SLAC NATIONAL ACCELERATOR LABORATORY

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U.S. DEPARTMENT OF ENERGY

Micromagnetic Simulation of Ultrafast Skyrmion Dynamics in Fe/Gd

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Motivation

Novel physical phenomena often present opportunities for technological advancement, offering insights into unexplored material properties and behaviors that can drive innovation. Magnetic materials serve as a prime testbed for discovering and applying novel spin phases. For example, spin textures can emerge from complex magnetic interactions and geometric effects, which we can understand by exploring their "phase diagram."

In magnetic materials exhibiting long-range spin-spin correlations, the order parameter is often magnetization. The symmetries within this parameter space directly influence material properties. Of particular interest is the skyrmion, a spin vortex with nontrivial topology, acting as a quasiparticle with valuable properties. Chief among these is its long lifetime and the potential to be manipulated with far lower currents than typical information carriers, such as electric charges, making skyrmions an ideal platform for high-performance information technology.

Our project aims to explore the ultrafast time dynamics of the skyrmion phase under the influence of an external magnetic field (H field) using micromagnetic tools. This requires, first of all, developing an understanding of the dynamics that inform how to encode and manipulate information within these quasiparticles as quickly as possible, and secondly, utilizing the novel tools enabled by LCLS-II X-ray free-electron lasers to characterize these changes.

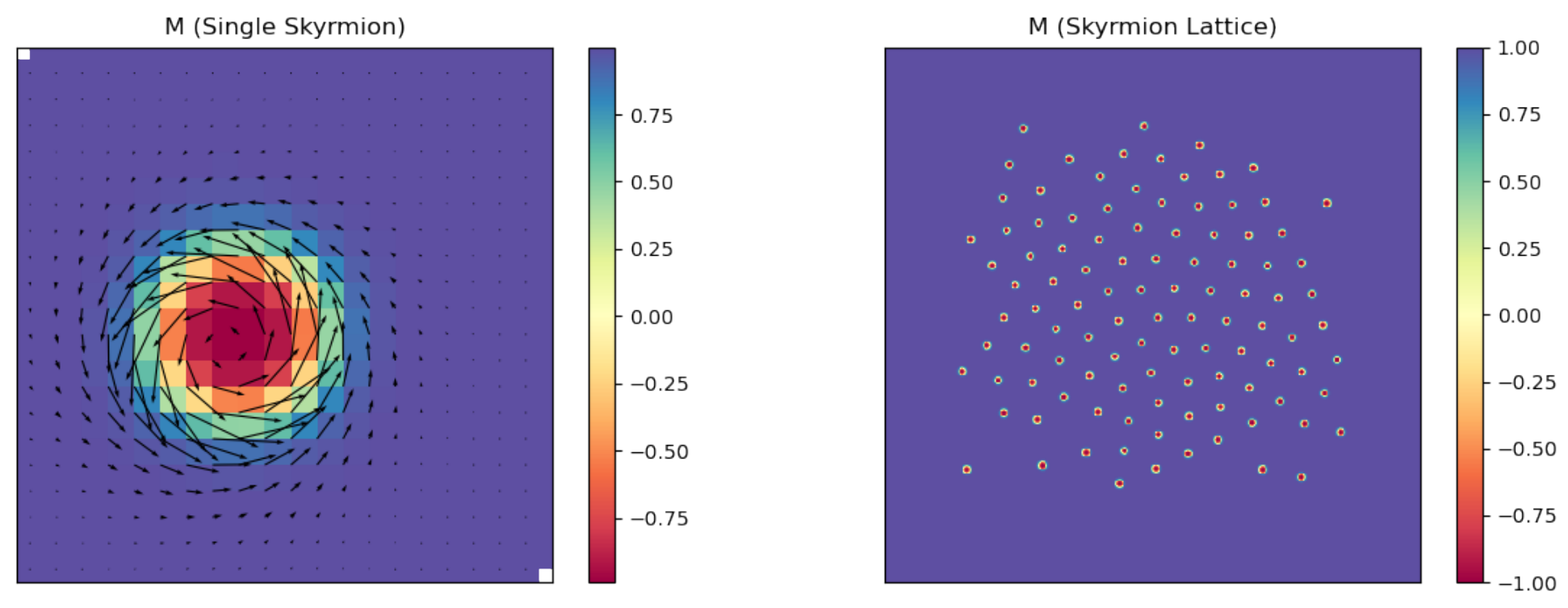

Fig 1. plots of the magnetization of a single skyrmion (left), and a looely packed skyrmion lattice (right). Magnitude of in plane magnetization correspond to arrow length, and out of plane magnetization is represented by the colorbar.

