NOVEL MATHEMATICAL METHODS IN MATERIAL SCIENCE: APPLICATIONS TO BIOMATERIALS (Online) 21w5232

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1 Overview of the Field

Many biological materials involve the entanglement of filamentous matter. Topological transitions of entanglement and knotting are associated with changes in the material properties and function of these systems. Mathematical models of physical systems can provide powerful methods to rigorously predict and control material properties and function. However, topological effects are often omitted in return of more coarse grained models. In addition to the challenges related to obtaining experimental data and modeling complex systems at multiple length scale resolutions, a challenge in studying the topology of materials is the lack of the mathematical and computational tools that can rigorously assess knotting and entanglement.

2 Recent Developments and Open Problems

Experimental and computational advances enable the visualization of topological complex systems, such as chromatin in the cell nucleus, microtubules in the meiotic spindle and liquid crystal structures, all of which emphasize the need to study structure and entanglement in these systems. Recent advances in knot theory enable the characterization of entanglement even when the filaments may have distinct ends. Incorporating topological information in continuum models and extracting topological information from continuous models of biological matter and experiments, remains a challenge.

The aim of this workshop was to bring together Mathematical communities with researchers from Physics, Materials Science and Biology with the goal to create new mathematical models of complex fluids that account for topological effects in biopolymers that can bridge length and time scales. The workshop had international participants from Pure and Applied Mathematics, from Biology, Chemical Engineering and Physics in various stages of their careers. The workshop also included a presentation by NSF Officers about the funding opportunities for new collaborations and early career scientists.

3 Presentation Highlights

Some of the presentation highlights of this workshop were related to chromatin reorganization inside the cell nucleus. Experimental results were presented that found that undifferentiated chromatin behaves like a Maxwell fluid, while differentiated chromatin shows a coexistence of fluid-like (sol) and solid-like (gel) phases [1]. In parallel, recent theoretical predictions and experimental evidence for a strain-controlled mechanical phase transition in biopolymer networks below Maxwell's isostatic point was presented [2]. Novel modeling methods demonstrated that the time evolution for a system at a specific confinement with increasing activity can be characterized by a series of elementary topological events where nematic disclinations divide, merge, annihilate, and crossover [3]. It was shown that liquid crystal models can help predict the properties of DNA in bacteriophage P4 and the formation of knots [6].

Other presentations in this workshop brought attention to the relation between single chain properties and global organization of macromolecules in the cell. It was shown experimentally that subtle differences in nucleosomal DNA folding, extend beyond twist and have implications for nucleosome disassembly and higher-order structures [4]. Simulations were used to examine how the knotting of semi-flexible chains varies inside channels of different size and how the size and complexity evolves during the free or externally-driven dynamics of the chain [5]. The dynamics of DNA trefoils and configurations of DNA Hopf links with relevance to kinetoplast DNA were also discussed.

In this workshop, experimental and modeling results were juxtaposed to computational and theoretical results of coarse grained models of biopolymers, using random walks. Monte Carlo simulations are a big part of understanding the statistical properties of knots. Methods adapting BFACF to polygons in R3, and also attempts at trying to coerce the (very fast) pivot algorithm to respect topology were presented [12]. Link statistics for self-avoiding polygon models in small tubes were also discussed [7]. Theoretical results of random walks were extended using topologically constrained Gaussian random walks (TCRW) to other architectures. Using this framework, Flory's approximate expression for the mean square fluctuation of the end-to-end vector with respect to functionality was proved [8].

Novel methods in knot theory for measuring entanglement of closed and open curves were presented. Methods of generalized approximation of an open curve by a knot [9], as well as measures of complexity of open curves in 3-space with no approximation by a knot were presented [10]. Finally, entanglement and knotting in periodic structures was discussed [11].

4 Scientific Progress Made

The presentations showcased the scientific progress made in the area of topology of materials. In addition to the presentations, the workshop consisted of several working groups which met every day. The areas of focus were: chromatin organization, cytoskeleton and active matter, entanglement in confinement, topology and periodic entanglement, entanglement of open curves, entanglement of triple helices of nucleic acids. The discussions led to new ideas for modeling triple helices, based on lattice ribbons or on theta-graphs. Key questions related to the effect of confinement of macromolecules where identified, such as how prime versus composite knots vary in confinement, which is also related to the localization of knots in a larger chain. Systems where entanglement may be more important than others, such as spectrin versus actin filaments in the cytoskeleton were discussedThe discussions also pointed out that some systems may be modeled better by open knots and links, while others by graphs and that the cell may consist of a mixture of both. Novel ideas for measuring entanglement of open graphs based on singular knots diagrams and integration over the 2-sphere were suggested.

5 Outcome of the Meeting

The meeting brought together scientists from different backgrounds, working on mathematics of materials or topological effects on materials, who exchanged ideas and methods. New collaborations were formed and several participants continued to have follow up meetings. One manuscript was published so far from discussions from this meeting [13], co-authored by a distinguished emeritus Professor, a post-doctoral scholar and an Assistant Professor.

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