Mechanics and Motility of Cells

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Oral presentations

Spontaneous Rotation in 2d and 3d active colonies

Mehrana Nejad[1]

[1]University Of Oxford, Oxford, United Kingdom

We use numerical simulations and linear stability analysis to show that activity leads to the formation of nematic order and the emergence of spontaneous rotation of droplets in both two and three dimensions.

In 2d the rotation is caused by the formation of a chiral +1 defect at the center of the drop. We show that competition between elasticity and surface tension determines the stability of the shape of the interface. In particular, when surface tension is small, the droplet forms elongated isotropic arms that fold and form a rotating annulus.

In 3d a +1 disclination line forms at one side of the droplet and leads to both spontaneous rotation and spontaneous polar symmetry breaking. As a result, growing extensile colonies form an oblate ellipsoid while rotating, and contractile droplets grow to form a prolate ellipsoid while they maintain their rotational motion perpendicular to the elongation.

Exploring force distributions in epithelial cell sheets by applying tools from granular statistical theory.

Charlotte Benney, Isaac Chenchiah, Silke Henkes

[1]University Of Bristol, Bristol, United Kingdom

Understanding embryonic development, the process in which a simple ball of cells is transformed into a complex organism with tissues and organs, is a key question of biology. An important factor in this transition is the active mechanics of epithelial cell sheets that arise from the actomyosin in the cytoskeleton, driving radical changes to the topology and structure of an embryo. In order to investigate these active forces, we model an epithelial cell sheet as a two-dimensional triangular tiling.

In the limit of the sheet being in mechanical equilibrium, we can adapt the statistical mechanics of granular materials to investigate the cell model. We implement a Monte Carlo simulation from the Force Network Ensemble (FNE), called the wheel move, to sample the force configurations on the periodic triangular lattice model. We formulated a recurrence relation to generalise the regular hexagonal wheel move to disordered/irregular polygons, a more appropriate model for cells. Furthermore, we prove and utilise the ergodicity of the generalised wheel move for bounded and periodic force networks. Creating a force tiling, known in the FNE field as a Maxwell-Cremona diagram, we investigate global conserved quantities in order to formulate a statistical mechanical theory for forces in the cell model, analogous to the statistical theory for granular matter.

We systematically find states of self-stress where tensions are balanced by compressive apical forces. We also find evidence of tension chains along junctions, while retaining truncated normal distributions for junctional tension and apical pressures separately.

How do bacteria collectively migrate in densely packed colonies?

Nathan Costin[1], Oliver Meacock[2], James Wheeler[1], William Durham[1]

[1]Department of Physics and Astronomy, The University Of Sheffield, Sheffield, United Kingdom, [2]Department of Fundamental Microbiology, University of Lausanne, Lausanne, Switzerland

The pathogen Pseudomonas aeruginosa moves across surfaces using microscopic grappling hooks called pili. This form of motility allows cells in densely packed colonies to collectively move into new territory and acquire nutrients. However, it is not known how these cells avoid jamming, which wholly arrests movement and is widely observed in other active matter systems. Here we use a combination of massively parallel cell tracking, mathematical modelling, and fluorescent fusions that label key components of the pili system to investigate how individual cells modify their behaviour in densely packed colonies. We find that cells actively reverse direction to move in the same direction of their neighbours, which drives a highly polarised state which allows colonies to expand more rapidly. Our results suggest that the behaviour of individual Pseudomonas cells orchestrates their large scale collective movement.

Seeing soft samples with atom beams

Paul Dastoor[2], David Ward[1], Katie Brown[1], Nick von Jeinsen[1], Matthew Bergin[2], Benjamin Butler[1]

[1]University Of Cambridge, Cambridge, United Kingdom, [2]University of Newcastle, NSW, Australia

The advent of the scanning helium microscope (SHeM) has realised a long standing desire to construct a neutral atom beam instrument for real space imaging. SHeM has been shown to reveal topographical structure completely non-invasively without the addition of any surface coating or contrast agents which has significant applications in studying delicate samples, especially soft samples. We now present our latest results showing the techniques application to the imaging of biofilm surfaces topographically with the potential of revealing more information drawn from it's unique contrast mechanisms.

