IP1
Perceptual Dynamics in an Ambiguous World

When experiencing an ambiguous sensory stimulus (e.g., the vase-faces image), subjects may report haphazard alternations (time scale, seconds) between the possible interpretations. I will describe dynamical models for neuronal populations that compete through mutual inhibition for dominance - showing alternations, behaving as noisy oscillators or as multistable systems subject to noise-driven switching. In highly idealized formulations networks are percept specific without direct representation of stimulus features. Our recent work involves perception of ambiguous auditory stimuli (e.g., http://auditoryneuroscience.com/topics/streaming-galloping-rhythm-paradigm); the models incorporate feature specificity, tonotopy, so that perceptual selectivity is emergent rather than built-in.

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IP2
Invited Plenary Speaker - Title Tbd - Swanson

TBD

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IP3
Modelling Plant Cell and Tissue Growth

Plant growth typically occurs through the coordinated anisotropic expansion of plant cells. Growth is regulated by hormones and is driven by high intracellular pressures generated by osmosis. This machinery allows a plant primary root, for example, to penetrate soil in a direction guided by gravity, while seeking out nutrients and avoiding obstacles. I will describe the biomechanical aspects of a multiscale model for root gravitropism recently developed with colleagues at the Centre for Plant Integrative Biology at the University of Nottingham, UK. This incorporates descriptions of cell walls as fibre-reinforced viscoelastic polymer networks and adopts upscaling approaches to efficiently describe the growth of multicellular tissues.

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IP4
Invited Speaker - Title Tbd - Lander

TBD

Arthur Lander
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IP5
Invited Plenary Speaker - Title Tbd - Galvani

TBD

Alison Galvani
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IP6
Is Good Cholesterol Always Good? New Insights about HDL from an In-Silico Model of Lipoprotein Metabolism and Kinetics

Individuals with higher endogenous plasma levels of high-density lipoprotein-cholesterol (HDL-C), the so called good cholesterol, have a lower risk of developing cardiovascular disease (CVD) an effect that is generally attributed to the role of HDL particles in the reverse cholesterol transport process. Nevertheless recent efforts to increase HDL-C levels pharmacologically have failed to lower CVD risk in patients. To understand this apparent paradox, we developed a novel in-silico model of lipoprotein metabolism and kinetics [1]. Our model highlights the geometrical aspects of HDL structure and dynamics, and suggests why certain HDL-C raising therapies have not been successful to date. 1.Lu J, Hbner K, Nanjee MN, Brinton EA, Mazer NA. An in-silico model of lipoprotein metabolism and kinetics for the evaluation of targets and biomarkers in the reverse cholesterol transport pathway. PLoS Comput Biol. 2014 Mar 13;10(3):e1003509. doi: 10.1371/journal.pcbi.1003509. eCollection 2014 Mar.

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IP7
Early Warning Signs and Critical Transitions in Ecology: Corals, Theory, Pitfalls, and Advances

I will start by describing specific ecological systems that have multiple stable states, lakes and coral algal grazer systems giving models of the latter. I will then discuss approaches for predicting sudden shifts in the face of slow parameter change. The approach will depend on developing a simple stochastic model and using this model to describe the data. A key element in describing the results will be the use of receiver-operator curves. This part of the talk will include both possibilities and pitfalls. I will then discuss how the use of data can both help and be misleading in judging the efficacy of warning signals.

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IP8
Synthetic Biology and Biocomputation: Life Redesigned

Synthetic biology is bringing together engineers, computational scientists and biologists to design and construct biological circuits out of proteins, genes and other bits of DNA, and to use these circuits to rewire and reprogram organisms. These re-engineered organisms are going to change our lives in the coming years, leading to cheaper drugs, "green" means to fuel our car and clean our environment, and targeted therapies to attack "superbugs" and diseases such as cancer. In this talk, we highlight recent efforts to create synthetic gene networks and programmable cells, and discuss a variety of synthetic biology applications

in biocomputing, biotechnology and biomedicine.