Methods

Using the material parameters measured in S Montoya, et al.[1], and the mumax 3 micromagnetic simulation package[2], we set out to simulate the following:

> Phase diagram shown by Mz as function of applied field (Fig 1.), including hysteresis dependent effects on the spin texture of the system, replicating the phase diagrams experimentally measured in S. Montoya, et al. [1]
>
> Time dynamics of the Fe/Gd system when excited with a 2 picosecond gaussian pulse, using the aforementioned phase diagram to inform our choices of static field.
>
> Time resolved behavior of the magnetization, as well as that of the winding number. This provides an additional means to distinguish the phase between the various skyrmion and stripe phases, and to characterize the evolution of the topology. Simulation of the winding number is made available through the mumax3 software.

With this, we are able to build an understanding of the ultrafast response of the skyrmion phase, and inform experimental interrogation of helimagnetic materials, such as Fe/Gd, when in the skyrmion phase. This is enabled by the GPU acceleration tools made available by mumax3[2], allowing us to reliably and rapidly simulate dynamics in quantum materials via discrete methods (RK23, finite difference).

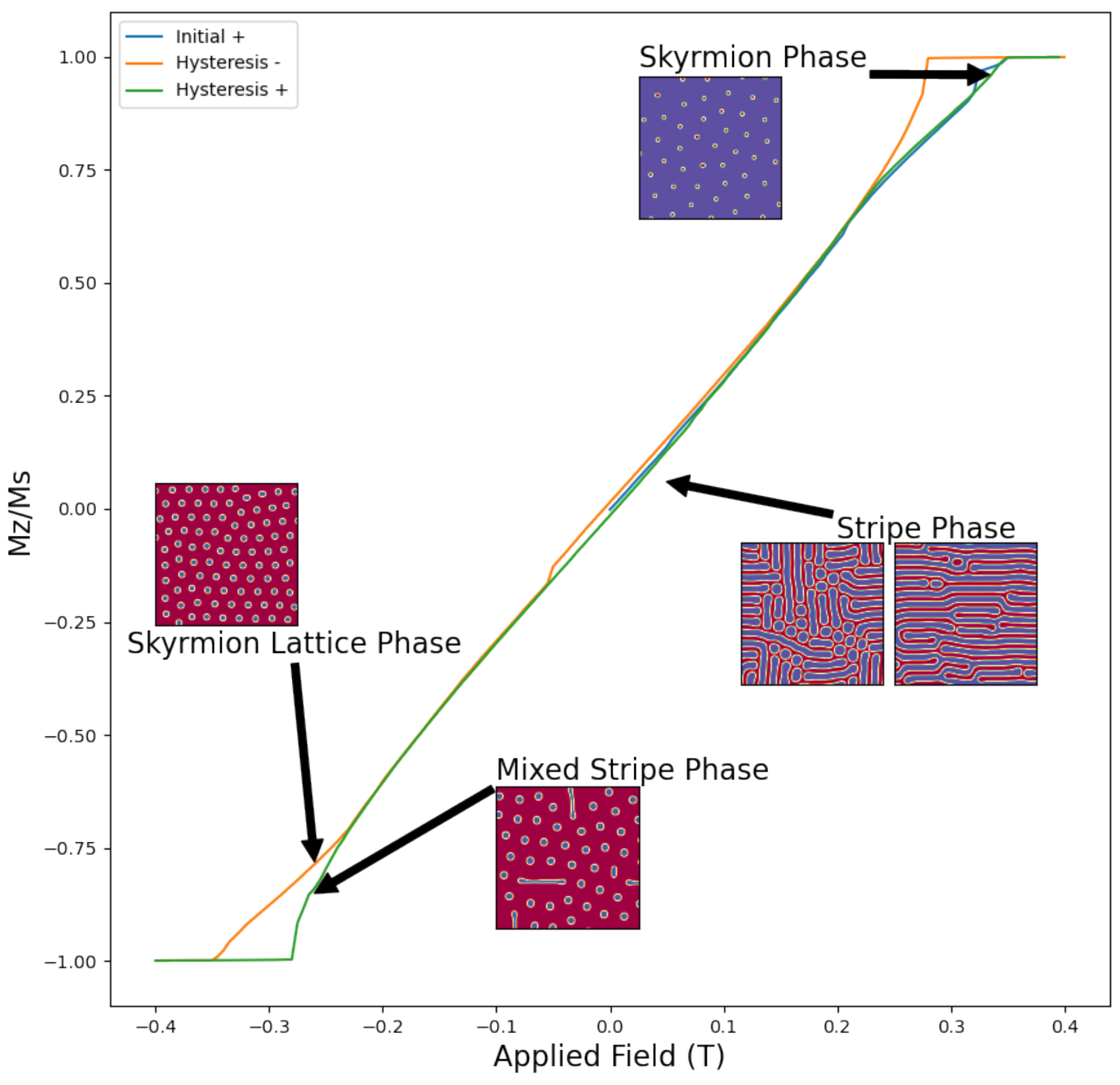

Fig 2. Hysteresis plot of total magnetization in Fe/Gd as a function of the applied field (c-axis), with examples of the phase inset. Magnetization is plotted as a fraction of the saturation magnetization of Fe/Gd, with the phases determined loosely by the prevalence of stripes and the density of skyrmions.

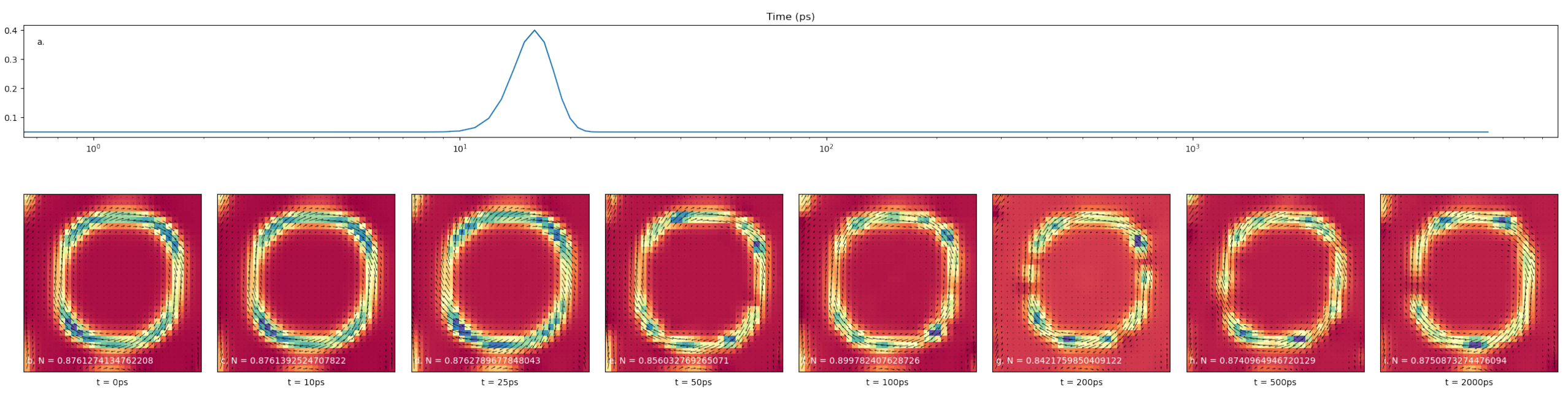

Fig 3. a) Log plot of B field excitation for a sample under static field of .050T. b-i)Time evolution of a single skyrmion in a mixed stripe phase on the upward sweep on the hysteresis curve, relaxing from the above pulse. Winding number is also listed, and determined numerically.

