1] Gen Tatara, Hiroshi Kohno, Junya Shibata, Phys. Rep. 468, 213-301 (2008), 10.1016/j.physrep.2008.07.003, arXiv:0807.2894.
[2] Jiadong Zang, Maxim Mostovoy, Jung Hoon Han, and Naoto Nagaosa, 10.1103/PhysRevLett.107.136804.
[3] Hong Chul Choi, Shi-Zeng Lin, Jian-Xin Zhu, Phys. Rev. B 93, 115112 (2016), 10.1103/PhysRevB.93.115112, arXiv:1601.00933.
[4] Ye-Hua Liu, You-Quan Li, J. Phys.: Condens. Matter 25 076005, 10.1088/0953-8984/25/7/076005, arXiv:1206.5661.
[5] Junichi Iwasaki, Wataru Koshibae, and Naoto Nagaosa, Nano. Lett. 2014, 14, 4432-4437, 10.1021/nl501379k.