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CP1

A Mathematical Model of Intermittent Androgen Suppression Therapy for Treatment of Advanced Prostate Cancer

Advanced prostate cancer is often treated with androgen deprivation therapy (ADT) which facilitates the death of androgen-dependent (AD) cancer cells. Androgen-independent (AI) cancer cells may increase with continuous ADT so that intermittent androgen suppression (IAS) therapy is utilized to delay the onset of AI cells. We model the dynamics of IAS therapy with a system of ordinary differential equations and determine the optimal times to collect data relative to model parameters in order to develop better treatment protocols.

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CP1

Can Mathematical Models Predict the Outcomes of Prostate Cancer Patients Undergoing Intermittent Androgen Suppression Therapy?

Prostate cancer is often treated by intermittent androgen deprivation therapy since prostate cells depend on androgens for proliferation and survival. We extend an existing prostate cancer model and test the model's predictive accuracy when only a subset of the data is used to find parameter values. The results are compared with those of an existing linear model. We also develop a second method for testing the accuracy in predicting the duration of off-treatment periods.

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CP1

Variance Reduced Model for Tumor Growth

One of the major challenges when using individual-based models for tumor growth is to reduce the computational cost. We consider an individual-based model for tumor growth, which is continuous in space and time and coupled with a set of reaction diffusion equations to model the environment. We propose a novel variance reduction scheme to reduce the computational cost, based on a control variate that is obtained from a kinetic description.

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CP1

On the Accumulation of Mutations in Cancer

In this work we consider the problem of modeling the stochastic accumulation of somatic mutations in cancer. The integration of mathematical modeling and statistical analysis with sequencing and clinical data represents a new powerful approach for better understanding the evolutionary dynamics of cancer, and for implementing quantitative approaches to cancer classification and treatment. By considering, for the first time, all relevant phases of a tissues history - the model makes unexpected predictions, validated by the analysis of sequencing data: what is the number of somatic mutations that occur prior to the onset of neoplasia? How many rate-limiting mutations are needed for cancer to occur? The talk is partially based on: Tomasetti C, Vogelstein B, Parmigiani G. Half or more of the somatic mutations in cancers of self-renewing tissues originate prior to tumor initiation. Proc Natl Acad Sci USA 2013, 110(6):1999-2004.

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CP2

A Simple Model Incorporating Demographic and Epidemiological Processes in a Spatially Heterogeneous

In this talk, we explore an epidemic model incorporating demographic processes in a spatially heterogeneous environment in which the individuals are subject to a random movement. Our analytical and numerical results reveal that the persistence of the population and disease outbreak be ignited by both individuals mobility and environmental heterogeneity.

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CP2

An SIRS Epidemic Model with Non-Exponential Probability for Temparary Immunity

We consider an SIRS model for disease dynamics that accounts for temporary immunity whereby recovered individuals return to the susceptible class. We allow for a general

probability function of remaining immune such that the model is a system of integro-differential equations (IDE). We show how the IDEs can be approximated by a system of delay-differential equations. We then show that different probabilities, whose parameters have been chosen such that they have equal moments, generate equivalent dynamical output. For the case of a linear function we can derive bifurcation equations that determine how the moments affect the intensity and duration of epidemics.

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CP3

Comparison of a Deterministic and Stochastic Model for the Transmission Dynamics of Influenza

We consider an extension of the SEIR model for the transmission dynamics of influenza. We describe two stages of the infection, an early and a late stage, in the later stage the infected may or may not take medicine, in addition a fraction from both these groups may be hospitalized. We perform rigorous analysis of the system. It is shown that for the basic reproductive number R_0 the disease free equilibrium is stable and the system has an endemic equilibrium for R_0. We next consider an analogous Continuous Time Markov Chain (CTMC) based model. Numerical simulations are used to estimate the mean, variance and probability distributions for the various states and are compared to the steady state solutions of the deterministic model. The expected time to extinction in the CTMC model is also estimated.

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CP3

A Mixed-Strategy Game Theoretical Approach for Infectious Disease Prevention by Social Distancing

We describe a population game in which individuals are allowed to decide between adopting different social distancing strategies in order to lower infection risk and maximize payoffs. When the reduction in infection risk is a convex function of the cost of social-distancing, there is a unique pure-strategy game equilibrium. When the reduction in infection risk is not convex, the existence of equilibria becomes more complicated. We will discuss three cases vis--vis different costs of infection.