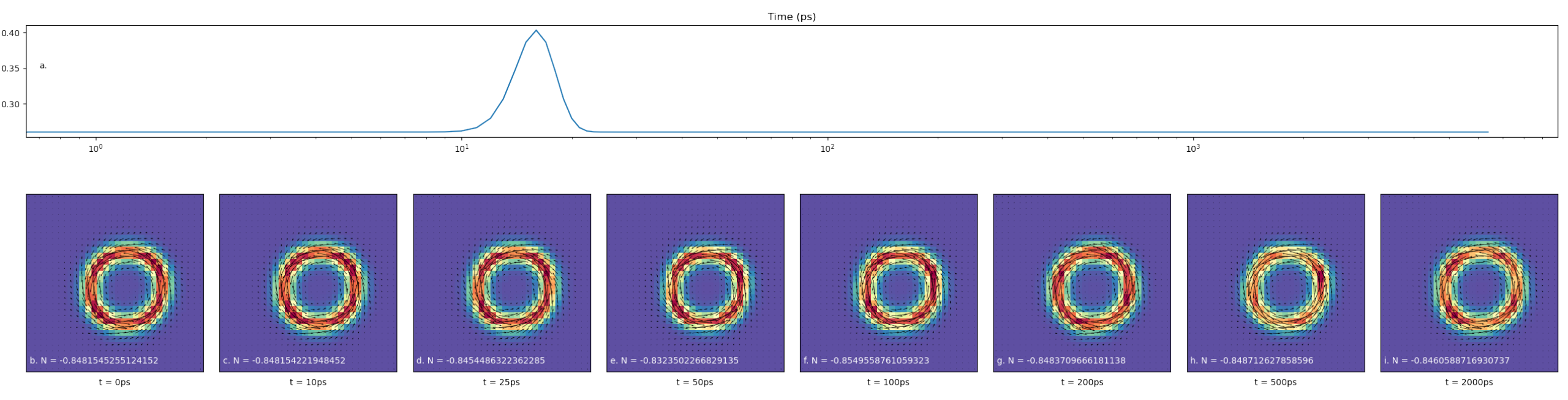

Fig 4. a) Log plot of B field excitation for a sample under static field of .260T. b-i)Time evolution of a single skyrmion in a skyrmion lattice phase on the upward sweep on the hysteresis curve, relaxing from the above pulse. Winding number is also listed, and determined numerically.

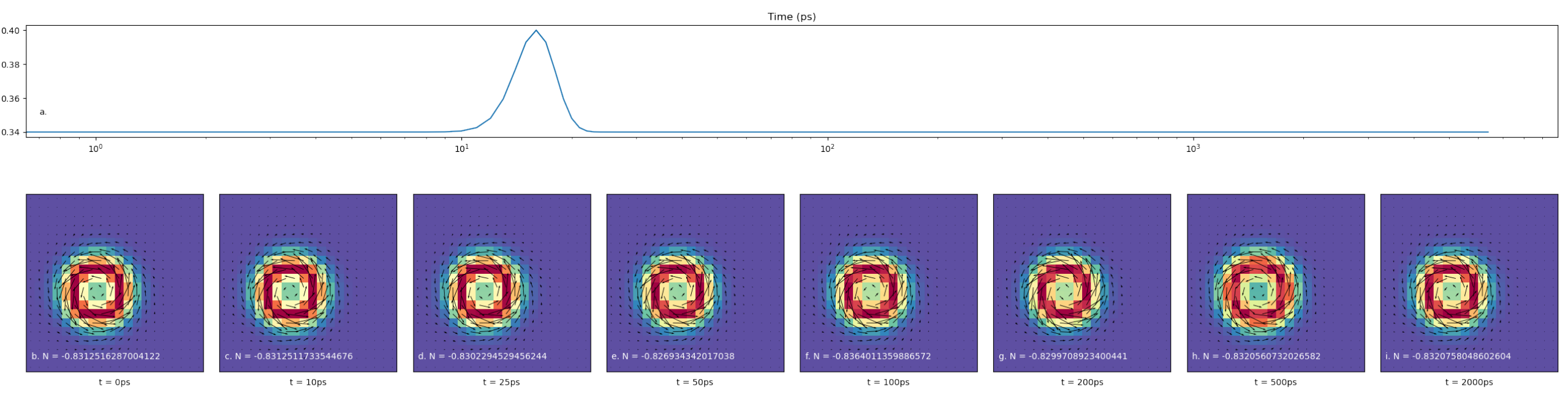

Fig 5. a) Log plot of B field excitation for a sample under static field of .334T. b-i)Time evolution of a single skyrmion in a skyrmion lattice phase on the upward sweep on the hysteresis curve, relaxing from the above pulse. Winding number is also listed, and determined numerically.

Results

Through analysis and visualization of our simulation results, we are able to see a number of informatice features in the real-space behavior of both the magnetization and the winding number:

> Non- relaxing behavior affecting the magnitude and spatial distribution of topological charge, and magnetization (Figs 3-5), existing well beyond the picosecond timescale of our pulse.
>
> Coherent modes emerge in both the magnetization, and in the winding number, with clear periodicity and a lifetime lasting into the nanosecond timescale (Fig 6)
>
> Distinct modes in the magnetization (dMz/Mz) and the winding number (dN/N), whose differing periodicity (Fig 6) imply that these are two separate and competing modes
>
> Phase dependence on the time resolved dynamics of both the magnetization and winding number, rather than a dependence on the static field, demonstrating the significance of the topology on the system.

This real space picture pushes us to analyze this data through the FFT, to better resolve the frequency-space and momentum-space behavior of the oscillatory modes we see. This also points us towards the methods of time-resolved RXD and RIXS made available to us by LCLS-II to understand and verify these results in real samples.

