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Field: Computational Biophysics
Expected Graduation: Spring 2018

Phase characterization of microtubule-motor active nematic liquid crystals

Abstract

Active nematic liquid crystals have remarkable properties that are only now starting to be understood. These non-equilibrium systems self-organize and generate flows in solutions. We study a type of solution consisting of microtubule filaments and motor proteins. Both are biological components. Microtubules give structure to the cell, while motor proteins facilitate transport of molecules along microtubules. We compose simulations and extract data to quantify stresses, pressure, filament distribution, and the order of two-dimensional active nematic liquid crystals. We identify and quantify phases and phase transitions, and seek to describe the physical properties of steady-state configurations. By characterizing these systems, we contribute to the developing field of non-equilibrium statistical mechanics, and provide a framework for further research in driven nematic liquid crystals.

Prospectus

Microtubule filaments are a part of the structural, “cytoskeletal”, network of the cell and take part in non-equilibrium processes of the cell. Such processes include cell division, cell motility, and facilitating transport of molecules across the cell. Some processes involve microtubules being tethered together by crosslinking motor proteins. These motor proteins then walk to the filament’s positive end. If the bound pairs of filaments are anti-parallel (pointing in opposite directions), the walking motors drive microtubule sliding. When these component proteins are extracted and placed in a quasi-two-dimensional environment, they exhibit properties that are not observed in passive liquid crystals. At high concentrations of microtubules and motor proteins, these relatively simple interactions generate flows of solution and cause materials to self-organize. These novel properties motivate the development of non-equilibrium statistical mechanics and may lead to applications in new material technologies.

This research seeks to quantify properties of these kinds of two-dimensional active nematic liquid crystals. Such properties include shear stresses, pressure, microtubule distribution, and order parameters. Though comprising only a few distinct components, novel liquid crystal phases arise as parameters are varied. By varying motor concentration and motor walking speed, we will observe different structural phases. We will then characterize any such phases and quantify dynamic properties. The goal of our research is to learn what properties of these crosslinking motor proteins are necessary to induce observed phases and what attributes cause them. Previous computational research in the field has shown that simple models of microtubules and motors generate anisotropic extensile stresses and steric (rod-rod) interactions. The classification and characterization of these materials will provide a framework for future research in active nematic liquid crystals.

We have taken coarse-grain simulated data across a range of motor walking speeds and motor concentrations. Running simulations is computationally expensive, so this data narrows the parameter space and focuses our research. Once we collect preliminary data, we

will develop software to analyze the aforementioned properties of the system. For example, stresses describe how energy is being converted into motion, while computing the pair distribution function helps describe the steady-state order of a nematic phase. Taken together, our analysis characterizes macroscopic quantities that determine physical laws describing distinct phases and phase changes. This research furthers the field by identifying the phases of certain driven microtubule-motor systems and describing macroscopic observables.

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Timeline

- 08-01-2017: Collect data at low velocities and low concentrations of motors using updated code
- 09-30-2017: Write pair distribution code
- 10-03-2017: Thesis registration due (15:00)
- 10-20-2017: Finish writing correlation functions & run data through analysis code
- 10-30-2017: Identify specific interesting parameters to study further
- 11-14-2017: Make figures and organize data for Dr. Glaser's January paper
- 11-30-2017: Finalize figures and data for January paper
- 12-20-2017:
    - Have met with Dr. Glaser before winter break to go over what is left to be done for paper
    - Adjust goals for next semester based on this semester's progress
- 01-16-2017:
    - Make sure figures and data are finalized for January paper
    - Meet with Adam, Dr. Betterton, Dr. Glaser to reaffirm goals for spring semester
- 02-01-2018: Collect data for different parameters not yet studied
- 02-12-2018:
    - Outline of thesis completed
    - Analyze stresses, pressure, distribution or solution
    - Identify additional parameters to study based on analysis
- 02-26-2018: Draft 1 completed and submitted for feedback
- 03-12-2018: Draft 2 completed and submitted for feedback
- 03-14-2018:
    - Honors defense presentation completed
    - Draft 3 completed and submitted for feedback

- 03-19-2018: Final draft of thesis submitted to committee (about one week in advance of defense)
- 03-26-2018: Potential date of thesis defense (defense needs to be before April)
- 04-10-2018: Last day to defend & defense copy due (15:00)
- 04-13-2018: Final copy of thesis due on CU Scholar (23:59)