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Chiral structures across scales

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Background and Motivation:

Helical structures can be found across disciplines and scales, from micromagnetism (e.g., helical magnetic structures in bulk materials [1] or epitaxial films [2]) over molecular dynamics (a-helical structure in proteins), genomics (double-helical structure of DNA [3]), see **Fig. 1**, and biology (snails) to astrophysics (spiral structure of galaxies).

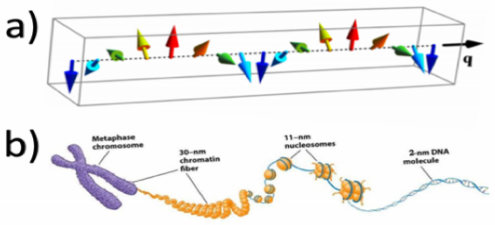


Figure 1: chiral structures; a) in magnetism, b) in biology

Interestingly, even though all of the helical phenomena may have a completely different origin and composition, they are very similar from the structural perspective and can also be reduced to a small amount of characteristic "scale parameters" being determined by microscopic factors. One of the core common challenges in this context is designing and identifying appropriate models for analysis and prediction of global steric effects from the known local properties on the microscopic scale. This challenge is mostly induced by the extreme computational complexity of a direct computation of macroscopic structures from microscopic properties - even with modern supercomputers it is still impossible to compute these relations.

In context of **DNA modeling** for example, the most recent molecular dynamics simulations of DNA were reported to cover only up to a couple of thousands of nucleotides [2] – whereas the biologically relevant modeling of the higher order folding of the DNA helix (Figure 1b) would require modeling billions of nucleotides. However, since even point-mutations (in non-coding domains) have been shown to significantly affect the chromatin conformation (the higher order folding of the helix) and herewith leading to severe disfunction of transcriptional/translational processes and even diseases [3], the prediction of position effects and quantification of their impact on changes in the global chromatin structure of pathogenic phenotypes remains one of the biggest challenges in modern molecular diagnostics.

In context of **magnetism**, helical structures form on different length scales (~ *nm* → *μm*) depending on the mi- croscopic details. The modelling of large helical structures, in particular in 3D, on the order of several hundred nanometers is out of reach by atomistic modelling and therefore effective models are needed and used instead. The latter work in particular well for homogeneous samples. However, in the case of non-neg- ligible impurities or

dislocations etc. the helical structures deform from their sim- ple alignment and can arrange into various patterns. In particular, local defects can influence the orientation of the helical structures as well as induce potential modulations, see **Fig. 2** for example configurations.

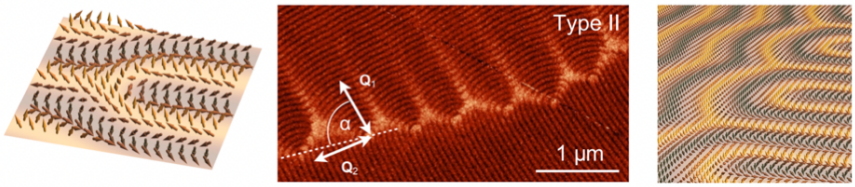
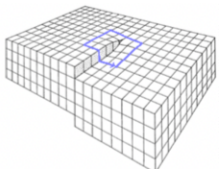


Figure 2. Helices with "defects", from Ref. [4].

Motivation for collaboration: Both PIs work on the development of data-driven methods as well as on data science aspects for the analysis and modeling of high-dimensional simulation and experimental data on multiple scales. The research of both PIs is particularly connected by the underlying question: **How modifications on microscopic local structures imply significant changes on a global macroscopic order in various setups,** focusing on either chromatin structures or magnetic textures. Here, we see outstanding perspectives for future collaboration particularly by learning and cross-fertilizing through complementary approaches common in the individual research fields.

2. Goals and project plan - Hypotheses (H) and Aims (A)



H1: There exists a statistically-significant data-driven mapping between the local microscopic parameterization of the Landau-Lifschitz-Ginsburg (LLG) model and the global ordering parameters (helical orientation, helical pitch vector and the phase shift) of the spatio-temporal solutions of the heterogenous LLG-model.

A1: To verify the hypothesis H1 we will adjust the pipeline from genomics developed in [6] (based on combination of generalized linear models from machine learning with the Linkage Probability measure probing for latent relations).

H2: Deploying the latent pattern recognition measures (latent entropy and latent dimension) recently developed for identification of material inhomogeneities, we can define a much better predictive relationship between 1D DNA sequence and the 3D packing of the DNA helix.

A2: To verify the hypothesis H2 we will combine the pipeline from [5] with the latent measures from [7]. Resulting methodology will then be applied to the whole-chromosome genomics data from the 1000 Genomes project and the relation to 3D HiC-data will be tested statistically. Also, we plan to profit from the magnetic community by deriving analogue equations for the effective models to study magnetic helices [8] for describing the bending (curvature) of the DNA structure.

3. Work packages and time line

The research will be carried out by a doctoral student under the joint

supervision of the two PIs. Based on the project plan outlined above, the work will be organized as follows. We will first address the H1 hypothesis with aims from A1. On that basis, we will proceed simultaneously in two directions: The method development direction, which continues with the back-mapping problem (i) and ends with the integration of all methods into one concurrent simulation scheme (ii), and approaching the H2 hypothesis with aims from A2.

4. Outlook

This research can be extended to more complicated inversion symmetry breaking structures such as whirls, which also appear across scales, as indicated in **Fig. 3**.

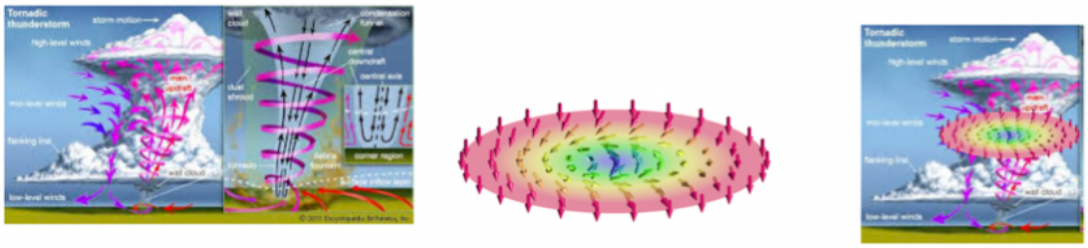


Figure 3: Whirls across scales, in magnetism and wind. Outlook to potentially collaborate with Volkmar Wirth.

References

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