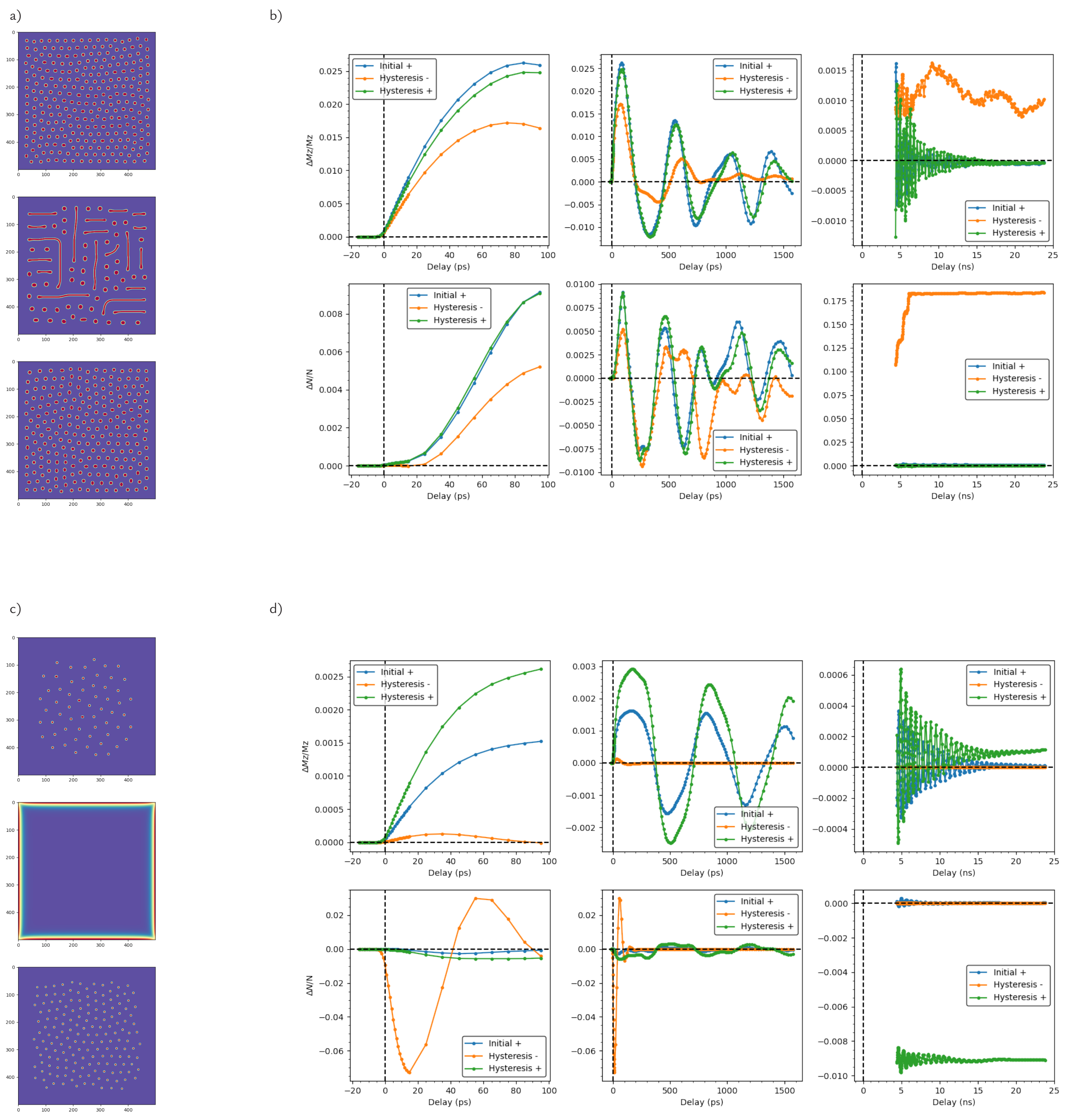

Fig 6. a) Real space plots of Fe/Gd at .260T from each point on the hysteresis curve (initial rise, downward sweep, upward sweep; top to bottom) b) Time domain plots for the .260T case, showing dMz/Ms and dN/N at various timescales c) Real space plots of Fe/Gd at .334T from each point on the hysteresis curve (initial rise, downward sweep, upward sweep; top to bottom) b) Time domain plots for the .334T case, showing dMz/Ms and dN/N at various timescales

Discussion

In our inspection of the Fourier transforms we can see various novel behaviors in the frequency and momentum spaces as follows:

> Highly pronounced frequency response for the magnetization of the sample, as well as a highly peaked response for the dynamics of the winding number, further highlighting the distinction between the two modes, and their experimental accessibility.
>
> Long lasting and highly pronounced responses to excitation in the momentum space, highly visible as an observable for a RIXS interrogation of Fe/Gd dynamics.

