Topological Analysis of Amplicon Structure in Breast Cancer Subtypes

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DNA copy number aberrations (CNAs) play an important role in cancer and can be experimentally detected using aCGH techniques. Amplicons, CNAs that extend over large sections of the genome, are difficult to study since they may contain multiple independent and dependent copy number changes. Here, we propose an algorithm to find the CNAs structure within a given amplicon. Our method relies on the observation that co-occurring CNAs can be encoded as 1-dimensional cycles. We found regions of co-amplifications in Luminal B, ERBB2/HER2/NEU amplified and Basal patients

Bridging protein rigidity theory and normal modes using kino-geometric analysis

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For over twenty years, pebble-game rigidity analysis and elastic network models (ENM) have provided tremendous coarse-grained insight into the dynamics of molecular mechanisms and function. However, the topological pebble game strongly depends on a network of non-covalent constraints, limiting its applicability and comparability to ENM. Here, we present an alternative, geometric approach which eliminates these drawbacks. Our analysis of the underlying rigidity matrix, the constraint Jacobian J, brings together topological rigidity and ENM, providing a basis for the full spectrum of collective motions. It allows to directly compare and contrast motion modes obtained from both traditional approaches.
Non-covalent constraints, like hydrogen bonds, encode a hierarchy of protein motions, ranked by increasing singular values. This hierarchy predicts energetic perturbations associated with each mode. The spectrum of singular values yields a fold-specific footprint, differentiating stiffer alpha-helical from beta-sheet proteins. Collectivity, encoded by the Shannon entropy, is significantly lower for motions obtained by topological rigidity versus ENM, and generally higher for beta over alpha folds. However, kino-geometric sampling with motion planning approximates conformational transitions closer than competing normal mode based methods. Overall, these results indicate that hydrogen bond networks have evolved with different protein folds to tailor structural dynamics and thus, fold-related function.

*poster presenter

Balanced rate and spiking model for oculomotor integrator

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The oculomotor neurons integrate a transient saccade into a persistent activity. Since the persistent activity is proportional to the intended position of the eyes in their orbit, integrator neurons are said to maintain a "memory of eye position". Mathematically, persistent activity is described in terms of "dynamical attractor" which means any self-sustained and stable state of a dynamical system. The question is that whether such attractor networks can be realized in the brain, biologically constrained models of persistent activity were needed? In this project, we focus on the network of the oculomotor integrator, and we will provide the necessary constraints on the synaptic strengths and on the time constants of the synapses in order for the network to have the persistent activity. Furthermore, the persistent activity is believed to be generated by feedback dynamics in the network. The oculomotor integrator has both positive feedback and negative feedback. In this project, we will introduce the negative-derivative form feedback which occurs when the network has same synaptic strength but offset in time. It will be shown that the negative-derivative feedback counteracts drift in persistent activity, and the negative-derivative feedback networks are robust to common perturbations such as the change or synaptic strength and loss of neurons. We will represent two models: a rate model and a spiking model. Both resulting derivative-feedback oculomotor models are robust to many commonly studied perturbations. In the rate model, we will show the firing rates remain more stable in the negative-derivative feedback models than those are in the positive feedback network against the change of the synaptic strength. In the spiking models, we will approximate the horizontal eye positions using the firing rates. We will show that even though some neurons are silent in the network, the rest neurons will compensate to spike in order to track the eye positions. However, there is a boundary for the optimal compensation for the loss of neurons. When too many neurons are silent, the balance between excitation and inhibition is disrupted, and the eye position representation is lost.

*poster presenter

Maximizing atrial fibrillation-selectivity of IKur inhibitors: in silico optimization of drug binding kinetics and state-dependence

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The atrial predominant (vs. ventricles) ultra-rapid delayed-rectifier K+ current (IKur) has been extensively studied as a promising target to treat atrial fibrillation (AF). However, evidence of antiarrhythmic efficacy of IKur-targeting compounds in human clinical trials is lacking, perhaps because preclinical assessment of candidate drugs relies on steady state drug concentration response curves rather than accounting for channel conformational state specificity and kinetics of drug binding. Here, we simulated a Markov-type model of IKur gating and drug-channel interaction within our comprehensive atrial cell model to reveal the ideal binding properties of IKur inhibitors that maximize AF-selectivity in normal sinus rhythm (nSR) and chronic AF (cAF). Specifically, we identified drugs exhibiting anti-AF properties at fast-pacing rates (prolongation of effective refractory period, ERP), while having little effect during normal heart rhythm (limited prolongation of action potential duration, APD). We also found that despite being downregulated (by 50% in our simulations), IKur contributes more prominently to APD and ERP in cAF than in nSR, and block of IKur in cAF has less cardiotoxic effects and increased efficacy. We propose that our in silico strategy can be implemented to identify the complex impact of IKur inhibitors at the different stages of AF-induced remodeling.

