PROGRAM AT A GLANCE

MONDAY, JUNE 28 (PDT)		TUESDAY, JUNE 29 (PDT)	
8:50 – 9:00	Opening remarks	8:50 – 9:00	Opening remarks
9:00 – 10:15	Oral pres. session 1: Quantum and Statistical Mechanics	9:00 – 10:15	Oral pres. session 3: Biomechanics
10:15 – 10:30	Coffee break (networking)	10:15 – 10:30	Coffee break (networking)
10:30 – 11:30	Keynote lecture 1: Christopher Cairo	10:30 – 11:30	Keynote lecture 2: Raymond E. Goldstein
11:30 – 12:30	Lunch break	11:30 – 12:30	Lunch break
12:30 – 14:15	Oral pres. session 2: Diseases + Protein Folding	12:30 – 13:30	Oral pres. session 4: Rheology
14:15 – 15:15	Career hour talks by our sponsors	13:30 – 14:45	Poster session
		14:45 – 13:00	Closing remarks

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KEYNOTE 1: CHRISTOPHER CAIRO

10:30 – 11:30 June 28 (PDT)

Sialic Acids in Membrane Organization and Receptor Function: Integrins and CD22

The plasma membrane contains a wide array of glycans and glycolipids, many of which are capped by sialic acids (also called neuraminic acid). As a result, sialic acids are front-line mediators of interactions between the extracellular surface and the external environment. Examples include host-pathogen interactions (e.g. influenza) and the recognition of host cells by leukocytes (white blood cells). Thus, the composition of sialosides in the membrane can influence receptor-receptor interactions critical to immunity and cellular function. Our group is investigating the influence of sialic acid on the function of adhesion and immune receptors through the development of tools that alter catabolism of membrane sialosides.

The human neuraminidases (NEU) are a family of four isoenzymes (NEU1, NEU2, NEU3, and NEU4) which have a range of substrate preferences as well as cellular and tissue localization. Our group has developed a panel of selective inhibitors, many with nanomolar potency, are being used to investigate how degradation of sialosides influences the function of cellular receptors. We use fluorescence microscopy to measure the size of receptor clusters and lateral mobility of receptors. These biophysical methods provide critical insight into the influence of NEU activity on membrane receptor organization.

We have examined the role of NEU enzymes on the function and organization of leukocyte adhesion receptors. We find that specific NEU enzymes can modulate integrin adhesion and affect leukocyte transmigration. In related work, we have examined the influence of synthetic glycoconjugates and inhibitors of NEU on the organization of the CD22 receptor of B cells. We propose that understanding the specific roles of NEU isoenzymes will identify new therapeutic strategies for autoimmunity, inflammation, and cancer.

About the speaker

Christopher W. Cairo is a Professor of Chemistry at the University of Alberta. He obtained a BSc in Chemistry from the State University of New York (SUNY) at Albany. He went on to graduate studies at the University of Wisconsin-Madison, with Prof. Laura L. Kiessling where he worked on multivalent carbohydrate-protein interactions. Chris then moved to an NIH-funded Postdoctoral fellowship with Prof. David E. Golan at Harvard Medical School where he studied the regulation of integrins in T cell adhesion. Chris joined the faculty of the University of Alberta in 2006 as an Assistant Professor of Chemistry and was promoted to Professor in 2021. He was a principal investigator in the Alberta Glycomics Centre, and is currently a Network Investigator with GlycoNet. The Cairo research group studies the function of glycoproteins and glycolipids in cardiovascular disease, cancer, and immunity. Their work takes place at the chemistry-biology interface with major projects targeting the design of inhibitors for the human neuraminidase enzymes, the recognition of carbohydrate antigens in immune response, and bioconjugate labelling strategies for glycolipids and glycoproteins.
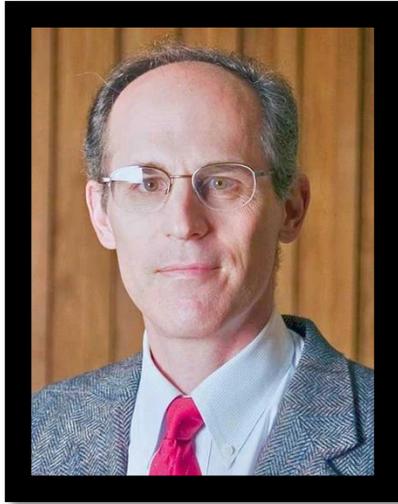
KEYNOTE 2: RAYMOND E. GOLDSTEIN

10:30 – 11:30 June 29 (PDT)

Cytoplasmic Streaming and the Swirling Instability of the Microtubule Cytoskeleton

Cytoplasmic streaming is the persistent circulation of the fluid contents of large eukaryotic cells, driven by the action of molecular motors moving along cytoskeletal filaments, entraining fluid. Discovered in 1774 by Bonaventura Corti, it is now recognized as a common phenomenon in a very broad range of model organisms, from plants to flies and worms. This talk will discuss physical approaches to understanding this phenomenon through a combination of experiments (on aquatic plants, Drosophila, and other active matter systems), theory, and computation. A particular focus will be on streaming in the Drosophilaoocyte, for which I will describe a recently discovered "swirling instability" of the microtubule cytoskeleton.

About the speaker

Raymond Ethan Goldstein is Schlumberger Professor of Complex Physical Systems in the Department of Applied Mathematics and Theoretical Physics (DAMTP) at the University of Cambridge. Before his position at University of Cambridge started in 2006, he has held academic appointments at the University of Chicago, Princeton University and the University of Arizona. Raymond Goldstein is an internationally recognised leader in the fields of biological physics and nonlinear dynamics. He is distinguished for having made important mathematical contributions to those subjects as well as pioneering experimental discoveries. His broad-ranging contributions include classic work on the dynamics of pattern formation driven by long-range forces, the differential geometry of interfacial pattern formation, and the explanation for the shapes of stalactites. He has made seminal experimental contributions to the study of active matter, including developing a class of green algae as model organisms for the study of biological fluid dynamics, the physics of multicellularity, and the synchronisation of eukaryotic flagella.

