

Generating Magnetic Skyrmion Ground States with Generative Adversarial Networks

Bozhidar Trenchev, Srinandan Dasmahapatra, Marijan Beg, Ondrej Hovorka, Natalie Downing

University of Southampton

btrenchev1@gmail.com

Magnetic Skyrmions

Skyrmions are topologically protected non-trivial field configurations [1] observed in chiral magnetic materials [2]. Their **stability**, **nanometer size** and **coherent dynamics** [3] make them attractive candidates for applications such as **race-track-like memories** [4] and **reservoir computing** [5].

Skyrmionic states such as those on Fig. 1 are explored by **minimizing the total energy** of a random initial magnetisation configuration. Current numerical methods are **far from exhaustive** and **computationally expensive**.

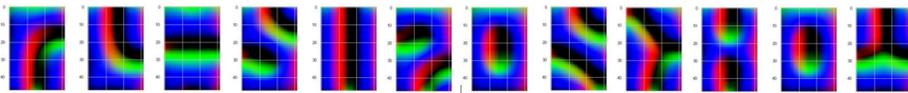


Fig. 1 Example training skyrmion samples of size (48, 32) generated with the micromagnetics simulation software Ubermag with OOMMF as computational backend.

Computational Micromagnetics

The **magnetization field** $\mathbf{M}(\mathbf{r}) = M_s \hat{\mathbf{m}}(\mathbf{r}) \in \mathbb{R}^3$ (a hat denotes a unit length vector) is computed using a **finite-difference method** where \mathbf{r} is restricted to a 2D lattice grid of size (48, 32) or (144, 96).

The **energy** of the system is computed as

$$E[\hat{\mathbf{m}}] = \int [w_{\text{ex}}(\hat{\mathbf{m}}) + w_{\text{dmi}}(\hat{\mathbf{m}}) + w_z(\hat{\mathbf{m}})] d^2\mathbf{r} \quad (1)$$

where $w_{\text{ex}}(\hat{\mathbf{m}})$, $w_{\text{dmi}}(\hat{\mathbf{m}})$, and $w_z(\hat{\mathbf{m}})$ are the symmetric exchange, the Dzyaloshinskii-Moriya and the Zeeman energy densities respectively.

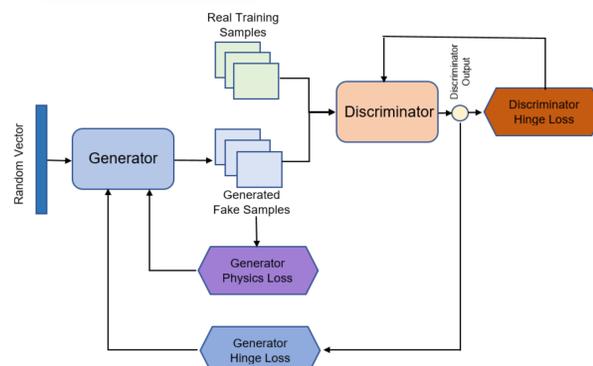
The first variational derivative of the energy functional $E[\hat{\mathbf{m}}]$ with respect to $\hat{\mathbf{m}}$ is called the **effective field** $\mathbf{H}_{\text{eff}}(\hat{\mathbf{m}})$. The magnetisation field dynamics is governed by the **Landau-Lifshitz-Gilbert (LLG) equation** [6]:

$$\frac{d\hat{\mathbf{m}}}{dt} = -\frac{\gamma_0^*}{1+\alpha^2} \hat{\mathbf{m}} \times \mathbf{H}_{\text{eff}} - \frac{\gamma_0^* \alpha}{1+\alpha^2} \hat{\mathbf{m}} \times (\hat{\mathbf{m}} \times \mathbf{H}_{\text{eff}}) =: \ell(\hat{\mathbf{m}}, \mathbf{H}_{\text{eff}}(\hat{\mathbf{m}})) \quad (2)$$

where γ_0^* is the modified gyromagnetic ratio and α is the Gilbert damping, dependent on the skyrmion-hosting material which for this study was chosen to be **FeGe** [7], whose $\alpha = 0.1$. Let $\mathbf{L}_\times := \hat{\mathbf{m}}(\mathbf{r}) \times \mathbf{H}_{\text{eff}}$. A dynamically **steady state** (equilibrium state) is reached when \mathbf{L}_\times is close to 0.

PhysGAN

Our network **PhysGAN**, implemented in Tensorflow and Keras, **reduces the search space** from a random initialisation using the **minimax game** with a **hinge loss** and a **physics loss** which helps reduce the energy of the generated samples and keep them consistent with the FeGe micromagnetic model.



We seek to **generate viable equilibrium configurations** using several custom **Generative Adversarial Networks** [8] that incorporate some of the micromagnetic **physical laws** into their architectures via **physics-aware loss functions**.

Physics Losses

Every L_{phys} loss is computed for a mini-batch of generated samples and reduced to a single number.

- **E loss:** the average $E[\hat{\mathbf{m}}]$;
- **\mathbf{L}_\times loss:** the average of $(\mathbf{L}_\times)^2$ or the norm $|\mathbf{L}_\times|$ or $|\mathbf{L}_\times|^2$;
- **Combined loss:** $\alpha E + \beta |\mathbf{L}_\times|^p$ for $p = 1, 2$;
- **LLG loss:** the average of $\ell(\hat{\mathbf{m}}, \mathbf{H}_{\text{eff}}(\hat{\mathbf{m}}))^2$ or the norm $|\ell(\hat{\mathbf{m}}, \mathbf{H}_{\text{eff}}(\hat{\mathbf{m}}))|$ or $|\ell(\hat{\mathbf{m}}, \mathbf{H}_{\text{eff}}(\hat{\mathbf{m}}))|^2$.