Collision-Free Poisson Motion Planning in Ultra High-Dimensional Molecular Conformation Spaces

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The function of protein, RNA, and DNA is modulated by fast, dynamic exchanges between three-dimensional conformations. Conformational sampling of biomolecules with exact and nullspace inverse kinematics, using rotatable bonds as revolute joints and non-covalent interactions as holonomic constraints, can accurately characterize these native ensembles. However, sampling biomolecules remains challenging owing to their ultra-high dimensional configuration spaces, and the requirement to avoid (self-) collisions, which results in low acceptance rates. Here, we present two novel mechanisms to overcome these limitations. First, we introduce temporary constraints between near-colliding links. The resulting constraint varieties instantaneously redirect the search for collision-free conformations, and couple motions between distant parts of the linkage. Second, we adapt a randomized Poisson-disk motion planner, which prevents local oversampling and widens the search, to ultra-high dimensions. Tests on several model systems show that the sampling acceptance rate can increase from 16% to 70%, and that the conformational coverage in loop modeling measured as average closeness to existing loop conformations doubled. Correlated protein motions identified with our algorithm agree with those from MD simulations.

*poster presenter

Spatiotemporal model of anaphylatoxic clouds explains key features of complement-mediated chemotaxis by human neutrophils

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When locating pathogens in tissue, human neutrophils must navigate a variety of competing chemical gradients. One such gradient is formed when complement proteins from human serum bind to a pathogen and release highly potent chemoattractants known as anaphylatoxins, forming a localized anaphylatoxic cloud. In this work, we formulate a diffusion-reaction problem describing the evolution of a generic chemoattractant concentration gradient around a source particle and derive a closed-form solution. We then apply this model to characterize the formation of an anaphylatoxic cloud under realistic physiological conditions, finding that the cloud forms rapidly (i.e. ~1-6 s), and that its steady-state concentration profile drops off sharply around the particle. Furthermore, the size of the source particle correlates positively with both the chemoattractant concentration and the spatial reach of the cloud. These theoretical predictions are confirmed by our single-cell measurements of the distances over which human neutrophils sense pathogens of different sizes. This integrative experimental/theoretical approach allows us to establish the minimum relative anaphylatoxin concentration that triggers a neutrophil chemotactic response. Our findings show that complement-mediated chemotaxis facilitates a final course correction of neutrophils migrating toward pathogens.

Bounds for the Minimum Step Number for Two-Component Links in the Simple Cubic Lattice

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Topological structures in the form of knots and links are found throughout nature and are commonly studied in the context of protein and DNA structure. A key question in the interpretation of biological results and in the design of polymers in nanotechnology is to determine the smallest number of monomers, the minimum step number, necessary to build a specific knot or link. Previous work has reported on bounds for the minimum step number for knots up to ten crossings in the simple cubic lattice and in confined regions of the lattice (i.e. slabs and tubes). Our work numerically estimates the minimum step number necessary to build two component links up to nine crossings in unconfined regions of the simple cubic lattice. We further extend the Monte-Carlo algorithm BFACF, used to sample conformations with a fixed knot type, to sample conformations with a fixed link type. In addition, we extend an algorithm that determines whether two minimal step number conformations of links are equivalent under rigid motion, enabling the classification of all minimal step number conformations into equivalence classes.

*poster presenter

Deep profiling of mouse splenic architecture with CODEX multiplexed imaging

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A cytometric imaging approach, called CO-Detection by indEXing (CODEX), that enables high parameter multiplexing of antibody-tagged target epitopes is used here to create high parameter imaging datasets of normal mouse and lupus (MRL/lpr) spleens. In this procedure, antibody binding events are rendered iteratively using DNA barcodes, fluorescent dNTP analogs, and an in-situ polymerization-based indexing procedure. Fluorescent signals from multiple rounds of indexing are computationally combined into a multi-channel image stack and subjected to image segmentation and quantification. A segmentation and linear model algorithm was developed to accurately quantify membrane antigen levels on dissociated cells as well as tissue sections. Leveraging the spatially resolved nature of CODEX multiplexed single-cell imaging data, quantitative de novo characterization of lymphoid tissue architecture was enabled and overlaid onto previously described morphological features. We observed an unexpected, profound impact of the cellular neighborhood on the expression of protein receptors on immune cells. By comparing normal murine spleen to spleens from animals with systemic autoimmune disease (MRL/lpr), extensive and previously uncharacterized splenic cell interaction dynamics in the healthy versus diseased state was observed. The fidelity of multiplexed imaging data analysis demonstrated here will allow deep proteomic analysis and systematic characterization of complex tissue architecture in normal and clinically aberrant samples.