We present the first SHeM images of an extracellular matrix (ECM). It is well known that biological cells detect and react to mechanical changes in the ECM using a coordinated mechanosensing apparatus composed of adhesion receptors, cytoskeletal networks, and molecular motors. Importantly, mechanosensing plays a significant role in converting physical triggers into biochemical responses at a cellular level and is a key mediator influencing various stages of development in range of diseases including cancer.

ECM imaging traditionally relies on conventional histology staining techniques for optical microscopy. However, a host of well-documented limitations restrict the ability of these techniques to provide even semi-quantitative assessments of tissue ECM structure and morphology. Furthermore, histological staining is limited by its association with highly laborious sample preparation protocols. Consequently, to complement and advance beyond conventional staining techniques it is widely recognised that the field of ECM visualisation urgently requires the development of novel imaging capabilities.

Through our data, we will show that biofilm formation can be studied using the SHeM with topics such as the role that the ECM plays in determining bacterial biofilm formation and growth leading to understanding on how the mechanical microenvironment regulates biological cell processes responsible for growth and transmigration. The SHeM provides the unique ability to image the important interactions between surface topography and bacterial biofilm formation and growth without damaging or influencing the delicate biology of these systems.

The SHeM technique is finding application in the study of the ECM, initial data suggests that beyond the selective imaging of ECM topography the technique may offer a method of imaging the matrix stiffness to be imaged through it's sensitivity to surface phonons and a quantitively chemical sensitivity of the samples.

A reaction-diffusion model of flagellar beating matches beating patterns of eukaryotic microswimmers

James Cass[1], Dr. Hermes Gadelha[1]

[1]University Of Bristol, Bristol, United Kingdom

Eukaryotic flagella are cellular appendages used to propel organisms through fluid. Dynein motor proteins power beating of the flagellum by hydrolysing ATP and exerting axial forces between the microtubules that make up the cylindrical internal structure known as the axoneme. It is well understood that passive elements constrain sliding motions and this leads to bending deformations. Research is ongoing, however, to explain how the collective activity of individual dyneins can result in the self-sustaining stable oscillations of the flagellum that are seen in microswimmer experiments. Progress in this area could have implications for male infertility treatments and the design of artifical swimmers.

Most previous modelling studies have assumed that the energy supplied by the motors is dissipated in the external fluid, with little dissipation occuring internally, but recent experimental studies have called this into question. In this talk I present a self-sustaining reaction-diffusion model of flagellar beating with an internal dissipation mechanism that is able to reproduce the flagellar beating patterns of both Chlamydomonas Reinhardtii and bull sperm for appropriate parameters.

Poster presentations

The dynamics model of time-varying infectious disease based on machine learning

Dr. Guangyi Jia[1], Miss Jinxuan Luo[1]

[1]School of Science, Tianjin University of Commerce, Tianjin, China

The outbreak and spread of COVID-19 have significantly influenced global economics and people's lives. By the end of August 31, 2022, there have been 599,071,265 confirmed cases of COVID-19 and reported 6,467,023 deaths in the world, according to the most recent WHO real-time statistics. COVID-19 has severely impacted lifestyles worldwide. It is meaningful to exploit effective dynamics models to exactly predict the development trend of COVID-19 patients. Among various prediction models, the mathematical model of infectious disease dynamics has been extensively used to forecast the COVID-19. However, in the actual development of the epidemic, as the national governments continue to take effective control and prevention strategies, the self-isolation and protection awareness of susceptible people are increasingly enhanced, both of which will cause the infection coefficients to change over time. Besides, the accumulation of clinical experience and the development of vaccines further make the healing factor constantly change. All of these variation factors are not taken into account by the infectious disease dynamics. In view of this, we proposed a time-varying model with specific parameters on the basis of machine learning. In this model, we make full use of polynomial regression and back propagation (BP) neural network to fit the time-varying parameters, and then optimize the epidemic transmission model via adjusting parameters. By using the gradient search technology, BP neural network minimizes the mean square error of the actual output value and the expected output value of the network. The final fitting results show that our proposed method can be utilized to more effectively predict the variation tendency of COVID-19 patients than the current infectious disease dynamics.

The role of pH for in-situ biofilm detection on venous catheters

Dr Laura Confalonieri[1]

[1]The University of Edinburgh, Edinburgh, United Kingdom

The formation of bacterial biofilms on venous catheters is a major cause of failure, resulting in the need for invasive procedures to remove and replace the catheters, as well as the risk of lethal bloodstream infections [1, 2].

