Numerical study of DNA supercoiling
MSc Internship 2016

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Hosting Laboratory: équipe BIPOP de l'INRIA et du LJK (Grenoble)
`http://www.inrialpes.fr/bipop`

Practical details: Paid internship (INRIA scale), possibility to pursue a PhD on a 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 plays an important role in gene regulation. The long and thin DNA molecule is modeled as an elastic rod and its behavior under applied tension and torsion is studied experimentally and numerically[2, 5]. For large torsion loads, the molecule winds on itself, a phenomenon called supercoiling. There exists 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 nor numerically.

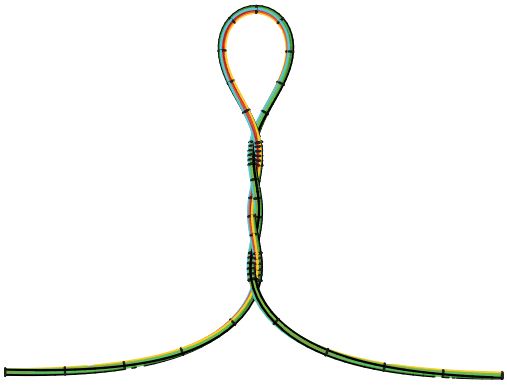

Figure 1: Plectonemic supercoiling

Objectives: The goal of this project is to study DNA supercoiling from a numerical point of view. To this end, various simulators for dynamic rods subject to contact, used by or developed at INRIA [1, 3, 4] will be adapted and applied to the simulation of DNA supercoiling, in the hope for revealing new geometrical structures. A static simulator for thin elastic rods will also be investigated to complete the study.

Required skills: Good skills in numerical analysis (modeling, numerical discretization of ODEs and PDEs, finite elements, optimization) as well as in algorithmic and programmation (C/C++ and/or Python) are required. Curiosity and taste for applications in mechanics and structural biology would be appreciated.

References

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

[3] R. Casati and F. Bertails-Descoubes. Super space clothoids. *ACM Transactions on Graphics (Proc. ACM SIGGRAPH'13)*, 32(4):48:1–48:12, July 2013.

[4] G. Daviet, F. Bertails-Descoubes, and L. Boissieux. A hybrid iterative solver for robustly capturing Coulomb friction in hair dynamics. *ACM Transactions on Graphics (Proc. ACM SIGGRAPH Asia'11)*, 30:139:1–139:12, 2011.

[5] 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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