ORAL PRESENTATIONS

(15 min ea. ~10 min presentation, ~5 min setup and Q/A)

Session 1: Quantum and Statistical Mechanics
9:00 – 10:15, June 28 (PDT)

9:00 – 9:15	Yu-Chen Cheng	Generalizing Gibbsian Statistical Ensemble Theory for Strongly Coupled Heterogeneous Systems
9:15 – 9:30	Matthew Leighton	Scaling Laws and Performance Trade-offs for Collective Transport
9:30 – 9:45	Miranda Louwerse	Information Thermodynamics of the Transition-Path Ensemble
9:45 – 10:00	Steven Blaber	Steps Minimize Dissipation in Rapidly Driven Stochastic Systems
10:00 – 10:15	Luke Reynolds	Fractional T1 Relaxation from Magnetization Transfer in Wood: Applications to Brain MRI?

Generalizing Gibbsian Statistical Ensemble Theory for Strongly Coupled Heterogeneous Systems

Yu-Chen Cheng (9:00 – 9:15)

The probability distribution of a function of a subsystem conditioned on the value of the function of the whole, in the limit when the ratio of their values goes to zero, has a limit law: It equals the unconditioned marginal probability distribution weighted by an exponential factor whose exponent is uniquely determined by the condition. We apply this theorem to explain the canonical equilibrium ensemble of a system in contact with a heat reservoir. Since the theorem only requires analysis at the level of the function of the subsystem and reservoir, it is applicable even without the knowledge of the composition of the reservoir itself, which extends the applicability of the canonical ensemble. Furthermore, we generalize our theorem to a model with strong interaction that contributes an additional term to the exponent, which is beyond the typical case of approximately additive functions. This result is new in both physics and mathematics, as a theory for the Gibbs conditioning principle for strongly correlated systems.

Scaling Laws and Performance Trade-offs for Collective Transport

Matthew Leighton (9:15 – 9:30)

Motor-driven intracellular transport of organelles, vesicles, and other molecular cargo is a highly collective process. An individual cargo is often pulled by a team of transport motors, with numbers ranging from only a few to over 200. We explore the behaviour of these systems using a stochastic model for motor-driven transport of molecular cargo by N motors which we solve analytically. We investigate the N-dependence of important quantities such as the velocity, precision of forward progress, energy flows between different system components, and efficiency; these properties obey simple scaling laws with N in two opposing regimes. Finally, we explore performance bounds and trade-offs as N is varied, providing insight into how different numbers of motors might be well-matched to different types of systems depending on which performance metrics are prioritized.

Information Thermodynamics of the Transition-Path Ensemble

Miranda Louwerse (9:30 – 9:45)

The reaction coordinate describing a transition between reactant and product is a fundamental concept in the theory of chemical reactions. Within transition-path theory, a quantitative definition of the reaction coordinate is found in the committor, which is the probability that a trajectory initiated from a given microstate first reaches the product before the reactant. Here we demonstrate an information-theoretic origin for the committor, show how it naturally arises from selecting out the transition-path ensemble from the equilibrium ensemble, and prove that the resulting entropy production is fully determined by committor dynamics. Our results provide parallel stochastic-thermodynamic and information-theoretic measures of the relevance of any system coordinate to the reaction, each of which are maximized by the committor, providing further support for its status as the 'true' reaction coordinate.

Steps Minimize Dissipation in Rapidly Driven Stochastic Systems

Steven Blaber (9:45 – 10:00)

Since its inception nearly 200 years ago, a central theme of thermodynamics has been the design of energetically efficient engines. In our modern world the engines grow ever smaller, down to the micro- and nano-scale of biological molecular machines, where stochastic fluctuations are large. To achieve fast operating speeds, these small-scale machines are driven by rapid changes in control parameters (control protocols). By focusing on the fast limit, we show that for any stochastic system driven sufficiently rapidly, the most energetically efficient driving always consists of jumps at the beginning and end of the protocol, spending the entire duration at the point which optimally balances the relaxation rate with jump size. Our results are of practical use in thermodynamic computing, single-molecule experiments, and free-energy estimation.

Fractional T1 Relaxation from Magnetization Transfer in Wood: Applications to Brain MRI?

Luke Reynolds (10:00 – 10:15)

Spin-lattice (T1) relaxation is widely used in NMR to characterize chemical structure, molecular dynamics, and to provide a contrast mechanism for in-vivo imaging. When tissue is heterogeneous and multi-compartment like brain tissue, however, it becomes difficult to model and assign physiological meaning to T1 relaxation due to the transfer of magnetization between pools during relaxation. Using wood as a model system, we explore the deviation from a standard exponential in the relaxation component stemming from this transfer. Fractional calculus offers a generalized exponential function to fit relaxation data from which a potentially unique parameter associated with the sample's inhomogeneity results. We show the improved fit to the data of the fractional model compared to standard exponentials in wood as well as a lipid bilayer system and posit a white matter mapping technique based on the added fractional fit parameter.

Session 2: Diseases + Protein Folding
12:30 – 14:15, June 28 (PDT)

12:30 – 12:45	Keng-Shuo Pi	Interaction of U24 and Phosphorylated U24 from Human Herpes Virus Type 6B with Fyn SH3 and Nedd-4L WW3* Domain
12:45 – 13:00	Hans Ghezzi	Understanding the Impact of Gut Physical Perturbations on Bacterial Abundance
13:00 – 13:15	Lauren Walgren	Synergy between Antimicrobial Peptides Derived from Aurein 2.2 and IDR- 1018 and Commonly used Antibiotics
13:15 – 13:30	Shawn Hsueh	Epitope Scaffolding using Alpha-synuclein Cyclic Peptides to Generate Oligomer-selective Antibodies for Parkinson's Disease
13:30 – 13:45	Pranav Garg	Misfolding-Associated Exposure of Natively Buried Residues in Mutant SOD1 Facilitates Binding to TRAF6
13:45 – 14:00	Lei Yu	Systematic Differences between Current Molecular Dynamics Force Fields to Represent Local Properties of Intrinsically Disordered Proteins
14:00 – 14:15	Jiayu Li	The Mechanical Folding-Unfolding Mechanism of Cytochrome C Probed by Single-Molecule Optical Tweezers

Interaction of U24 and Phosphorylated U24 from Human Herpes Virus Type 6B with Fyn SH3 and Nedd-4L WW3* Domain