Meta-analysis of Cytometry Data Reveals Racial Differences in Immune Cells

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While meta-analysis has demonstrated increased statistical power and more robust estimations in studies, the application of this commonly accepted methodology to cytometry data has been challenging. Different cytometry studies often involve diverse sets of markers. Moreover, the detected values of the same marker are inconsistent between studies due to different experimental designs and cytometer configurations. As a result, the cell subsets identified by existing auto-gating methods cannot be directly compared across studies. We developed MetaCyto for automated meta-analysis of both flow and mass cytometry (CyTOF) data. By combining clustering methods with a silhouette scanning method, MetaCyto is able to identify common cell subsets across studies, thus enabling meta-analysis. Applying MetaCyto on a set of 10 heterogeneous cytometry studies with a total of 5966 samples allowed us to identify multiple cell populations exhibiting differences in phenotype and abundance across races. Software is released to the public through GitHub

*poster presenter

Characterizing Synergy in Biology: Simulating Radiation Damage During Interplanetary Voyages as an Example

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In biology, synergy is important but no systematic mathematical quantification general enough to cover most cases of interest has been available. It is often taken for granted that comparing “effects” (e.g. mouse tumor prevalences) due to a mixture of “agents” (e.g. a mixture of alpha-particle and beta-particle radiations) to adding the effects of all mixture components can characterize synergy and antagonism. However, pharmacologists and toxicologists have long known that this simple effect additivity characterization is wrong if components’ individual dose-effect relations are highly curvilinear. Various replacements for simple effect additivity are currently utilized.

We here describe “incremental effect additivity”. It characterizes no-synergy/antagonism mixture dose-effect derivatives as linear superpositions of component dose-effect derivatives, using mappings from mixture effects to component doses in the calculation.

As examples we: (a) reanalyze published results on murine tumors and chromosome aberrations induced by high energy radiations which simulate components of the interplanetary radiation mixture; and (b) calculate corresponding baseline no-synergy/antagonism incremental effect additivity dose-effect relations for planned mixture experiments.

Incremental effect additivity is applicable even when mixture components have highly curvilinear dose-effect relations. It has fewer limitations than other replacements for simple effect additivity, but shares drawbacks common to almost all known synergy quantifications.

*poster presenter

Computational modeling of biological systems with peridynamics

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Computational modeling can be used to better understand how processes that are well defined on the cellular and sub-cellular scales manifest on the tissue scale. In particular, computational modeling can be used to predict the population scale mechanical behavior of tumors from cellular scale behavior. Though much work has been done in this field, many open questions remain. Here we show how the dual-horizon peridynamic framework can be adapted to model biological systems, particularly tumors, and discuss why peridynamics is well equipped to handle many of the challenges associated with mechanical modeling of biological systems. Then, we discuss recent applications of this agent-based modeling technique, where we investigate the influence of cellular scale division angle during cell proliferation on macroscale tissue growth and the influence of cellular scale cell death mechanisms on macroscale tissue shrinkage.

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[2] Lejeune, E., & Linder, C. (2017). Quantifying the relationship between cell division angle and morphogenesis through computational modeling. Journal of Theoretical Biology, 418, 1-7.

Developmental Shape Transition in Cowrie Seashells

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Cowries are a family of sea snail -- prevalent off the coast of Africa, in the Indian Ocean, and in the Pacific -- that undergoes a transition from laying shell down in a typical seashell spiral to spiraling inward and thickening the shell en route to maturity. This developmental path involves the formation of teeth-like ridges on the underside of the shell. Here we present modeling work that builds on the physics of wrinkling elastic sheets and mathematical approaches to the form and development of seashells to provide an avenue towards understanding the process underlying this transition. We also present experimental data on the link between geometry of the shell and material coupling of soft-body mantle growth and shell deposition. Our calculations, based on elasticity theory and geometry, link a behavioral change in the lifecycle of the mollusc to this under-studied shape transition. Coupling mechanics to shell repair mechanisms and development provides a physical understanding of the emergent structure of Cowrie shells.