A standardised method for real-time biofilm detection in hospital settings is still missing. Working with Kimal, a UK-based manufacturer of medical devices, we are investigating the role of pH for in-situ biofilm detection.

Gradual pH changes have been reported to occur in biofilms as a results of anaerobic metabolism [3]. By embedding pH-sensitive dyes in the catheters' coating, we are aiming to reveal the bacterial colonisation of plastic catheters by a simple colour change.

Biocompatible polyurethane hydrogels were combined with pH-sensitive dyes to obtain pH-sensitive films which are not prone to leaching. Some of the most relevant bacteria for catheter-related infections were cultured in standard laboratory growth media and human plasma from healthy donors. Test results showing films' colour change in response to pH change following the bacterial growth will be presented (Figure 1).

The observed colour change was quantified via absorption spectra acquisition. The peak ratio of the red and the blue components of the spectra revealed as a useful tool to identify growing pathogens.

The pH change was found to be dependent on the growth medium and conditions. This stimulated further studies of metabolic pathways simulations via Flux Balance Analysis.

This work aims to provide a proof of concept for the potential use of pH-sensitive dyes for in-situ biofilm detection on medical devices. It opens the perspective for future applications in the health sector for a prompt identification of pathogens, finalised to a rapid selection of the proper antibiotic treatment.

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Predicting the efficacy of Visible-Violet disinfection of surfaces containing deposited airborne pathogens

Mr Prakash Sarnobat[1]

[1]Insight2Solution, Reigate, United Kingdom

Ultraviolet (UV) light plays a central role in the decontamination of Healthcare facilities. While it is very effective in decontaminating the air, any pathogens deposited from the air to any surface are not deactivated in a steady regular manner, as for safety reasons the use of UV requires the room to be regularly emptied of its occupants.

This work further investigates a relatively recent innovation but from a different point of view: Solid-state LED Light that is predominantly of Visible-Violet colour at 405nm wavelength (but bathed in a background of warm-white light), has been shown to deactivate surface pathogens both in the laboratory and in clinical trials. Such devices are referred to as High-Intensity-Narrow-Spectrum (HINS), first investigated by MacGregor et al (2010). The decontamination of the pathogens begins when they are released from the source into the air (as well as continuing after they reach any surface), and unlike for UV devices, a rigorous and definitive method of being able to predict this with sufficient accuracy has not yet been developed. Recent advances in computer simulations have enabled significant progress to be made.

We show that by using Computational Fluid Dynamics of air and pathogen movements in a hospital room, the ability of HINS devices to decontaminate air and surfaces can be predicted with sufficient accuracy. Also, the pathogen deposition rate and HINS decontamination rate was explored over a variety of ventilation rates (corresponding to different types of hospital rooms). It was shown for most surfaces that while the air-to-surface deposition rate reduces with increasing ventilation rate, the effectiveness of HINS devices is broadly consistent across several ventilation rates up to 25 ACH, reducing surface pathogen concentrations by up to two orders of magnitude. These results suggest that in rooms for which air-to-surface contamination is a major issue, the use of HINS devices can complement existing methods.

Metabolomics Markers of COVID-19 Are Dependent on Collection Wave

Holly-may Lewis[1], Yufan Liu[1], Cecile Frampas[1], Katie Longman[1], Matt Spick[1], Alexander Stewart[1], Emma Sinclair[1], Nora Kasar[1], Danni Greener[2], Anthony Whetton[1], Perdita Barran[3], Tao Chen[1], Deborah Dunn-Walters[1], Debra Skene[1], Melanie Bailey[1]

[1]University Of Surrey, Guildford, United Kingdom, [2]Frimley Health NHS Trust, Camberley, United Kingdom, [3]University of Manchester, Manchester, United Kingdon