Training Strategies

1. Train the Generator only on L_{phys} ;
2. Train the Generator with both L_{phys} and hinge loss with the Discriminator;
3. First perform hinge-loss-only training or strategy 2 training for several epochs, then train only on L_{phys} .

The training data consists of equilibrium-state skyrmion magnetizations, 'seen' by the network as images.

Evaluation

For every combination of strategy and L_{phys} , samples were generated from a newly-instantiated PhysGAN trained for 1000 epochs. Results were checked **how physically plausible** they were according to the following criteria:

- Are the **samples diverse** and visually **similar** to the **training data**;
- Is the L_{phys} being **reduced** over the epochs;
- Is the average energy density E (AED) and the average cross product \mathbf{L}_\times (ACP) of a batch of generated samples close to reference values computed from the training data which are AED: -8.19×10^4 , ACP: $[1.76, 6.78, 1.83] \times 10^{-4}$.

Results

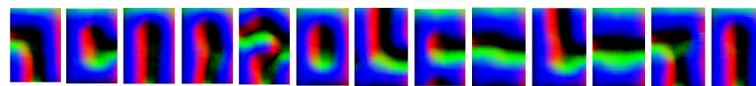


Fig. 2 Output of size (48, 32) of a PhysGAN trained with E loss and strategy 2 for 1000 epochs. AED: -7.7×10^4 , ACP: $[-2623, 1820, 820]$.

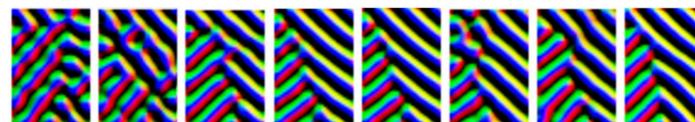


Fig. 3 Output of size (144, 96) of a PhysGAN output (AED: -10^5); trained with strategy 3 on E loss for 100 epochs. Samples from left to right are from epoch 6 to 41 with step of 6. It is noticeable how the Generator finds a more optimal state as the training progresses.

Results

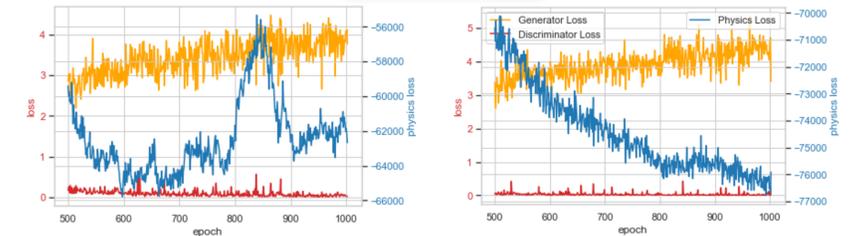


Fig. 4 Left: The average hinge losses and E loss for the last 500 epochs of the training of 10 PhysGANs with only hinge loss, the E is calculated as a score, not applied to the generators' gradients. One such PhysGAN had AED: -6.6×10^4 , ACP: $[-2268, 160, -6512]$. Right: The losses of the training of 10 PhysGANs with E loss and strategy 2 for the last 500 epochs.

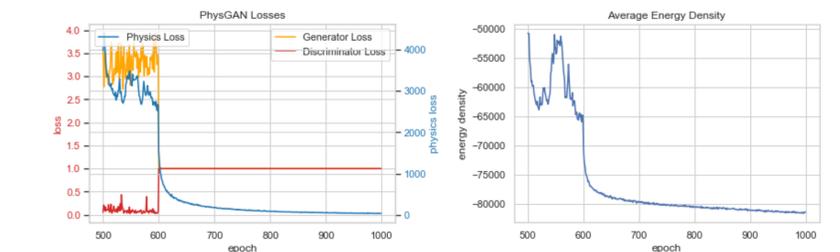


Fig. 5 Left: The losses of a PhysGAN; last 500 epochs; trained with strategy 3 and $|\mathbf{L}_\times|^2$. Switch to $|\mathbf{L}_\times|^2$ -only-training at 600th epoch. AED: -8.2×10^4 , ACP: $[98, -2070, 913]$; Right: AED.

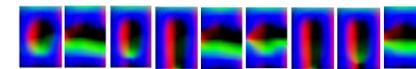


Fig. 7 Output of the Fig. 5 PhysGAN. More diverse samples.

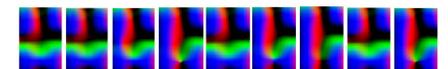


Fig. 8 Output of a PhysGAN trained with strategy 3 and $\ell(\hat{\mathbf{m}}, \mathbf{H}_{\text{eff}}(\hat{\mathbf{m}}))$ loss. Less diversity.

Training with **strategy 1** always led to **mode collapse**. The PhysGANs trained with **strategy 2 and 3** generated **diverse samples** which looked **similar to the training data** as shown in Fig 2 and Fig. 3. The Discriminator and Generator losses maintain **equilibrium** as seen in Fig. 4, whilst reducing the L_{phys} . Strategy 3 also had better L_{phys} reduction, **smoother samples**, but **partial mode collapse**. All losses are good at reducing AED, but the \mathbf{L}_\times and LLG losses reduce the ACP more. Inclusion of L_{phys} makes the generated skyrmions **more consistent** with the **physics model**.

Conclusion

The proposed PhysGAN shows promising although not yet perfect results regarding physics data generation. Future work improvements:

- **Conditional PhysGAN**;
- Vary the parameters dependent on the material. Check what magnetizations arise. This might assist the discovery of **new helimagnetic materials**;
- Apply the core ideas of the PhysGAN to **other scientific domains**.

References

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