*poster presenter

Thermodynamics and Statistical Mechanics of Viral Evolution: Non-Equilibrium Behavior

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We study a model of viral evolution, in which viruses have a barrier to cell entry, mediated by their match to cell “key”, followed by a viral-type dependent immune response by the cell, and finally a probability to reproduce and mutate. These mutated viruses then go on to attack other cells in the model. Previously we found equilibrium behavior, featuring a phase transition as a function of temperature and immunity [PLOS One 2015 https://doi.org/10.1371/journal.pone.0137482]. Here we describe our studies of the behavior of this model as a dynamical system, and the nonequilibrium evolution of the quasispecies distribution including metastable states and other unexpected features.

Methylomic and transcriptomic perturbations associated with autism at birth in umbilical cord blood samples from the prospective MARBLES study

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Autism spectrum disorders (ASD) have complex etiologies, likely involving multiple genetic and environmental insults in perinatal life. Biomarkers for ASD at birth would facilitate earlier diagnosis and treatment. The MARBLES prospective study is an enriched risk cohort that enrolls couples who have already had a child with ASD and follows their subsequent pregnancy. To identify DNA methylation biomarkers predictive of ASD diagnosis, we investigated human umbilical cord blood samples from the MARBLES study by whole-genome bisulfite sequencing (WGBS) and expression microarray. ASD subjects had lower global percent CpG methylation compared to typically-developing (TD) controls ($p=0.01$). 2619 differentially-methylated regions (DMRs) were also identified. Methylation in DMRs was associated with behavioral outcomes and could distinguish ASD from TD subjects. DMR methylation was associated with gene expression at 1411 genes, as measured by expression microarray. DMR-associated genes were enriched in cell signaling by ubiquitination, immune response, and nucleosome regulatory functions (FDR < 0.01). Global hypomethylation in ASD cord blood suggests a methylation deficiency during perinatal life. Identified DMRs and differentially expressed genes are relevant to ASD and have potential as a diagnostic tool. These results are expected to improve understanding of ASD etiology and aid in future preventative and therapeutic treatments

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*poster presenter

Data-driven evaluation of drug-inducible larval zebrafish behaviors

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Behavioral screens are increasingly used in neuroactive compound discovery. A method called behavioral barcoding detects responses to physical stimuli in larval zebrafish. Multiple behaviors are quantified rapidly—about 200 compounds in 2,000 larvae per hour—but which behaviors are informative for neuropharmacology is unknown. We have developed a system with extremely high throughput and flexibility. By collecting and analyzing a large dataset of well-characterized neuroactive drugs and their behavioral effects, different stimuli and computational features can be evaluated. In addition, these reference compounds form behavioral anchors: Compounds that induce similar behaviors are likely to share pathways. This massively expands a guilt-by-association paradigm to discover novel neuroactive compounds and understand neurochemical pathways.

A Systems Biology Approach to Understanding Cell Fate Heterogeneity in Streptomyces Coelicolor

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Actinomycetes are filamentous soil bacteria with a multitude of significant biological properties. In particular, the model actinomycete Streptomyces coelicolor is a rich source of secondary metabolites such as medically relevant antibiotics. In addition, they undergo a multicellular developmental life cycle; they begin as spores, germinate into filamentous vegetative hyphae, and eventually raise aerial hyphae that differentiate into spores to begin the cycle again. Early genetic studies have linked secondary metabolism production to the onset of development. However, how these networks are integrated remains poorly understood at a systems level. My project aims to determine if a simplified genetic model is sufficient to explain how cells make the choice to either become aerial hyphae or produce secondary metabolites. To this end, I intend to develop a computational method to accurately predict parameter values that drive these networks. This knowledge can be used to analyze spatiotemporal expression data and make accurate predictions of expression profiles that result from genetic manipulation.

*poster presenter

Developing a human ventricle-torso model for investigating ventricular activity and electrocardiograms

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A human ventricle-torso model is a valuable tool in understanding impaired cardiac electrical activity and its manifestations on the electrocardiograms (ECGs). In this study, a 3D human ventricle-torso model was developed and used to assess the effects of acute ventricular ischaemia and bundle branch block on ECGs. The 3D anatomical ventricular model was stimulated using an improved endocardium stimulation profile. The simulated ventricular electrophysiological data were then incorporated into an anatomical model of the human torso with heterogeneous conductivities. Using the ventricle-torso model, the body surface potential was calculated, from which 12-lead ECGs were extracted. The simulated ECGs under the normal conditions were compared with experimental data. Single cell models of acute ventricular ischaemia were developed and incorporated into the ventricle-torso model. Various locations of the ventricular ischaemic zones were considered. In simulating the bundle branch blocks, both left and right bundle branch blocks were modelled. The computed ECGs were in good agreement with documented clinical observations under these conditions. In conclusion, the developed ventricle-torso model is a useful platform linking the ventricular electrophysiology and ECGs under normal and diseased conditions. The model may be applied to assess the efficacy and safety of antiarrhythmic drugs in future.