Ultimately, what we see is strong responses that we can measure and characterize through Tr-RXD and RIXS, to affirm our simulated picture of these dynamics, and explore an underutilized space in ultrafast x-ray science

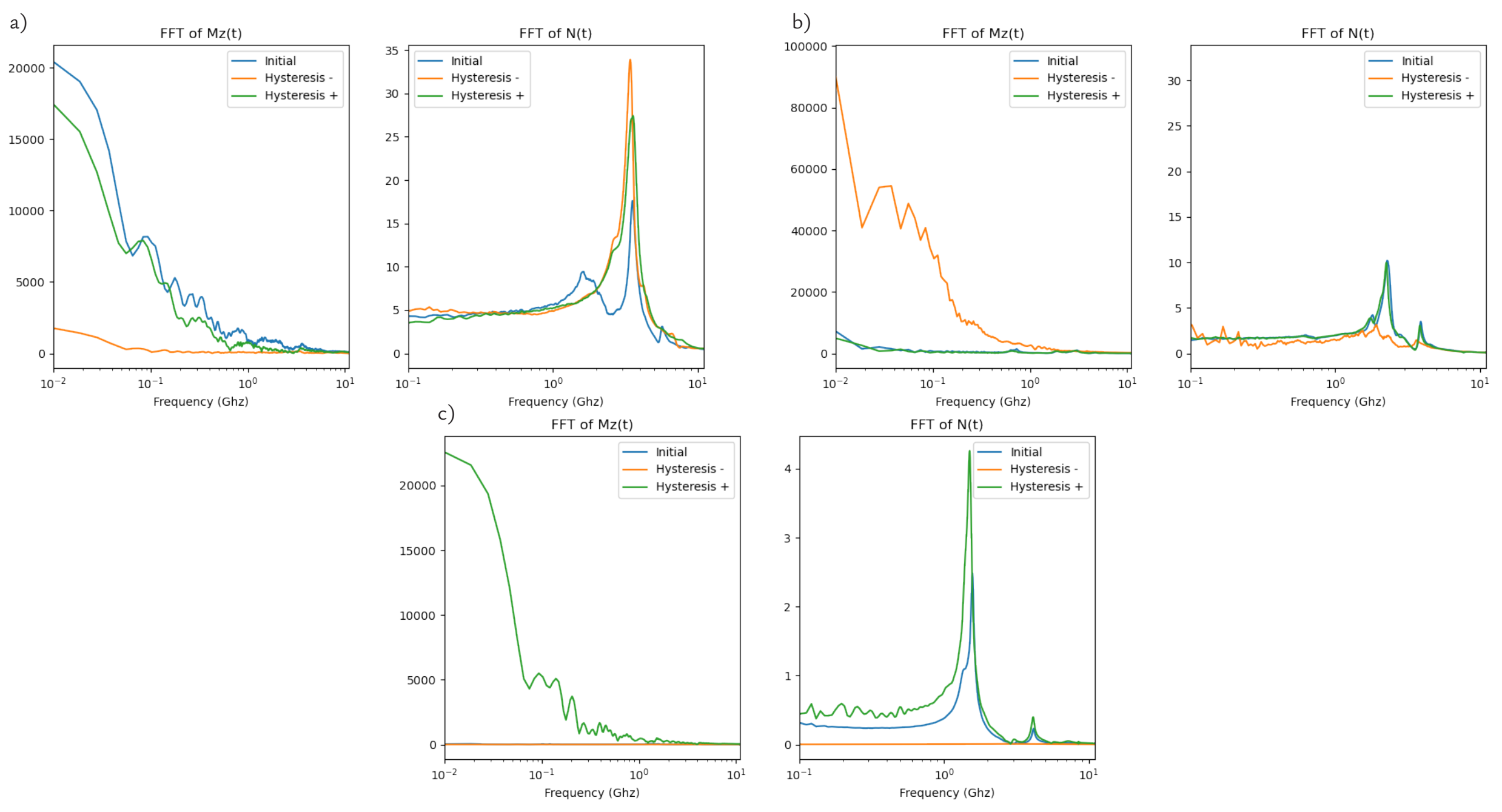

Fig 7. Plots of the simulated frequency domain response for each static field of .050T (a), .260T (b), .334(c), showing the intensity of the response (y-axis) at a given GHz frequency (x-axis), for both dMz/Mz (left) and dN/N(right).