Keng-Shuo Pi (12:30 – 12:45)

Recent work has shown that U24, a putative tail-anchored membrane protein unique to Roseoloviruses (i.e. Human Herpesvirus (HHV) type-6A, -6B and -7), may play a role in multiple sclerosis (MS). Two hypotheses on how HHV may be implicated in MS have been proposed: 1) molecular mimicry; and 2) endocytic recycling. In particular, these explorations indicated the importance of phosphorylation and charges on bindings affinities between U24-6A and important proteins such as Fyn-SH3 and Nedd4 for the molecular mimicry and endocytic recycling models, respectively. Herein, the interaction of U24-6B and its phosphorylated variant (pU24-6B) with hNedd4L-WW3* as well as Fyn-SH3 domains will be quantified. Results obtained from isothermal titration calorimetry (ITC) have shown that U24-6B binds to human Nedd4L-WW3* (KD= 4.7 ± 0.3) slightly better than U24-6A, while similar binding affinities were observed for pU24-6B (KD= 0.88 ± 0.01 μM) and pU24-6A (KD= 0.76 ± 0.03 μM) with hNedd4L-WW3*. Interestingly, binding interactions between phosphorylated U24-6A and -6B with Fyn-SH3 showed a larger number of perturbed residues than the unphosphorylated versions of the peptides, as evidenced through 15N- HSQC NMR titrations. These results will be discussed in light of the two models linking the highly seroprevalent HHV-6A and 6B variants to MS.

Understanding the Impact of Gut Physical Perturbations on Bacterial Abundance

Hans Ghezzi (12:45 – 13:00)

The human gut is inhabited by a diverse community of microorganisms including bacteria, archaea and viruses, which make up our microbiota. Microbial dynamics, including the establishment and maintenance of bacterial communities, can be rapidly and drastically impacted by the gut physical environment. Specifically, changes to gut osmolality (a measure of concentration of molecules) such as in the case of laxative use, celiac disease or Crohn's disease can lead to perturbations of the gut ecosystem, and impact human health. Our research investigates the direct effects of osmolality on the growth of individual bacteria, as a predictor of bacterial abundance. We hypothesize that the physical environment has a major direct impact on bacterial availability, alongside other indirect effects of physical perturbations such as changes to bacterial-host and inter-bacterial interactions. To investigate this, we bi-colonised germ-free mice with two gut commensals, Bacteroides thetaiotaomicron VPI-5482 and Muribaculum intestinale G6, and induced osmotic diarrhea by administering water with increasing concentrations of an osmotic laxative. We show that hyperosmotic stress negatively affected in vivo abundance of both bacteria in a dosage-dependent matter. Our results suggest that that the gut physical environment may govern microbial abundance, as osmotic stress linearly inhibited bacterial growth dependent on gut osmolality. Altogether, understanding the impact of physical perturbations on the gut microbiome is key to develop novel approaches in personalised medicine.

Synergy between Antimicrobial Peptides Derived from Aurein 2.2 and IDR- 1018 and Commonly used Antibiotics

Lauren Walgren (13:00 – 13:15)

Antibiotic resistance has become a large public health problem due to the frequent and unrestricted use of antibiotics. Thus, there is an urgent need to find novel antibacterial therapeutics or a combination of antibacterial agents to treat antibiotic-resistant bacteria. This study investigated the synergy between two antimicrobial peptides (AMPs) and broad-spectrum antibiotics used against a number of ESKAPE pathogens, namely P. aeruginosa, S. aureus, A. baumannii and E. faecium. One of the AMPs, denoted peptide 73, was derived from the natural host defense peptide aurein 2.2 [1,2]. The other AMP (IDR-3002) was derived through in silico quantitative structure-activity relationship (QSAR) models [3]. The minimum inhibitory concentration (MIC) of each AMP was evaluated against each of the 4 strains listed above. Based on the MIC found for each AMP, a checkerboard assay was performed to investigate the synergy between the peptides and antibiotics, as expressed by the fractional inhibitory concentration (FIC). Neither peptide showed synergistic effects with antibiotics when tested against the Gram-positive bacteria (S. aureus and E. faecium). However, each AMP combined with polymyxin B showed synergistic activity against antibiotic sensitive strains of P. aeruginosa and A. baumannii. The results will be presented in light of using AMP/antibiotic combinations to combat antibiotic resistance.

Epitope Scaffolding using Alpha-synuclein Cyclic Peptides to Generate Oligomer-selective Antibodies for Parkinson's Disease

Shawn Hsueh (13:15 – 13:30)

Effectively scaffolding epitopes on immunogens, in order to raise conformationally selective antibodies through active immunization, is a central problem in treating protein misfolding diseases, particularly neurodegenerative diseases such as Alzheimer's disease or Parkinson's disease. We seek to selectively target conformations enriched in toxic, oligomeric propagating species while sparing healthy forms of the protein which are often more abundant. To this end, we scaffolded cyclic peptides by varying the number of flanking glycines, to best mimic a misfolding-specific conformation of an epitope of alpha-synuclein enriched in the oligomer ensemble, as characterized by a region most readily disordered and solvent-exposed in a stressed, partially denatured protofibril. We screen and rank the cyclic peptide scaffolds of alpha-synuclein in silico based on their ensemble overlap properties with the fibril, oligomer-model, and isolated monomer ensembles. We introduce a method for screening against structured off-pathway targets in the human proteome, by selecting scaffolds with minimal conformational similarity between their epitope and the same primary sequence in structured human proteins. Ensemble comparison and overlap was quantified by the Jensen-Shannon Divergence, and a new measure introduced here---the embedding depth, which determines the extent to which a given ensemble is subsumed by another ensemble, and which may be a more useful measure in sculpting the conformational-selectivity of an antibody.