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CP3

Abms for Infectious Diseases Spreading and Ill-Posed Problems

Usually rules and behavior of agents in ABMs are not known exactly. In the general case a problem of ABMs parameters evaluation is so called ill-posed one and therefore it can have no unique solution for available data describing emergent patterns under consideration or can have unique but unstable solution with respect to small changes of these data. In my talk I will illustrate that for a model of influenza epidemic spreading in a city.

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CP3

Analysis of Labour Productivity in the Presence of Substance Abuse

Substance abuse impedes the productivity of employees and reduces economic growth. Efficient management of an organizations workforce must involve eradicating drug use. In this paper, we formulate and analyse a mathematical model for labour productivity in the presence of substance abuse transmission dynamics that includes intervention strategies. We investigate the existence and stability of equilibria and use Pontryagin's Maximum Principle to derive necessary conditions for the optimal control of the disease. Numerical simulations are performed to illustrate the analytical results.

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CP4

Nonlinear Stochastic Dynamics of Sensory Hair Cells

Hair cells are mechano-receptors in vertebrate senses of hearing and balance. In lower vertebrates sensory hair cell exhibits spontaneous oscillations of hair bundle and membrane potential. We use modelling to study how mechanical and electrical oscillations emerge, interact and contribute to the overall sensitivity and selectivity of the hair cell. We show that oscillatory regimes result in enhanced sensitivity to harmonic stimuli. Irregular spontaneous dynamics is best suited for sensing broad-band slowly changing external stimuli.

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CP4

Large Deviations of An Ergodic System of Hebbian Neurons

We investigate finite-size effects in a system of neurons interacting ergodically. Our model consists of N Hodgkin-Huxley neurons, with external noise. The noise is correlated in an ergodic manner, meaning that its probability law is invariant under a uniform translation of the neurons. We asymptote N to infinity and apply the theory of Large Deviations to determine in which direction the system is most likely to deviate from its limit equation.

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CP4

Fast-Slow Analysis of Neural Excitability with Synaptic Noise

By considering a stochastic Morris-Lecar model with the inclusion of synaptic noise, we study neural excitability using a systematic perturbation analysis. In this presentation, I will talk about our understanding and findings of synaptic noise on neural excitability.

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CP5

A Fractional Order Model of Electroporation

Electro-chemotherapy and gene electro-transfer have recently emerged as promising new cancer therapies that use locally applied electric fields to facilitate the transport of either chemotherapeutic drugs or genes into tumor cells using the cell membrane electroporation. The continuous evolving microstructure of tissues and tumors affect the distribution of the applied electric field. To account for such complex and mostly unknown dynamics, we propose a novel fractional order model for the local electric field distribution.

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CP5

Parameter Inference Using Variance Fitting for Markov Models of Voltage Gated Ion Channels

Voltage gated ion channels play a central role in neuronal and electric signaling and are experimentally studied by the voltage clamp technique with single channel or whole cell current recordings. In this talk we address the inverse problem of identifying rate parameters in Markov chain models that describe the transition between the conformational states the channel can sojourn in. Assuming that single channel data from repeated observations is available we utilize model predictions of the current variance and directly compare it with the sample variance derived from the data. Cost functions that account for variance fitting may feature landscapes in the parameter space with more pronounced curvatures than mean based approaches such that parameter unidentifiability or model ambiguity may be weakened or even overcome.

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CP5

Compatibility of Slender Bodies and Surface Traction at Low Reynolds Number

The past forty years have witnessed an ever-increasing interest in applications of slender-body dynamics (such as Kirchhoff rod theory), in particular with regard to the shape, movement, or material parameters of biomolecules or materials. In most applications, hydrodynamic interactions (i.e. surface traction often approximated by resistive force theory) have been of utmost importance since the biologically relevant scales usually result in very small Reynolds number. However, the formulation of classical Kirchhoff slender-body assumes no surface traction in the development of the constitutive relation. We will discuss an asymptotic approach to reconciling this apparent inconsistency and provide velocity bounds for which the compatibility of Kirchhoff rod and resistive force theory hold.