The effect of COVID-19 infection on the human metabolome has been widely reported, but to date all such studies have focused on a single wave of infection. COVID-19 has generated numerous waves of disease with different clinical presentations, and therefore it is pertinent to explore whether metabolic disturbance changes accordingly, to gain a better understanding of its impact on host metabolism and enable better treatments. This work used a targeted metabolomics platform (Biocrates Life Sciences) to analyze the serum of 164 hospitalized patients, 123 with confirmed positive COVID-19 RT-PCR tests and 41 providing negative tests, across two waves of infection. Seven COVID-19-positive patients also provided longitudinal samples 2–7 months after infection. Changes to metabolites and lipids between positive and negative patients were found to be dependent on collection wave. A machine learning model identified six metabolites that were robust in diagnosing positive patients across both waves of infection: TG (22:1_32:5), TG (18:0_36:3), glutamic acid (Glu), glycolithocholic acid (GLCA), aspartic acid (Asp) and methionine sulfoxide (Met-SO), with an accuracy of 91%. Although some metabolites (TG (18:0_36:3) and Asp) returned to normal after infection, glutamic acid was still dysregulated in the longitudinal samples. This work demonstrates, for the first time, that metabolic dysregulation has partially changed over the course of the pandemic, reflecting changes in variants, clinical presentation and treatment regimes. It also shows that some metabolic changes are robust across waves, and these can differentiate COVID-19-positive individuals from controls in a hospital setting. This research also supports the hypothesis that some metabolic pathways are disrupted several months after COVID-19 infection.

Characterizing flexibility and mobility in the natural mutations of the SARS-CoV-2 spikes

Prof Rudo Roemer[1], Dr Dom Bellini[2]

[1]University Of Warwick, Coventry, United Kingdom, [2]MRC Laboratory of Molecular Biology, Cambridge , United Kingdom

We perform in-silico modelling of the SARS-CoV-2 spike protein and its mutations, using structures from the Protein Data Bank (PDB), to ascertain their dynamics, flexibility and rigidity. Identifying the precise nature of the dynamics for the spike proteins enables, in principle, the use of further in-silico design methods to quickly screen both existing and novel drugs that may hinder these natural dynamics. We use a recent protein flexibility modelling approach, combining methods for deconstructing a protein structure into a network of rigid and flexible units with a method that explores the elastic modes of motion of this network, and a geometric modelling of flexible motion. We also conduct this analysis on synthetic structures of some newer variants (α, β, γ, δ, λ, ο) for some of which structure files are not yet available from the PDB. All proteins are thermalised for at least 1ns with NAMD to human body temperature before the flexibility analysis.

Effect of Cerium Oxide (CeO2) on Antibacterial Properties of Synthetic Cancellous Bone Scaffolds

Lemiha YILDIZBAKAN[1], Neelam IQBAL[1], Thuy DO[2], Elena JONES[3], Peter GIANNOUDIS[4], Animesh JHA[1]

[1]School of Chemical and Process Engineering, University of Leeds, Leeds LS2 9JT, United Kingdom, [2]Division of Oral Biology, St James University Hospital, School of Medicine, University of Leeds, Leeds LS9 7LN, United Kingdom, [3]Clinical Sciences Building, St James University Hospital, School of Medicine, University of Leeds, Leeds LS9 7LN, United Kingdom, [4]Academic Department of Trauma and Orthopaedic, School of Medicine, University of Leeds, Leeds General Infirmary, Leeds LS2 9JT, United Kingdom

Bone is a complex living tissue with significant metabolic and regenerative activities, which are disrupted when the tissue is damaged. The damaged bone in the open fracture is predisposed to infection, which must be eradicated prior to new bone formation in the healing phase. A compromised healing phase of bone regeneration may lead to bone non-union or missed union and mal-union, needing further surgical intervention. According to the Trauma and Orthopaedic Surgery collected data between 1995 to 2010 were obtained, the rate of non-union and postoperative limb deformity increased from year to year in England and Wales. Total expenditure over 15 years was £8.2m (1).