Misfolding-Associated Exposure of Natively Buried Residues in Mutant SOD1 Facilitates Binding to TRAF6

Pranav Garg (13:30 – 13:45)

Amyotrophic lateral sclerosis (ALS) is a fatal neurodegenerative disease primarily impacting motor neurons. Mutations in superoxide dismutase 1 (SOD1) are the second most common cause of familial ALS. Several of these mutations lead to misfolding or toxic gain of function in the SOD1 protein. Recently, we reported that misfolded SOD1 interacts with TNF receptor-associated factor 6 (TRAF6) in the SOD1-G93A rat model of ALS. Further, we showed in cultured cells that several mutant SOD1 proteins, but not wild type SOD1 protein, interact with TRAF6 via the MATH domain. Here, we sought to uncover the structural details of this interaction through molecular dynamics (MD) simulations of a dimeric model system, coarse grained using the AWSEM force field. We used direct MD simulations to identify buried residues, and predict binding poses by clustering frames from the trajectories. Metadynamics simulations were also used to deduce preferred binding regions on the protein surfaces from the potential of the mean force in orientation space. Well-folded SOD1 was found to bind TRAF6 via co-option of its native homodimer interface. However, if loops IV and VII of SOD1 were disordered, as typically occurs in the absence of stabilizing Zn2+ ion binding, these disordered loops now participated in novel interactions with TRAF6. On TRAF6, multiple interaction hot-spots were distributed around the equatorial region of the MATH domain beta barrel. Expression of TRAF6 variants with mutations in this region in cultured cells demonstrated that TRAF6 residue T475 facilitates interaction with different SOD1 mutants. These findings contribute to our understanding of the disease mechanism and uncover potential targets for the development of therapeutics.

Systematic Differences between Current Molecular Dynamics Force Fields to Represent Local Properties of Intrinsically Disordered Proteins

Lei Yu (13:45 – 14:00)

The prevalence of intrinsically disordered polypeptides (IDPs) and protein regions in structural biology has prompted the recent development of molecular dynamics (MD) force fields for the more realistic representations of such systems. Using experimental NMR backbone scalar 3J-coupling constants of the intrinsically disordered proteins alpha-synuclein and amyloid-beta in their native aqueous environment as a metric, we compare the performance of four recent MD force fields, namely AMBER ff14SB, CHARMM C36m, AMBER ff99SB-disp, and AMBER ff99SBnmr2, by partitioning the polypeptides into an overlapping series of heptapeptides for which a cumulative total of 276 us MD simulations are performed. The results show substantial differences between the different force fields at the individual residue level. Except for ff99SBnmr2, the force fields systematically underestimate the scalar 3J(HN,Ha) couplings, due to an underrepresentation of beta-conformations and an overrepresentation of either alpha- or PPII conformations. The study demonstrates that the incorporation of coil library information in modern

molecular dynamics force fields, as shown here for ff99SBnmr2, provides substantially improved performance and more realistic sampling of local backbone phi,psi dihedral angles of IDPs as reflected in good accuracy of computed scalar 3J(HN,Ha)-couplings with < 0.5 Hz error. Such force fields will enable a better understanding how structural dynamics and thermodynamics influence IDP function. Although the methodology based on heptapeptides used here does not allow the assessment of potential intramolecular long-range interactions, its computational affordability permits well-converged simulations that can be easily parallelized. This should make the quantitative validation of intrinsic disorder observed in MD simulations of polypeptides with experimental scalar J-couplings widely applicable.

The Mechanical Folding-Unfolding Mechanism of Cytochrome C Probed by Single-Molecule Optical Tweezers

Jiayu Li (14:00 – 14:15)

Cytochrome c (cyt c) is an important type of electron transfer protein involved in both aerobic and anaerobic respiration processes. It is also one of the most studied proteins due to its easiness to obtain and characterize by spectroscopic methods. The 104 amino acid-protein is highly helical, and contains a heme cofactor bounded by two thioether bonds and two coordination bonds. The ensemble folding-unfolding behavior of cyt c in denaturant has been extensively studied with hydrogen exchange experiment, and a foldon-dependent multiple-step folding-unfolding mechanism has been proposed. Here we used single-molecule optical tweezers to probe the mechanical folding-unfolding behavior of cyt c at the single-molecule level. We found that folded cyt c has a very narrow unfolding force distribution centered at ~30 pN. Cyt c mostly unfolded in an all-or-none fashion, while a short-lived intermediate could sometimes be observed in relatively low-force unfolding events. The refolding always happened in two-state fashion at ~4 pN. In addition, we found that the apo-form cyt c, which is long-believed as a random-coil, displayed some intrachain interactions. Our results may provide important new insights to our understanding of the folding and stability of cyt c as well as metalloproteins in general.

Session 3: Biomechanics
9:00 – 10:15, June 29 (PDT)

9:00 – 9:15	Daniele Agostinelli	Nutations in Growing Plant Shoots: Endogenous and Exogenous Factors in the Presence of Elastic Deformations
9:15 – 9:30	Mouad Boudina	Vortex-induced Vibrations as a Soft Coral Strategy to Enhance Food Capture
9:30 – 9:45	Manish Kumar	Effect of External Flows on Sperm Flagellar Dynamics
9:45 – 10:00	Daniele Agostinelli	Morphological Control of Receptor-mediated Endocytosis
10:00 – 10:15	Naba Mukhtar	Simulating Epithelial-Mesenchymal Transition in Cell Sheets

Nutations in Growing Plant Shoots: Endogenous and Exogenous Factors in the Presence of Elastic Deformations
Daniele Agostinelli (9:00 – 9:15)

Growing plant shoots exhibit circumnutations, namely, oscillations that draw three-dimensional trajectories, whose projections on the horizontal plane generate pendular, elliptical, or circular orbits. A large body of literature has followed the seminal work by Charles Darwin in 1880, but the nature of this phenomena is still uncertain and a long-lasting debate produced three main theories: the endogenous oscillator, the exogenous feedback oscillator, and the two-oscillator model. After briefly reviewing the three existing hypotheses, I will discuss a possible interpretation of these spontaneous oscillations as a Hopf-like bifurcation in a growing morphoelastic rod.

