Numerics for DNA supercoiling
MSc Internship / PhD 2019

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Hosting Laboratory: d'alembert institute for mechanics
`http://www.dalembert.upmc.fr`

Practical details: Paid internship with a possibility to pursue a PhD on a same/similar topic.

Context: It is now clear that DNA mechanical properties deeply influence the biology of the cell. In particular the flexibility of the DNA molecule play a important role in gene regulation. The long and thin DNA molecule is modelled as an elastic rods and its behaviour under applied tension and torsion is studied experimentally and numerically[1, 4]. For large torsion loads, the molecule winds on itself, a phenomenon called supercoiling. There is a large diversity of supercoiling configurations, see for example the plectonemic state in Figure 1. Beyond the well-known formation of plectonemes, it is now suspected that other structures might exist in tight geometrical conditions. However, no one has been able so far to exhibit such new configurations, neither experimentally or numerically.

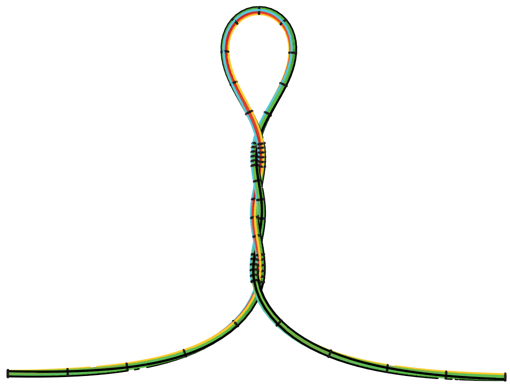

Figure 1: Plectonemic supercoiling

Objectives: The goal of this project is to study DNA supercoiling from theoretical and numerical points of view. Experiments indicate the possibility of different supercoiling topologies depending on salt concentration and mechanical constraints [2, 3]. We wish to investigate these supercoiling topologies theoretically and develop a static simulator for thin elastic rods under hard-core or long-range self-repulsion.

Required skills:

- Curiosity and taste for applications in mechanics and structural biology.
- Good skills in modelling of mechanical/elastic systems.
- Good skills in numerical analysis (modelling, numerical discretisation of ODEs and PDEs, finite elements, optimization) as well as in algorithmic and programmation (Mathematica, C/C++ , and/or Python)

References

[1] C. Bustamante, Z. Bryant, and S. B. Smith. Ten years of tension: single-molecule dna mechanics. *Nature*, 421(6921):423–427, 2003.

[2] John F. Marko and Sébastien Neukirch. Competition between curls and plectonemes near the buckling transition of stretched supercoiled dna. *Phys. Rev. E*, 85(1):011908, 2012.

[3] John F. Marko and Sébastien Neukirch. Global force-torque phase diagram for the dna double helix: Structural transitions, triple points, and collapsed plectonemes. *Phys. Rev. E*, 88:062722, 2013.

[4] S. Neukirch and J. F. Marko. Analytical description of extension, torque, and supercoiling radius of a stretched twisted DNA. *Phys. Rev. Lett.*, 106(13):138104, 2011.

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