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CP6

Sensitivity Analysis and Treatment of Hepatitis C Virus Infection

The interplay between two types of immune responses, antibodies and CTL cells, is explored in the context of hepatitis C virus (HCV) infection. The competition for HCV is explored with sensitivity analyses, considered under three main steady states: co-existence, dominant CTL response, and dominant antibody response. Sensitivity functions allow temporal ranking of parameters, in relation to their degree of influence in viral load. Comparisons between steady states with and without treatment are discussed.

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CP6

The Effect of Systemic Estrogen and Cortisol on the Inflammatory Phase of Wound Healing

A complex combination of interactions initiates and regulate the inflammatory phase of the wound healing response. Many chronic wounds arise due to an improper transition out of this phase. To understand regulation of this transition, we developed a model for key inflammatory cells during wound healing that accounts for the effects of cortisol and estrogen. Latin Hypercube sampling was performed to determine feasible parameters for the model. Experimental

data was used to validate this model.

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CP6

Modeling Effects of Drugs of Abuse on Hiv-1 Dynamics

Complications of HIV-1 infection with simultaneous drugs of abuse are an emergent problem. I will present a within-host viral dynamics model that incorporates effects of drugs of abuse on HIV-1 infection. Our model agrees well with experimental data from Simian Immunodeficiency Virus infections in morphine-addicted macaques (animal model of HIV). I will discuss how our model helps evaluate morphine-induced alterations in viral dynamics, steady state viral load, and basic reproduction number.

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CP6

The Role of Interleukin-2 in Immune Response Regulation

The immune system has many adaptive and dynamic components that are delicately regulated to ensure appropriate, precise, and rapid response to a pathogen. Inadequate immune response can lead to prolonged disease, while an excessive or under-regulated response can lead to autoimmunity. We are interested in the role cytokines play in maintaining this balance. Through the use of mathematical models, we attempt to understand cytokine signaling including problems leading to autoimmunity and MS treatment by Daclizumab.

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CP7

Simulation-Based Simplification of Non-Linear Feed-Forward Models

Mechanistic modeling of signaling or metabolic pathways is highly valuable for understanding and predicting basic biology, disease, and therapy. However, due to the complexity of biological systems it is necessary to make simplifying assumptions to reduce the degrees of freedom of any model. Here we demonstrate in a simple, yet biologically relevant, case an approach using simulation and data to simplify non-linear feed-forward models. We apply this to a model of hepatic de novo-lipogenesis.

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CP7

Spatial Uniformity of Solutions of Reaction-Diffusion Pde's

Motivated by the question of pattern formation, we study the behavior of the solutions of reaction-diffusion PDE's. Applying some techniques from modern functional analysis, such as logarithmic Lipchitz constants and logarithmic norms, we provide conditions for global convergence to uniform solutions. We then illustrate the result by a simple biomolecular model.

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CP7

Scale-Invariant Sensing of Singularly Perturbed Biomolecular Models

Feedforward motifs such as a simple incoherent feedforward loop have been the subject of extensive research in systems biology, and they are inherent in cellular systems ranging from bacteria to mammalian cells. Additionally, it was observed that multiple time scales are typically inherent in such motifs. Experimentally, it has been shown that certain incoherent feedforward molecular circuits can (approximately) exhibit a scale invariance property, namely, scale invariance of the complete output trajectory with respect to a rescaling of input magnitudes. Even though they may not exhibit the perfect scale invariance property, such circuits can often possess an approximate scale invariance property, and we study conditions under which systems with different time scales can possess the approximate scale invariance property, estimate the accuracy with which this property can be established, and illustrate our theoretical predictions on three examples.

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CP7

On the Perfect Reconstruction of the Topology of

Gene Regulatory Networks

The network inference problem consists in reconstructing the topology or wiring diagram of a dynamic network from data. Solving this problem is specially important for gene regulatory networks, because in many cases regulation mechanisms are unknown or cannot be detected directly. Even though this problem has been studied in the past, there is no algorithm that guarantees perfect reconstruction of the topology of a dynamic network. In this talk we will present a framework and algorithm to solve the network inference problem for discrete networks that, given enough data, is guaranteed to reconstruct the topology of a dynamic network perfectly. The framework uses tools from algebraic geometry.