For preventing possible infection or to eliminate a present infection, antibacterial scaffolds are needed for restoring bone growth in the damaged area. The “ideal” scaffold must support the healing of the healthy bone via enhanced osteogenesis and angiogenesis and provide biomechanical loading in an aseptic environment. Additionally, the growth factors are required for inducing bone growth. We have focussed on the engineering of stimulating union and preventing the non-union of tissues in a damaged bone. Additionally, the designed material should promote bone mineralization, formation of intrinsic vasculature, and anti-bacterial properties. a cancellous scaffold derived from the mixture of chitosan, iron oxide doped brushite (CaHPO4.2H2O) calcium phosphate, and cerium oxide phase mixture; the latter is known for enhancing osteogenesis and controlling infection (2). The cancellous structure is designed to mimic the natural cancellous bone hierarchy that will allow mineralization and vascularization, and have antibacterial properties for preventing or eliminating the infection. The mineral mixture of chitosan, cerium oxide, and iron-doped brushite was fabricated via precipitation and freeze-drying. The nanoparticle of mixed valent cerium oxide (Ce3+, Ce4+) plays important role in controlling the antibacterial properties, and also shows low cytotoxicity for osteoblast proliferation(3). The mixed valence state of cerium oxide is an essential pathway for controlling antibacterial action, which may arise as a result of low pH (<5) in an infected environment and high pH~6.8-7.2 in a healthy cell environment. To evaluate the antibacterial properties of the developed scaffold has been tested with two different bacterial cultures (gram+ and gram-). Results of the bacterial experiment in vitro demonstrated that the developed scaffold has the potential to prevent bacterial proliferation.

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Fast 3D coarse-grained simulation of interacting elastohydrodynamic filaments and solid body microhydrodynamics

Paul Fuchter[1], Dr Hermes Bloomfield-Gadêlha[1]

[1]Department of Engineering Mathematics, University of Bristol, Bristol, United Kingdom

Elastic filaments are vital to numerous biological, physical and engineering systems, from cilia driving fluid in the lungs to robotic powered micro-swimmers and microfluidic chips. Simulating these structures requires intricate balance of 3D elastic, body, active and hydrodynamic moments. In this talk we will discuss a generalised 3D coarse-graining formulation that is fast, efficient, numerically stable, and easy-to-implement and customise. Our method allows efficient simulation of collections of 3D elastic filaments coupled hydrodynamically, with both flexural and torsional deformations, in addition to hydrodynamic and contact-contact interactions with free or fixed solid bodies and micro-structures with arbitrary shapes. The method exploits the exponential mapping parametrisation for high-precision tracking of 3D rotations of each interacting unit, allowing fast and efficient computation. Spheres are used as 'building blocks' for a flexible, straightforward and intuitive construction of arbitrary three-dimensional geometries. We highlight the strengths of the method in a series of non-trivial applications. These include multi-flagellated swimmers, sperm-egg elastohydrodynamic scattering and multi-cilia interaction driving particle transport, all in 3D. Applications to lab-on-a-chip devices with multiple passive and/or active filaments within a complex geometry, mono-to-multi flagellated or kinematic swimmers, Brownian polymer and DNA dynamics, and micro-, soft-robotics are also straightforward.

PolyScope: a 3D-printed minimal microscopic system for microswimmer tracking

Wesley Shao[1], Dr. Hermes Gadêlha[1]

[1]University of Bristol, Bristol, United Kingdom

The innovative technology of additive manufacturing('3D printing') brings up opportunities to democratize microscopy. Devices with high magnifying powers could be designed of individualization, produced in mass and re-innovated with ease. However, due to separation between the innovating and applying communities, such a paradigm currently fails to fulfill its full potential. Here, an innovative 3D-printed microscopic system: PolyScope, is presented as a specific device for observation of microswimmers. Applied to static, motile and living targets, the system shows capability for educational and researching usage. Besides, since its structure can be easily modified to change magnifying features, PolyScope bears high flexibility of modification. The further developement and application of PolyScope would not only make microscopic technology more accessabile, but also benefit the exploration on an universal method of purpose-guided device development.

Reproducing mulitiscale dynamics of myosin's cooperative behaviour using a discrete mechanical model

Mr Benjamin Warmington[1], Dr Hermes Bloomfield-Gadêlha[1], Professor Jonathan Rossiter[1]

[1]Department Of Engineering Mathematics, University Of Bristol, Bristol, United Kingdom

Models describing the collective behaviour of non-processive myosin motors are limited by their reliance on modelling populations of motors. This allows them to demonstrate dynamics of an actin filament, but provides little insight on the dynamics of the molecular motors themselves. In this talk we will discuss a mechanical model abstracting myosin heads as a discrete series of periodically couple, oscillating force producing units. Using this model we have replicated typical sawtooth displacement profiles seen in the results of both experiments and previous continuous models. We then show that in producing these profiles individual oscillators can self-organise into stable synchronisation patterns, allowing the system to exert a greater force than when disordered. We found there is a positive relationship between resisting force and number of coupled oscillators. This allows the total force produced by the oscillators to increase and minimises velocity reduction of the system, acting similarly to a differential control. Finally we created a physical replica of the model, recognising the potential a system that demonstrates self-organisation and morphogenic control has in the field of robotic actuation.