Vortex-induced Vibrations as a Soft Coral Strategy to Enhance Food Capture

Mouad Boudina (9:15 – 9:30)

Soft corals are flexible marine species that deform under a flow of water. Some records of the bipinnate sea plume (A. bipinnata) reveal a curious motion: while the stem sways back and forth at low-frequency with a wave surge, the branches suddenly vibrate at high frequency, with small amplitude, and transverse to the water flow. We explain the origin of these vibrations, and find their impact on soft corals. Finite-element implementation of the wake-oscillator model for an elastic slender rod favours vortex-induced vibrations as the most probable cause of the observed fast branch motion. Since soft corals are passive filter feeders that catch particles brought by currents, we hypothesise that these vibrations may affect their feeding rate. Using a monolithic fluid-structure interaction finite-element solver and Python code, we integrated the trajectories of spherical particles around a circular cylinder and calculated the capture rate. We found that vibrating cylinders capture up to 40% more particles than fixed cylinders at frequency synchronisation. Therefore, vortex-induced vibrations plausibly enhance the food capture and offer soft corals a better nutrition.

Effect of External Flows on Sperm Flagellar Dynamics

Manish Kumar (9:30 – 9:45)

The swimming sperm of many external fertilizing marine organisms face complex fluid flows during their search for egg cells. Aided by chemotaxis, relatively weak flows and marine turbulence enhance sperm-egg fertilization rates through hydrodynamic guidance and mixing. However, strong flows can mechanically inhibit flagellar motility through elastohydrodynamic interactions - a phenomenon that remains poorly understood. We explore the effects of flow on the buckling dynamics of sperm flagella in an extensional flow through detailed numerical simulations, which are informed by microfluidic experiments and high-speed imaging. Compressional fluid forces lead to rich buckling dynamics of the sperm flagellum beyond a critical dimensionless sperm number, Sp, which represents the ratio of viscous force to elastic force. For non-motile sperm, the maximum buckling curvature and the number of buckling locations, or buckling mode, increase with increasing sperm number. In contrast, motile sperm exhibit an intrinsic flagellar curvature due to the propagation of bending waves along the flagellum. In compressional flow, this preexisting curvature acts as a precursor for buckling, which enhances local curvature without creating new buckling modes and leads to asymmetric beating. However, in extensional flow, flagellar beating remains symmetric with a smaller head yawing amplitude due to tensile forces. We also explore sperm motility in different shear flows. In the presence of Poiseuille flow, the sperm moves downstream or upstream depending on the flow strength along with net movement toward the centerline.

Morphological Control of Receptor-mediated Endocytosis

Daniele Agostinelli (9:45 – 10:00)

Receptor-mediated endocytosis is one of the most common mechanisms by which cells internalize particles. This process is driven by adhesion forces between the external particle and the cell membrane, due to specific interactions such as ligand-receptor bindings, or non-specific ones such as electrostatic, van der Waals, and hydrophobic forces. These adhesive forces provide the energy that is necessary to overcome the energetic cost of wrapping the particle. Previous studies revealed that spherical nanoparticles can be endocytosed only within a specific range of radii, which is determined by the balance between the adhesion energy and the membrane deformation energy. Numerical studies showed that the fundamental biophysics of spherical nanoparticles holds also for other simple geometries, which exhibit different entry modes. However, the effect of more complex morphologies remains largely unexplored, despite its importance for the development of new strategies in the context of biomedical diagnostics and therapeutics. In this study, we investigate the endocytosis of a spherical nanoparticle equipped with protrusions, and we find the region in the space of the relevant parameters where the internalization process is energetically favorable. We discuss the implications of these results in suggesting a new strategy for the design of viral antibodies, and nanoparticles for targeted diagnosis and drug delivery - via a geometrical control of endocytosis.

Simulating Epithelial-Mesenchymal Transition in Cell Sheets

Naba Mukhtar (10:00 – 10:15)

Epithelial-mesenchymal transition (EMT), a process in which immotile cells that line surfaces in the body become motile mesenchymal cells, play a crucial role in major processes such as wound healing, embryo development, and cancer growth; therefore, examining the dynamics behind individual and collective cell migration would allow for a better understanding of these processes. It has been previously observed that the protein YAP is activated by external mechanical stimuli and affects the expression and activation of the proteins E-cadherin and Rac1, which are involved in intercellular adhesion and migratory ability respectively. It has also been demonstrated that the mechanical stimulation of expanding cell sheets leads to the formation of finger-like projections and EMT, as well as quantitative differences in properties between cells near the sheet edge and cells away from it. Such cell sheets can be simulated using Morpheus, an agent-based modelling and simulation environment. In this talk, I will propose an ODE model for YAP/Rac1/E-cadherin dynamics and demonstrate that the resulting Morpheus simulation gives results consistent with several observations seen in vitro.

Session 4: Rheology
12:30 – 13:30, June 29 (PDT)

12:30 – 12:45	Chike Okwara	The Mechanical Properties of Neurospheres
12:45 – 13:00	Minghuan Xu	Effect of Extensional Rheology on Enhancing the Retention of Agricultural Sprays
13:00 – 13:15	Yun-Han Huang	Effects of Aging on the Shelf Life and Viscoelasticity of Polymer-based Microcapsules
13:15 – 13:30	Bharath Antarvedi Goda	Mechanics of Soft Material Cutting

The Mechanical Properties of Neurospheres
Chike Okwara (12:30 – 12:45)

Stem-cell-derived tissues are excellent models for investigating mechanisms of tissue formation and responses to physiological and mechanical cues. Neuronal spheroids, also known as neurospheres, have attracted particular interest for studying brain diseases. A lot is now known about the differentiation and maturation of neurospheres, as well as their responses to biochemical cues. However, understanding of their mechanical properties pales in comparison, especially considering recent insights about how mechanical stimuli trigger the onset of neurodegenerative conditions. In the current study, we have taken formative steps to fill this knowledge gap. Our study is the first to investigate the mechanical properties of living neurospheres under uni-axial compression. We observed that neurospheres exhibit viscoelastic behaviour at low strains and plastic deformation at larger strains. However, the results also demonstrate the need for further method development in order to properly account for biological variability and sample heterogeneity.

Effect of Extensional Rheology on Enhancing the Retention of Agricultural Sprays

Minghuan Xu (12:45 – 13:00)

The use of agrochemicals such as pesticides and fertilizers has contributed much to improving the output and quality of agricultural crops. However, agrochemicals are commonly delivered by spray nozzle systems, and in the process, substantial amount of the agrochemicals may be lost to the surrounding environment. This leads to overuse of agrochemicals to achieve target levels in plants and in turn leads to environmental pollution and economic losses.Our study focuses on the retention of spray droplets after they reach the target surface, which can be limited by droplets splashing, rebounding, or rolling off the surface, Here, a novel approach is presented for quantifying the retention efficiency. This approach enables testing of the influence of polymer additives for enhancing retention efficiency of both real and model agricultural sprays. The results demonstrate that increasing the extensional rheology of the spray solution can increase the retention efficiency on both synthetic surfaces as well as plant surfaces.