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CP8

Mutational History Dominates Clonal Selection Within Evolving Tumors

Natural selection acting on clonal diversity within tumors is thought to drive tumor progression, but details remain obscure. Evolutionary mathematical models of the angiogenic switch predict the emergence of hypovascular necrosis caused by hypertumors—"cheating" clones that free-ride on vasculature organized by cooperative clones. Here we show that hypertumors should rarely evolve because the deterministic evolutionary trajectory is overwhelmed by stochastic mutational history. These results highlight mutation pressure as a significant evolutionary force in cancer.

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CP8

Stationary Stability for Evolutionary Dynamics in Finite Populations

We extend the theory of evolutionary stability to multidimensional finite populations with mutation, connecting the theory of the stationary distribution of the Moran process with the Lyapunov theory of evolutionary stability for the replicator dynamic. We show essentially that the local extrema of the stationary distribution minimize the relative entropy of the current population state and the "expected next state" computed by weighting the adjacent states by the appropriate transition probabilities. This holds for a variety of selection processes including the increasingly popular Fermi selection. We present several complete computational examples for illustration and we show that the classical stability theory of the replicator dynamic is recovered in the large population limit. If time allows, we describe extensions to populations evolving on graphs.

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CP8

Linear Algebra of the Quasispecies Model

Eigen's quasispecies model is a famous 'almost linear' system of ODEs, for analysis of which intricate methods of classical and quantum mechanics, statistical physics, and elaborate numerical algorithms were applied. In a nutshell, the analysis boils down to studying the leading eigenvalue and the corresponding eigenvector of the matrix describing mutation–selection process. Our approach to this problem is to use the methods of linear algebra. Using the fact that the mutation matrix has a special form, a change of the basis is suggested such that in new coordinates a number of exact results can be obtained.

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CP8

Species coexistence under eco-evolutionary dynamics

Ecological mechanisms for coexistence of interacting species have been studied extensively. In light of recent evidence that feedbacks between ecological and evolutionary processes are more common and substantial than originally thought, we examine how these feedbacks mediate coexistence in a three-species interaction. We model these processes using a Lotka-Volterra and quantitative genetics framework and use singular perturbation theory to analyze coexistence for this model.

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CP9

Pest Persistence and Eradication in a Deterministic Model for Sterile Insect Release

The release of sterile insects is an environment friendly pest control method used in integrated pest management programs. New deterministic population models that include sterile male release are derived and explored numerically.

The differential equations account separately the effects of mating failure due to sterile release and the frequency of mating encounters. When insects spatial spread is incorporated through diffusion terms, computations reveal the possibility of steady pest persistence in finite size patches.

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CP9

Quantifying the Relationships among Natural Selection, Mutation, and Stochastic Drift in Multidimensional Finite Populations

The interrelationships of the fundamental biological processes natural selection, mutation, and stochastic drift are quantified by the entropy rate of Moran processes with mutation, measuring the long-run variation of a Markov process. The entropy rate is shown to behave intuitively with respect to evolutionary parameters such as monotonicity with respect to mutation probability (for the neutral landscape), relative fitness, and strength of selection.

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CP9

The Information Player: a Novel Strategy That Dominates Zero Determinant and Other Known Strategies in Multiplayer Evolutionary Games

We present a long-history strategy capable of quickly inferring opponent strategies and building coalitions in population games using statistical inference and machine learning techniques. These "information players" very effectively invade existing strategies including tit-for-tat, win-stay-lose-shift, and zero determinant strategies, and conversely block invasion by these strategies, even in the presence of substantial ambient noise (errors in play). Crucially, information players initially seek not to maximize their *score*, but rather their *information* about the opponent's strategy.

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CP9

Quantifying the Impact of the Recent Invasive Species, Pomacea insularam

Pomacea insularam, or applesnail, is a relatively new species to the Gulf Coast region and threatens local sugar and rice crops, due to their relatively low predation rates at high sizes and seemingly fast population growth, resulting in significant vegetation consumption. In collaboration with the National Wetlands Research Center, we present the estimation of vital rates in a size-structured mathematical model from a population observed in a laboratory setting. We compare these results and estimates of population sizes and growth dynamics with the calibrated model to preliminary field data, highlighting necessary modifications necessary to adapt the model to this natural setting, such as the incorporation of predation. We discuss the possible impact of this species and potential for its control.

