## TOPOLOGICALLY INFORMED GUESSES IN CHAIN OF STATES METHODS TO CALCULATE THERMAL ACTIVATION BARRIERS IN MICROMAGNETIC SYSTEMS

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The height of the energy barriers separating metastable states is the most crucial feature in the thermal stability of magnetic information storage devices. In most systems, the transition state cannot be determined analytically, and must be found using numerical procedures. A family of proposed algorithms used to computationally identify transition states are the Chain-Of-States methods. Among these we can find the String Method, the Nudge Elastic Band Method, and the geometric Minimum Action Method and their refinements [1-3]. The common approach of these methods is that they first guess a sequence of states that connects the two energy minima and then let this chain of states evolve downwards in energy. At convergence, the transition state can be identified from the final chain of states.

In this talk, we will present our work on calculation of the energy barriers in nanomagnetic disks with strong Dzyaloshinskii-Moriya Interactions. These systems have a rough energy landscape with many minima. The different energy minima can be characterized by their Skyrmion numbers, a topological quantity that measures the number of times the magnetization winds around the unit sphere in the region occupied by the device. We highlight the importance of incorporating information about the topological features of energy minima in the initially guessed chain-of-states to be used as input for the calculation. Two key advantages of our improved guesses are a dramatic reduction on the steps necessary to reach convergence, and avoidance of accidental insertion of topological defects which produce singularities of the energy landscape.



Fig. 1. Initial paths can be generated by using the topological features between two states (left and right) and smoothly transform between them. Blue regions represent upward magnetization skyrmion cores in an otherwise downward magnetized device (red). The white domain walls can be smoothly transformed between configurations to avoid accidental insertion of topological defects.

## References

- [1] Weinan E, Weiqing Ren and Eric Vanden-Eijnden. *String method for the study of rare events*. Phys Rev. B **66**, 052301 (2002)
- [2] P. F. Bessarab, V.M.Uzdin, Hannes Jónsson. Method for finding mechanism and activation energy of magnetic transitions, applied to skyrmion and antivortex annihilation. Computer Physics Communications 196, 335-347 (2015)
- [3] M. Heymann, E. Vanden-Eijnden, *The geometric minimum action method: A least action principle on the space of curves* Communications on Pure and Applied Mathematics 61, 1052 (2008)

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