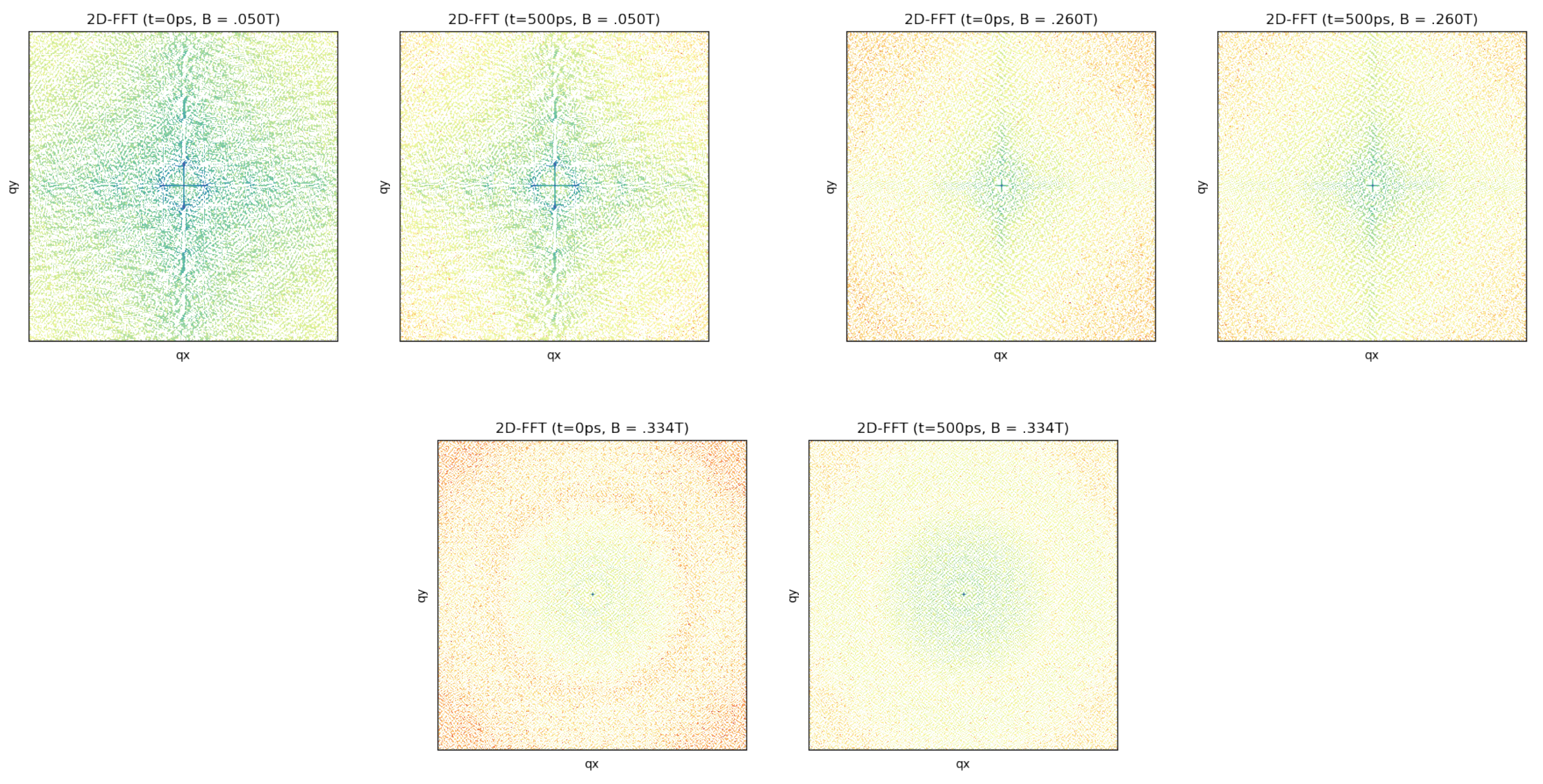

Fig 8. 2D-FFT of the magnetization plotted in momentum space intensity of our simulations, with the .050T and .260T taken from the hysteresis downsweep, and the .334 data taken from the hysteresis up sweep. Plots are shown in log scale.