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CP10

Bursting in Networks of Integrate and Fire Neurons

We use mean field analysis to study bursting in networks of identical, pulse-coupled neurons. The individual neurons are represented using a class of two-dimensional integrate and fire model. The mean field model is a system of switching ordinary differential equations and the transition to bursting involves both standard and nonsmooth bifurcations. The results of the mean field analysis are compared with numerical simulations of large networks.

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CP10

Robust Design of Polyrhythmic Neural Circuits

Neural circuit motifs showing multiple coexistent rhythms are building blocks of neural networks. We study robustness of such circuitry to sustain rhythms by revealing statistics of their switches due to random perturbations. We find a threshold of coupling strength beyond which accidental switching between rhythms occurs frequently. We elucidate mechanisms underlying this stochastic arrhythmia, and show how the type of coupling enhance rhythm robustness. Our findings are applicable to a broad class of oscillator systems.

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CP10

Characterization of Transient and Spatially Distributed High-Frequency Oscillations in the Brain with Quasi-Periodic Time Scales

Spatially distributed neural oscillations with characteristic frequencies $\geq$80 Hz have recently been identified in non-invasive electroencephalograms. These high-frequency oscillations (HFO) are transient and are thought to be modulated by abnormal and dynamic neurophysiological processses. In continuous multi-day recordings, it is possible to estimate HFO dynamics and their corresponding time scales. In this study we show that transient HFO dynamics have quasi-periodic time scales, with periods of occurrence that are modulated by relatively rare electrophysiological events.

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CP10

Relating Spiking Neural Network to Partial Differential Equations

In this talk we show that a spiking neural network without the constraint of symmetry can be approximated by the FitzHugh-Nagumo equations. The well-known FitzHugh-Nagumo equations are much easier to analyze than an enormous system of differential equations, describing the activity of each spiking neuron.

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CP11

Fractional Model for Neurovascular Coupling

Functional magnetic resonance imaging (fMRI) is an indirect measure of brain activity. To describe the chain from neural activity to the measured fMRI signal namely the Blood Oxygen Level Dependent (BOLD) signal, we propose to use a system of fractional differential equation inspired from the dynamical Balloon Model [K. J. Friston et al, 2000. Nonlinear responses in fMRI: the Balloon model, Volterra kernels, and other hemodynamics. NeuroImage 12, 466 477]. We show that thanks to its non-locality and memory properties, fractional derivatives constitute a powerful tool for the neurovascular coupling.

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CP11

Glucose and Temperature Compensation in the Neurospora Circadian Clock: Mathematical Modeling and Experimental Validation

Circadian rhythms play a vital role in an organisms functions anticipating daily changes in its environment. The period of circadian oscillator is relatively insensitive to changes in physiological temperature and nutrients (e.g. glucose), which are referred to as temperature and glucose compensation, respectively. In this study, we constructed a mathematical model of the Neurospora circadian clock, and investigated molecular mechanisms of glucose and temperature compensation. Our model shows that temperature compensation is achieved by an intricate balance of synthesis and degradation of FRQ and WC-1. We experimentally validated loss of glucose compensation in wc-1 overexpression mutant and maintenance of nuclear abundance of FRQ as predicted in the model.

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CP11

Molecular Mechanisms That Regulate the Coupled Period of the Mammalian Circadian Clock

In the mammalian circadian clock, intercellular coupling synchronizes rhythms with the period close to the population mean of individual periods. With the theory of weekly coupled oscillators, we found that the coupled period stays near the population mean if transcriptional repression oc-

curs with piecewise-linear protein sequestration, but not highly non-linear Hill-type regulation in individual cells. This shows that the behavior of coupled oscillator with the same topology changes depending on the mechanisms underlying individual oscillator.

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CP11

In Vivo Volume and Hemoglobin Dynamics in Red Blood Cells

Human red blood cells (RBCs) lose ∼30% of their volume and ∼20% of their protein during their ∼100-day lifespan in the bloodstream. We use measurements of RBC size and protein concentration to derive a model for the physical processes controlling RBC volume and hemoglobin. We show that common models of vesicle shedding alone are sufficient to explain surface area lost but insufficient to explain the lost volume and hemoglobin mass. We use single-cell measurements of human RBCs to validate the models and to define requirements for alternative explanations.