Effects of Aging on the Shelf Life and Viscoelasticity of Polymer-based Microcapsules

Yun-Han Huang (13:00 – 13:15)

Microcapsules have a wide range of applications in industries such as targeted drug delivery and encapsulation of functional food ingredients. While many studies have focused on characterization of their mechanical properties, very few studies monitored the change of mechanical properties as they age. Such changes are of critical importance to product performance. In this work, we examine the effect of aging on polymer-based microcapsules with liquid cores. Our findings suggested that the structure, color, stability, and even the density of individual microcapsules change over the aging process. Furthermore, the stiffness of the microcapsules increased significantly and they became more viscoelastic over time. A cantilevered-capillary force apparatus is used to make precise measurements of these properties.

Mechanics of Soft Material Cutting

Bharath Antarvedi Goda (13:15 – 13:30)

Cutting is a ubiquitous process with a wide range of implications. We have a very good theoretical understanding of fracture and cutting mechanics of ductile and brittle materials but very little attention has been paid to understand the mechanics of failure and cutting of soft materials. Understanding them is crucial and will benefit several sectors ranging from biotech to food processing. Traditionally, in the soft mechanics cutting literature, the focus has been on food processing and wire cutting of bulk soft materials and cannot be generalized to other processes. Oftentimes, the soft materials are thin, and there is a need to account for the trade-off between cutting force and stability or buckling resistance of the film being cut. It has been found from the experiments that this phenomenon is well understood by leaf cutter ants that have evolved with the capability to cut leaves with minimal effort. My work focuses on learning the mechanics of cutting from nature and develop a mathematical theory that can be applied to solve challenges faced in thin-film cutting and failure.

POSTER SESSION

14:00 – 15:00, June 29 (PDT)

Row 1, Column 1	David Holloway	Controlling the Number of Cotyledons in Conifer Embryos
Row 1, Column 2	Hadi Zadeh-Haghighi	Radical Pairs may Explain Xenon-induced Anesthesia and Lithium Effects on Hyperactivity
Row 2, Column 1	Lauren Walgren	Synergy between Antimicrobial Peptides Derived from Aurein 2.2 and IDR- 1018 and Commonly used Antibiotics
Row 2, Column 2	Albert Kong	Enhanced Packing and in Micropillar Arrays through the Introduction of Tilt
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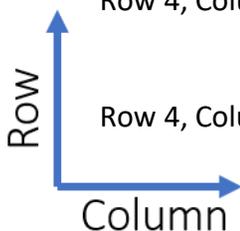
Column

Controlling the Number of Cotyledons in Conifer Embryos

David, Holloway (Row 1, Column 1)

Conifers, unlike flowering plants, generate variable numbers of cotyledons (embryonic 'seed leaves'). Conifer cotyledons do not form all over the dome-shaped embryo, but form in a single ring at a particular distance from the tip. A 3-fold increase in this ring radius from 55 to 180 μm corresponds to the experimentally observed range of 2 to 10 regularly-spaced cotyledons. In the flowering plant Arabidopsis, leaves are also initiated at a particular distance from the growing tip. Molecularly, this is at a 'trough' between two expression domains, of REV (an HD-ZIP III protein) above the leaves and KAN below the leaves. REV and KAN are mutually inhibitory via miRNAs (tasiARF from REV, miR166 from KAN). This is at least partly shared by conifers: overexpression of miR166 in larch decreases HD-ZIP III expression and affects cotyledon formation. We have developed a model for HD-ZIP III (H), KAN (K) regulation to investigate how their interface position is controlled - in particular, what allows for the 3-fold natural variability in conifer cotyledon ring radius. Simulating Arabidopsis H/K experimental perturbations contributes to a general mechanism for radial positioning, as well as quantitatively predicting radial shifts in new conifer experiments.

Radical Pairs may Explain Xenon-induced Anesthesia and Lithium Effects on Hyperactivity

Hadi Zadeh-Haghighi (Row 1, Column 2)

The human brain is a magnificent system with highly complex functionalities such as learning, memory, emotion, and subjective experience. Over the past decades, it has been proposed that that quantum physics could help answer unsolved questions in life science. Here we present a quantum model that could shed light on the mechanisms behind xenon-induced anesthesia and the lithium effects on hyperactivity. It has been shown that the process of xenon-induced general anesthesia involves electron transfer, and the potency of xenon as a general anesthetic exhibits isotopic dependence. It has also been observed that lithium's effects are isotope-dependent. Based on these findings, here we propose that xenon and lithium exert their effects by influencing the recombination dynamics of a naturally occurring radical pair involving oxygen. We develop a simple model inspired by the radical-pair mechanism in cryptochrome in the context of avian magnetoreception. Our model reproduces the observed isotopic dependence in the xenon anesthesia and the lithium treatment of hyperactivity. It predicts a magnetic-field dependence of the effectiveness of lithium on hyperactivity and the potency of xenon anesthetic, which provides one potential experimental test of our hypothesis. Our findings show that Nature might harness quantum entanglement for the brain's cognitive processes.

Synergy between Antimicrobial Peptides Derived from Aurein 2.2 and IDR- 1018 and Commonly used Antibiotics

Lauren Walgren (Row 2, Column 1)

Antibiotic resistance has become a large public health problem due to the frequent and unrestricted use of antibiotics. Thus, there is an urgent need to find novel antibacterial therapeutics or a combination of antibacterial agents to treat antibiotic-resistant bacteria. This study investigated the synergy between two antimicrobial peptides (AMPs) and broad-spectrum antibiotics used against a number of ESKAPE pathogens, namely P. aeruginosa, S. aureus, A. baumannii and E. faecium. One of the AMPs, denoted peptide 73, was derived from the natural host defense peptide aurein 2.2 [1,2]. The other AMP (IDR-3002) was derived through in silico quantitative structure-activity relationship (QSAR) models [3]. The minimum inhibitory concentration (MIC) of each AMP was evaluated against each of the 4 strains listed above. Based on the MIC found for each AMP, a checkerboard assay was performed to investigate the synergy between the peptides and antibiotics, as expressed by the fractional inhibitory concentration (FIC). Neither peptide showed synergistic effects with antibiotics when tested against the Gram-positive bacteria (S. aureus and E. faecium). However, each AMP combined with polymyxin B showed synergistic activity against antibiotic sensitive strains of P. aeruginosa and A. baumannii. The results will be presented in light of using AMP/antibiotic combinations to combat antibiotic resistance.