Conditions for hydrodynamic coordination in arrays of model cilia

Rachel Bennett[1]

[1]University Of Bristol, United Kingdom

On surfaces with many cilia, individual cilia coordinate their beat cycles in the form of metachronal waves. The coordinated beating facilitates self-propulsion of ciliated microorganisms and creates efficient fluid flow, which is important in several human organs. Here, we consider the connection between single cilium characteristics and the collective behaviour. A theoretical framework is presented using an array of model cilia coordinated by hydrodynamic interactions. We calculate the dispersion relation for metachronal waves and perform a linear stability analysis to identify stable waves. This framework shows how the wave vector, frequency and stability depend on the geometric properties of cilia in the array and the beat pattern of an individual cilium. Analytical results are compared with agent-based numerical simulations of hydrodynamically coupled cilia, and we find quantitative agreement with analytical predictions. These results show how information about individual cilia can be used to predict the collective behaviour of many cilia.

Active feedback generates convergence extension in a continuum model for epithelial tissues

Aondoyima Ioratim-uba[1], Silke Henkes[1,2], Tanniemola Liverpool[1]

[1]University Of Bristol, Bristol, United Kingdom, [2]Lorentz Institute for Theoretical Physics, Leiden University, Leiden, The Netherlands

Epithelial tissues undergo significant structural changes during development. An example is convergent-extension, which has been observed during gastrulation. It involves tissue elongation in one direction, accompanied by narrowing in the perpendicular direction. However, we lack a mechanistic understanding of how these changes occur. We present a continuum model for an epithelial tissue embedded in a viscous liquid. The force exerted by the tissue on the fluid is balanced by friction. The tissue is viscoelastic, and its stress tensor is separated into a passive and an active component. The passive stress relaxes viscoelastically. The active stress is controlled by an anisotropic distribution of myosin molecular motors. The evolution of the myosin distribution has a positive feedback (catch bond) between myosin distribution and applied tension so that the tissue can work against applied tension. We study the system analytically using linear response theory and explore numerical solutions of the full nonlinear problem.

Droplets in the cell nucleus: Linking polymer dynamics with liquid-liquid phase separation

Sam Cameron, Rachel Bennett, Tanniemola Liverpool

[1]University Of Bristol, Bristol, United Kingdom

The interplay of DNA elasticity and liquid droplet formation within the cell nucleus is modelled by coupling discrete, bead-rod polymers with a continuum (Flory-Huggins) field theory of liquid-liquid phase separation. Nucleation sites placed along the polymer beads provide a mechanism of droplet formation or exclusion. We have developed a fully parallel, scalable software package to solve the resulting (stochastic) equations of motion. The resulting dynamics show qualitative agreement with experimental observation of droplet formation in the cell nucleus. We aim to use this theory to obtain into the physical mechanisms which drive DNA clustering within liquid droplets, a phenomenon which is thought to be relevant in certain types of cancer.

Counterbend of Tapered Elastic Filament-Bundles

Natasha Avery

Elastic filament-bundles are ubiquitous in nature, from flagella and cilia to DNA and protein chains. In flagella it is observed that a high curvature at the base induces a counter curvature at the distal end, this is known as the counterbend phenomenon. Similar experimental conditions show a much higher counterbend with near constant curvature in rat sperm compared to sea urchin sperm. We predicted that this was due to differences in structure between the flagella. Mammalian sperm possess tapered outer dense fibers surrounding the axoneme whereas sea urchin sperm lacks such structures. To discern the effects of four different rates of taper on the static, post-buckled geometries of filament-bundles, we used a geometrically exact sliding filament model. We found that counter curvature positively correlates to the rate of taper. This is most easily observed when the basal compliance is low and sliding resistance through the filament is high. However, we are yet to qualitatively recreate the near constant curvature seen within rat sperm counterbend, which suggests there are other factors not accounted for in the model.