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CP12

Unravelling the Impact of Obstacles in Diffusion and Kinetics of An Enzyme Catalysed Reaction

We develop a two-dimensional lattice-based Monte Carlo simulation to model enzyme-catalyzed reactions in diffusion-limited conditions to investigate effects of obstacle density and size on reactant diffusion and rate coefficients. Our results show that these factors affect first- and second-order rates. We also find that particle rotations and weak force interactions affect rate coefficients. Our simulations suggest that the anomalous kinetic observed in cellular crowded environments can appear in less restricted conditions than previously reported.

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CP12

Mathematical Modeling of the Hypothalamic-Pituitary-Adrenal Axis in Relation to Major Depression

Both circadian and ultradian oscillations are seen in the levels of the hormones of the Hypothalamic-Pituitary-Adrenal axis, including cortisol. With a model consisting of non-linear ordinary differential equations, we investigate enzyme reactions taking place inside the cortisol-producing adrenal cortex cell to see, whether the presence of potential Goldbeter-Koshland switches is instrumental in generating the ultradian oscillations. The performances in model reduction of the standard quasi-steady-state approximation (sQSSA) and the total QSSA are compared.

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CP12

Modeling the Spatio-Temporal Dynamics of Small Gtpase Activity at Dendritic Spines

Signaling through small GTPases at dendritic spines is crucial for synaptic plasticity, a cellular correlate for learning and memory. We implement a computational method in order to model the spatio-temporal dynamics of GTPase activity accounting explicitly for the spine geometry. A question that motivates our research is how does the activity of the GTPase Cdc42 localize persistently to spine membranes despite its rapid lateral diffusion.

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CP12

In Vitro Assay Geometry Affects Estimates of the Cell Diffusivity and Cell Proliferation Rate

Cells respond to biochemical and physical cues during wound-healing and tumour progression. *In vitro* assays used to study these processes are typically conducted in one geometry. In this work, we investigate the capacity of cell populations to spread in two different *in vitro* assay geometries by comparing estimates of the effective cell diffusivity and effective cell proliferation rate.

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CP13

A Continuous Model of Ant Foraging with Pheromones and Trail Formation

We propose and numerically analyze a PDE model of ant foraging behavior. Ant foraging is among the most interesting behaviors in the animal kingdom, and a prime example of individuals following simple behavioral rules based on local information producing complex, organized and "intelligent' strategies at the population level. One of its main aspects is the widespread use of pheromones, which are chemical compounds laid by the ants used to attract other ants to a food source. We consider a continuous description of a population of ants and simulate numerically the foraging behavior using a system of PDEs of chemotaxis type. We show that, numerically, this system accurately reproduces observed foraging behavior, such as trail formation, optimization of routes, and efficient removal of food sources. Furthermore, we present a preliminary mathematical analysis of a simplified version of the model.

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CP13

Using Homogenization to Estimate Random-Walk Motility from Gps Collar Data in Variable Landscapes

We compute the probability of an animal passing through various habitat patches between known GPS collar locations using solutions of a homogenized ecological diffusion model. From these probabilities we can obtain the time an animal spends in a particular habitat type to use in estimating motility coefficients. We apply this method to parameterize a model of the spread of chronic wasting disease in mule deer in Utah.

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CP13

Respect Versus Disrespect for Ownership: An Iterated Hawk-Dove Game with Relocation Costs

The classic Hawk-Dove game predicts that when "Bourgeois" respect for ownership arises as a pure convention, so does "anti-Bourgeois" disrespect. Why is the former so common in nature, the latter so rare? An iterated model can yield stable strategy mixtures with any degree of partial respect between 0 and 1. This poster describes how their basins of attraction depend on both the relocation costs of "infinite regress" and the probability of further interaction.

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CP13

The Dynamics of Foraging Activity in Harvester Ants

Collective foraging is ubiquitous in social animals. Its utility is largely dependent on the efficient use of social information to communicate changes in environmental profitability and coordinate the actions of individual group members. Here, we develop a simple compartmental model of foraging activity in harvester ant colonies based on non-spatial, interaction-mediated worker recruitment. Our analysis indicate that adaptive changes in worker availability relative to the frequency of contacts with successful foragers can allow colonies to sustain activity when worker activation rates are low. Simulated forager removals exploring the effects of short-term reductions in forager return rates (e.g. due to elevated predation on the trail) show good fits with empirical data. We discuss the biological interpretation of our results and motivate further improvements to the model.