Enhanced Packing and in Micropillar Arrays through the Introduction of Tilt

Albert Kong (Row 2, Column 2)

Micropillar arrays see use in many fields including bioinspired adhesives, carbon nanotube devices, experimental biochemistry, and microfluidics. In these fields, it may be desirable to either pack the micropillars as densely as possible or produce them to be as long as possible. A barrier to either metric is the phenomenon of condensation: where adjacent micropillars adhere to each other due to lateral Van der Waals forces. We show that by introducing tilt, the condensation of micropillars is stunted and arrays with denser packing or longer pillars are possible. For bioinspired adhesives, we show that a 30% improvement in packing efficiency is possible by simply introducing tilt.

General Model for the Mechanical Characterization of Hydrogels

Sridaran Rajagopal (Row 2, Column 3)

Hydrogels have found their application in the field of Chemistry, Biology, and Mechanics. They have been used to make Adaptive optics for ocular devices, Stretchable Ionics to make artificial skins, and make actuators in Microfluidics devices. An interesting application of Hydrogels is in the field of Tissue Engineering and mechanobiology. Hydrogels are used to impregnate cells to provide them stimulatory microenvironments that allow the cells to grow and proliferate. It is known from the literature that the mechanical properties of the microenvironments play a large role in the growth of cells. However, the mechanical properties of hydrogels are poorly understood. In this study, we will be focusing on understanding the coupled diffusion and deformation characteristics of these hydrogels. We will also propose a novel model to describe the mechanical behavior of these hydrogels. We will also understand the influence of the swelling ratio on the mechanical properties of the hydrogel as a function of deformation and time. Our model allows us to generalize the behavior of gels that soften as the equilibrium swelling ratio increases and gels that are observed to stiffen with increasing equilibrium swelling ratio.

Quantitative Interpretation of Cell Rolling Velocity Distribution

Adam Yasunaga (Row 2, Column 4)

Leukocyte rolling adhesion, facilitated by selectin-mediated interactions, is a highly dynamic process in which cells roll along the endothelial surface of blood vessel walls to reach the site of infection. The most common approach to investigate cell-substrate adhesion is to analyze the cell rolling velocity in response to shear stress changes. It is assumed that changes in rolling velocity indicate changes in adhesion strength. In general, cell rolling velocity is studied at the population level as an average velocity corresponding to given shear stress. However, no statistical investigation has been performed on the instantaneous velocity distribution. In this study, we first developed a method to remove systematic noise and revealed the true velocity distribution to exhibit a log-normal profile. We then demonstrated that the log-normal distribution describes the instantaneous velocity at both the population and single-cell levels across the physiological flow rates. The log-normal parameters capture the cell motion more accurately than the mean and median velocities, which are prone to systematic error. Lastly, we connected the velocity distribution to the molecular adhesion force distribution and showed that the slip-bond regime of the catch-slip behavior of the P-selectin/PSGL-1 interaction is responsible for the variation of cell velocity.

Eliciting the Effects of Phenotypic Heterogeneity on Cellular Growth and Antibiotic Response Using High-throughput Single-cell Assays

Shahla Nemati (Row 3, Column 1)

During the past decade, single-cell methods have greatly improved our understanding of cellular noise. This form of noise pertains primarily to gene expression, and can lead to the emergence of significant heterogeneity among isogenic cells under identical growth conditions. Cellular noise also pertains to antibiotic survival, where cells persist antibiotics without acquiring mutations. To probe these effects, single-cell investigations are required to uncover the cell-to-cell differences in growth or stress-response. To this end, we developed a polymer microarray for tracking single-cells over multiple generations and accurately extract optical-phase, and, thus cellular density information. We will present our findings on these assays, as well as the biophysical insight they enabled in the context of density homeostasis during growth and antibiotics response using E.coli as a model system.

Characterizing Structural Variants in RAD51B

Hossam Zaki (Row 3, Column 2)

DNA Double Strand Breaks (DSBs) are fairly common. Fortunately, there are several DNA damage repair pathways to fix these breaks and maintain genomic integrity. However, alteration of these pathways can cause genomic instability, leading to apoptosis or malignant phenotypes. It was found that in the International Cancer Genome Consortium, structural variants (SVs) were more prevalent in RAD51B than other genes involved in DSB repair. Furthermore, tumors with any mutation in RAD51B had a higher SV burden than tumors without RAD51B mutations. RAD51B has not been well characterized so we set out to assess its role in genomic instability using the PCAWG dataset. In this project, we characterized the variants of RAD51B as well as SV burden and other features of genomic instability within each tumor. Using these features we built a machine learning model to determine which variants of RAD51B are associated with features of genomic instability. Further studies will assess the role of the RAD51B variants we found to be associated with genomic instability in DSB repair. Further understanding of these variants could lead to biomarkers of tumors likely to respond to agents targeting DNA damage repair.

Non-equilibrium Structural Dynamics of Supercoiled DNA Plasmids
Cameron Hastie (Row 3, Column 3)

Many cellular processes occur out of equilibrium. This includes the site-specific unwinding of supercoiled DNA, which may play an important role in gene regulation. Here, we use convex lens-induced confinement (CLiC) microscopy to study plasmid unwinding using a fluorescent oligo probe complimentary to the unwinding site. We studied two model plasmid systems, pFLIP-FUSE and pUC19, and investigated the dynamics of DNA unwinding after a temperature perturbation. We used Monte Carlo Markov Chain (MCMC) methods to estimate the transition rates of the oligo-plasmid system. We found that structural transitions can be slow, and plasmids approaching the experimental temperature from a higher temperature had a slower transition rate than plasmids approaching from a lower temperature. Our findings highlight the importance of non-equilibrium effects when characterizing the complex structural dynamics of DNA and the mechanisms of gene regulation.