The Effects of Confinement on Transition Probabilities for Lower Crossing Topologies through Local Reconnection Moves

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Understanding the 3D organization of the human genome is an important challenge for structural biologists. Chromosome conformation capture (3C) based techniques have allowed experimental inquiry into the 3D organization of eukaryotic genomes, but these techniques are unable to discern fine-scale topological complexity within the nucleus. Additionally, since Eukaryotic chromosomes are long polymer chains confined within the nucleus, and it has been established that such chains in confinement are likely to be knotted. There are questions regarding the possibility of similar topological complexity in the genome. Through the study of local reconnection processes, which can result from aberrant repair of double-stranded breaks by recombination, we seek to understand how varying degrees of confinement can affect changes in the topology of DNA. Through the use of computer simulations, we investigated how local reconnection moves cause overall changes in the topology of polygonal chains and as a function of chain length and confinement. Our research shows that lower crossing topologies, such as the 3-crossing, 5-crossing, and 7-crossing knots, exhibit similar trends of transition probabilities for various degrees of volume occupancy. Furthermore, the probability of attaining a higher crossing topology from lower crossing topologies by a local reconnection move increases as volume occupancy increases.

*poster presenter

Pattern based classification approach for labeling medical records

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A Liquid-Crystal Model of Kinetoplast DNA

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Quantification of the entanglement complexity of the yeast genome reveals a bias towards simplicity

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Spatial confinement promotes the topological entanglement of DNA. While there have been a variety of proposed approaches to inferring 3D genome architecture from CCC data, assessing the reproducibility of solutions so obtained has received little attention. This problem was first raised by Segal and colleagues and addressed by defining four different statistical metrics, all of geometrical nature, which were later used to perform statistical inference. In this work, we investigate the problem of topological complexity and that of reproducibility in budding yeast by analyzing CCC data obtained by Duan et. Al. Our results show that the current approach of accessing reproducibility performs better that previous known methods. We also show that the topology entanglement of the yeast genome, inferred from 3D reconstructions of CCC data, is simpler that what we expected from randomly semi-flexible chains in confinement. We conclude that the ralb like configuration is sufficient to explain the entanglement simplicity of the yeast genome.

*poster presenter

Modeling pathways of DNA unlinking by site-specific recombination

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In *Escherichia Coli*, replication of circular chromosomes yields topologically linked DNA molecules. Topo IV, one of the type-II topoisomerases in E. coli, plays a major role in the decatenation of the newly replicated chromosomes. It has been shown that in the absence of Topo IV, site-specific recombinases XerC/D, in cooperation with the translocase FtsK, can also unlink the replication links [1,2]. The goal of this research is to explore the possible pathways of unlinking by XerCD-FtsK. We use computational methods to exhibit the recombination pathways and assign transition probabilities to each recombination step. Our results give strong support to the stepwise unlinking pathway proposed in [1,2].

Software Tool Development for Library-size Determination Using Quantitative Image Analysis

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Next-generation DNA Sequencing (NGS) workflows are complex, multistep procedures combining PCR and enzymatic reactions to prepare DNA fragments of specific concentration, purity, and length in ways that are compatible with a specific sequencing platform. The quality of the NGS library has the greatest influence on the success of a sequencing run, affecting both sequence validity and the number of reads. Many current quality-control (QC) protocols require expensive instruments and reagents to assess library length, specifically capillary gel electrophoresis tools such as Agilent's Bioanalyzer and TapeStation products. With the exponential growth of genome-wide analyses and large data sets that hinge on NGS, it is crucial to improve optimization, accuracy, and cost-effectiveness of each workflow step. Here we present a software package that assesses the size distribution of DNA fragments generated by Illumina®'s Nextera Tn5 transposition-based tagging/fragmentation protocol. The Nextera kit produces sequencing libraries through enzymatic shearing of input DNA, the products of which are distributed as continuous patterns in agarose-gel electrophoresis. Our image analysis tool is designed to efficiently analyze both banded and continuous gel-electrophoresis profiles with the goal of extracting information about purity, concentration, and average fragment size of fragmented DNA products. The method requires only modest imaging capabilities, and is a cost-effective and rigorous alternative characterization tool to augment existing methods for library QC.

*poster presenter