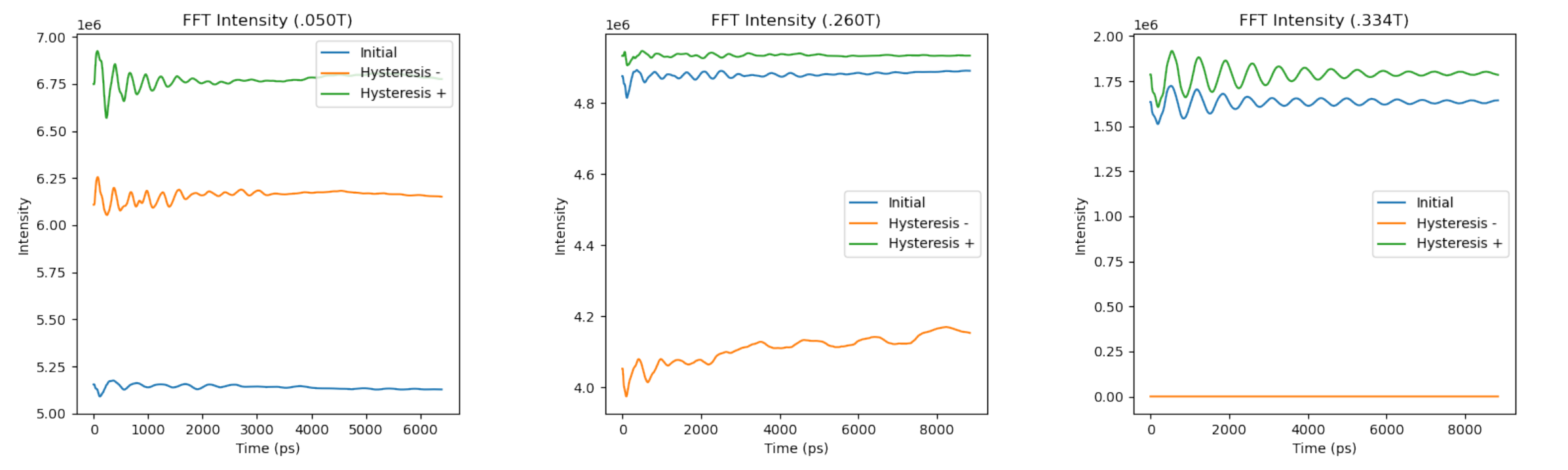

Fig 9. Plots showing momentum space intensity in regions of highest change over the duration of the simulation, sampled from a region around the center of the 2D plots shown above.

Conclusion

Throughout our simulations what we have seen is a robust and pronounced response to an excitation on the ultrafast scale, in a model developed from the well understood properties of Fe/Gd. We have seen the formation of distinct and coherent modes with nanosecond lifetimes, and minimal relaxation. This provides a stepping stone towards the elusive long lasting and rapidly writeable skyrmion, and its associated technological applications. With a picosecond excitation we see well defined changes that we can characterize with ultrafast techniques available to us at LCLS-II. Building on the work done in S. Zhang, et al [3], we can affirm the understanding in these simulations, and use Tr-RXD to directly measure the magnetization and crucially the topological charge in our sample. This provides a pathway to little-explored but novel physics on the ultrafast timescale, which we are readily able to characterize through pairing x-ray and ultrafast techniques.

To continue this work, we intend to narrow our excitation to a single skyrmion within the lattice phase, as a means to understand the ultrafast dynamics of skyrmion-skyrmion interaction that are crucial to their broader application. With only a picosecond-scale excitation we are able to see coherent modes arise on a nanosecond timescale, and can explore the competition that arises between these two modes. On the experimental side, we can use the Tr-RXD techniques described in S. Zhang, et al[3] in order to experimentally verify the highly pronounced responses we have seen in our simulations. This can be paired with RIXS measurements on LCLS-II in order to see the momentum space response that pairs with the real space understanding we have developed here. This offers an underused marriage of ultrafast and x-ray techniques to understand the topology of quantum materials in the time domain, and better understand the possibility for dynamic control of topological properties.

Acknowledgements

Thank you to the kind staff at SLAC and LCLS who have made this work possible:
Lingjia Shen, my mentor and advisor on this project, who has been indispensable throughout
The S3DF staff, for handling my unorthodox approach to computer resources
LCLS Internship Program Staff, for facilitating this whole endeavor
The developers of the mumax3 simulation package at Ghent University

References

[1] Montoya, S. A., et al. "Resonant properties of dipole skyrmions in amorphous Fe/Gd multilayers." Physical Review B 95.22 (2017): 224405.
[2] Vansteenkiste, Arne, et al. "The design and verification of MuMax3." AIP advances 4.10 (2014).
[3] Zhang, S. L., G. Van Der Laan, and T. Hesjedal. "Direct experimental determination of the topological winding number of skyrmions in Cu2OSeO3." Nature Communications 8.1 (2017): 14619.