Biopolymer Networks: Image Analysis, Reconstruction and Modeling

A thesis presented in partial fulfilment of the requirements for the degree of

Doctor of Philosophy

in

Physics

at Massey University, Manawatū,
New Zealand

Pablo Hernandez-Cerdan

2018

MASSEY UNIVERSITY
TE KUNENGA KI PŪREHUROA
UNIVERSITY OF NEW ZEALAND

It's not about the end, it's all about the path.
¡Buen camino!.

Abstract

The aim of this work is to extract the architecture of biopolymer networks from 3D images. This is motivated to further understand non-affine regimes, found during network formation and in low-density biopolymer networks, where the geometry of a network has a fundamental role in defining its mechanical properties.

Firstly, developed image analysis tools were extended to 3D and contributed to high-performance open-source libraries for image analysis. These developments in isotropic wavelets will help in extracting realistic networks by removing spurious noise generated during image acquisition.

Secondly, images of biopolymer gels from transmission electron microscopy (TEM), were used to reliably extract the network architecture. The imaged material was also studied with small-angle x-ray scattering (SAXS), and the comparison showed a strong agreement for network-size features.

Thirdly, spatial graphs were extracted from the image. A one-to-one map is provided between image and graph, keeping all the geometric information from the image. This then opened the door to using analytical tools from the complex networks field to characterize images.

Finally, statistical distributions extracted from three graph properties were used to reconstruct a completely in-silico network using a simulated annealing technique to generate new networks. This can be used as a computational exploration tool of how network behavior depends on network architecture.

Acknowledgements

A special thank to my supervisor Bill Williams whose support, openness, and vision of science is encouraging. As Brad would say, I will be forever indebted to your supervision and I add: and from all the stuff that I have learned from you beyond academia, specially your humane values and the love for dumplings. Thanks to Brad Mansel, Leif Lundin and Andrew Leis for the collaboration comparing scattering and imaging techniques, Allan Raudsepp for providing the confocal microscopy images for actin, and to all my group mates from the Biophysics and Soft Matter group, for all the shared moments, and how easy they made my adaptation to a new country. Finally, I am grateful to the MacDiarmid Institute for constantly providing the enrichment opportunity to meet other peer students and researchers, and to the staff of the Institute of Fundamental Sciences for its kindness dealing with all sort of issues.

In the personal side, I would like to thank my family, from who I have inherited, directly and indirectly, all the principles I stand for and made me realize how privileged I am to have them. And Martica! Without you here in New Zealand this quest would have been impossible, or faster, who knows, but way less enjoyable for sure. It has been a pleasure habernos re-encontrado por kiwi-land. And even we got married, in English!!, crazy, but made me feel extremely fortunate. Thanks really for all your support.

This research was supported by the MacDiarmid Institute, the Riddet Institute, and Massey University, New Zealand.

Contents

List of Figures

List of Publications

[1] Pablo Hernandez-Cerdan. “Isotropic and Steerable Wavelets in N Dimensions. A Multiresolution Analysis Framework for ITK.” In: *arXiv:1710.01103 [cs]* (Oct. 2017). arXiv: 1710.01103 [cs].

[2] Pablo Hernandez-Cerdan, Bradley W. Mansel, Andrew Leis, Leif Lundin, and Martin A.K. Williams. “Structural Analysis of Polysaccharide Networks by Transmission Electron Microscopy: Comparison with Small-Angle X-Ray Scattering.” In: *Biomacromolecules* (Jan. 2018). ISSN: 1525-7797. DOI: 10.1021/acs.biomac.7b01773.

[3] Hina Shah, Pablo Hernandez, Francois Budin, Deepak Chittajallu, Jean-Baptiste Vimort, Rick Walter, André Mol, Asma Khan, and Beatriz Paniagua. “Automatic Quantification Framework to Detect Cracks in Teeth.” In: *Medical Imaging 2018: Biomedical Applications in Molecular, Structural, and Functional Imaging.* Vol. 10578. International Society for Optics and Photonics, Mar. 2018, 105781K. DOI: 10.1117/12.2293603.

Abbreviations

AFM	Atomic force microscopy.
BGL	Boost Graph Library. c++ library.
CEWLC	Clickable extensible wormlike chain.
DFT	Discrete Fourier Transform, representation of data in frequency domain.
DGtal	Digital Geometry Tools and Algorithms. c++ library.
EtE	End to end.
EWLC	Extensible wormlike chain.
FE	Force extension (curve).
FFT	Fast Fourier Transform, specific algorithm of DFT.
ITK	Insight ToolKit. Image Analysis c++ library specialized to work with ND images.
LAOS	Large amplitude oscillatory shear (rheology).
LMP	Local maximum point.
MRA	Multiresolution framework.
MSD	Mean square displacement.
NP	Nucleation point.
PME	Pectin-methylesterase.
SAXS	Small angle X-ray scattering .
SEM	Scanning electron microscopy.
TEM	Transmission electron microscopy.
TV	Total Variation (regularization, denoising method).
WLC	Wormlike chain.