Non-equilibrium Structural Dynamics of Supercoiled DNA Plasmids
Albert Kamanzi (Row 3, Column 4)

Nanoparticles are a promising solution for delivery of a wide range of medicines and vaccines. Optimizing their design depends on being able to resolve, understand, and predict biophysical and therapeutic properties, as a function of design parameters. While existing tools have made great progress, gaps in understanding remain because of the inability to make detailed measurements of multiple correlated properties. Typically, an average measurement is made across a heterogeneous population, obscuring potentially important information. In this work, we develop and apply a new method for characterizing nanoparticles with single-particle resolution. We use CLiC (Convex Lens-induced Confinement) microscopy to isolate and quantify the diffusive trajectories and fluorescent intensities of individual nanoparticles trapped in micro-wells for long times. First, we benchmark detailed measurements of fluorescent polystyrene nanoparticles against prior data, to validate our approach. Second, we apply our method to investigate the size and loading properties of lipid nanoparticle (LNP) vehicles containing silencing RNA (siRNA), as a function of lipid formulation, solution pH, and drug-loading. By taking a comprehensive look at the correlation between the intensity and size measurements, we gain new insights into LNP structure and how the siRNA is distributed in the LNP. Beyond introducing a new analytic for size and loading, this work opens the door to new studies of dynamics with single-particle resolution, such as LNP fusion and drug-release kinetics. The prime contribution of this work is to better understand the connections between microscopic and macroscopic properties of drug-delivery vehicles, enabling and accelerating their discovery and development.

Growth and Remodelling of Cell Tissue Undergoing Epithelial to Mesenchymal Transition

Matteo Ferraresso (Row 4, Column 1)

Epithelial to Mesenchymal Transition (EMT) is a fundamental biological process involved in embryonic development, wound healing, cancer and fibrosis. In EMT, polarized epithelial cells lose their cell-cell adhesion and assume a mesenchymal phenotype allowing for migration and drastically altering mechanical properties of tissues, often reducing functionality. The biochemical pathways that trigger EMT have been studied and are well understood, but recent studies have shown that the mechanics of the microenvironment also play a crucial role in EMT. Specifically tensile stress have been shown to enhance EMT and thus increase local growth and proliferation. Experiments inducing EMT on disk shaped stem cell cultures produce a geometry-specific vertical growth pattern. Initially the disk shaped cell culture homogeneously grows and expands, but boundary conditions and constraints create uneven stress and strain energy distributions across the continuum. It is hypothesized that the uneven differential growth in the tissue is triggered by the non-uniform stress and strain energy distributions, leading to locations of higher EMT expression, thus greater material expansion. We developed a MATLAB and ABAQUS model to implement growth remodelling based on mechanical stress micro-states applied to the disk cell culture geometry. The simulated vertical growth pattern matches that of experiments, therefore this model can potentially be used to predict growth patterns form the geometers. This model will serve to detect and predict severity of a multitude of conditions pathologies.

Multiscale Contributions to Skeletal Muscle Mechanics

Ryan Konno (Row 4, Column 2)

Skeletal muscle is a complex biological material, and has many individual components that contribute to its overall behaviour. At the microscopic level, inside the fibres of the muscle, there are sarcomeres which activate to contract the muscle and produce force. Meanwhile, these fibres are wrapped in a stiff matrix of collagen fibres, which provide a substantial amount of passive structural stiffness. However, understanding the way these microscopic components contribute to the macroscopic deformation is unclear. Experimentally, this is a difficult problem to investigate, and so we have developed a mathematical model that can capture the influence of individual components, such as the sarcomeres and extracellular matrix, on muscle mechanics. This work is critical not only in understanding the underlying mechanics of muscle, but in investigating the effects of muscular diseases, which significantly alter the microstructural components of muscle. This model can then be used to direct future clinical and experimental research.

Ecological Theory for "Medicine for the Microbiome"

Eric Jones (Row 4, Column 3)

Over the last two decades an association between microbiome composition and some human diseases has been unambiguously established. In my research I employ novel theoretical approaches to study simplified instances of the complex microbial dynamics of the microbiome, motivated by a desire to inform the mechanism of action and development of microbiome based bacteriotherapies. I use generalized Lotka-Volterra models as a testbed to develop ecological theory that analytically and numerically explores the efficacy of direct (e.g. fecal microbiota transplantation) and indirect (e.g. changes in diet) bacteriotherapies. In recent work, I augment these prior findings by introducing noise that represents the immigration of bacteria into and within the gut (additive noise) and variations in growth rate associated with the spatially inhomogeneous distribution of resources

(multiplicative noise). We use concepts from transition path theory to investigate how the role of noise affects these bacteriotherapies, and probe the relationship between the deterministic and stochastic systems by comparing isocommittor surfaces of the stochastic system to the separatrix of the deterministic system.

CAREER HOUR TALKS

(15 min ea. ~10 min presentation, ~5 min setup and Q/A)

14:15 – 15:15, June 28 (PDT)

14:15 – 14:30	UBC Mathematics Department
14:30 – 14:45	Institute of Applied Mathematics UBC
14:45 – 15:00	Pacific Institute for the Mathematical Sciences
15:00 – 15:15	SFU Science Faculty

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The Institute of Applied Mathematics promotes interdisciplinary research in the mathematical sciences at UBC by bringing together students and faculty who do mathematical work within a variety of disciplines. The Institute's faculty and student members come from many different departments and faculties across the university, including the physical, chemical, biological, and engineering sciences. Students affiliated with the IAM pursue interdisciplinary masters and doctoral studies in applied and computational mathematics.

The Pacific Institute for the Mathematical Sciences (PIMS) was created in 1996 by the community of mathematical scientists in Alberta and British Columbia, and subsequently extended to Washington State, Saskatchewan and Manitoba. Our mandate is to promote research in and applications of the mathematical sciences, to facilitate the training of highly qualified personnel, to enrich public awareness of and education in the mathematical sciences, and to create mathematical partnerships with similar organizations in other countries (with a particular focus on the Pacific Rim). PIMS funds Collaborative Research Groups, Post-Doctoral Fellowships and individual events on a competitive basis.

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