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CP14

Analyzing the Effects of a Non-Host Worm Population on the Spread of Whirling Disease in Trout

We present a mathematical model of the Host/Parasite system describing the Myxobolus Cerebralis parasite and the Tubifex worms that cause Whirling Disease in trout. A Non-Host worm is incorporated which competes with the Host producing a negative effect but also eliminates the parasite spores causing a positive, indirect effect. System dynamics, parameters and bifurcation analysis will be discussed.

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CP14

The Virus of My Virus Is My Friend: Modeling the Ecological Effect of Virophages

Virophages are viruses that rely on the replication machinery of other viruses for reproduction. We construct two mean field models of population dynamics between hosts, viruses and virophage to address how different modes of coinfection affect the ecological dynamics. We prove that virophage reduce the viral population and increase the host population at equilibrium. We also identify differences in the frequency and nature of coexistence within the two models.

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MS1

A Structured Model for the Transmission Dynamics of Mycobacterium Marinum Between Aquatic Animals

Abstract: Mycobacterium marinum (Mm), a genetically similar bacterium to Mycobacterium tuberculosis, affects a number of fish industries (fisheries, aquaculture, aquariums and research stocks) on a comparable scale to tuberculosis (TB) in humans. Because of this, and the practical advantages of working with animal models as opposed to humans, Mm infections in recently established fish models provide a unique opportunity for the study of mycobacterial infections. We derive a model of transmission dynamics of Mm in fish, which either involves consumption of an infected host or a source of bacteria to ensure activation into a highly infectious state. We derive a model of transmission within a food web, in which infected fish behavior is structured by infection severity. This is a key component as chronic (seemingly asymptomatic) infection is prominent in both fish and human TB. We develop a finite difference method to compute solutions of this model. We illustrate, via this numerical scheme, that this model can be used to reproduce experimental settings.

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MS1

Mathematics of Anti-Hpv Vaccines

Human papilloma virus (HPV) is a major sexually-transmitted disease that inflicts a significant public health burden globally. HPV causes various cancers and warts in females and males, notably cervical cancer in females (the second highest malignancy in women globally, accounting for over 250,000 deaths annually). The talk is based on the use of mathematical models to gain insight into the population-level impact of the two currently-available anti-HPV vaccines (Cervarix (by GlaxoSmithKline) and Gardasil (by Merck Inc.)).

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MS1

Transient Periodic Oscillations and the Dynamics of CTL Response to Viral Infections

Abstract not available at time of publication.

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MS1

Modeling Avian Influenza and Implications for Control

A mathematical model of avian influenza which involves human influenza is introduced to better understand the complex epidemiology of avian influenza. The model is used to rank the efficacy of the current control measures used to prevent the emergence of a pandemic strain. We find that culling without re-population and vaccination are the two most efficient control measures. Control measures applied to humans, such as wearing protective gear, are not very efficient. Furthermore, we find that should a pandemic strain emerge, it will invade, possibly displacing the human influenza virus in circulation at that time. Moreover, higher prevalence levels of human influenza will obstruct the invasion capabilities of the pandemic H5N1 strain. This effect is not very pronounced, as 1% increase in human influenza prevalence will decrease the invasion capabilities of the pandemic strain with 0.006%.

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MS2

Parameter Identifiability in Virus Infection Models

Confidence in the accuracy of estimated parameters is essential for the development of successful treatment protocols. Guidance when designing the experiment is needed for recovery of accurate parameters and identifiability. Noise associated with data collection affects that design. Here, we establish a computational method that investigates the effect of noise on the design of the experiment and the identifiability of parameters. Our method is applied to a model of hepatitis B infection.

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MS2

Early HIV Infection Predictions: Role of Viral Replication Errors

Less than 0.1% of circulating virus in any HIV+ individual is infectious. Non-infectious virus may arise from errors in viral replication or other processes; the specific mechanism does not affect deterministic modeling predictions. However, during the earliest stages of infection, viral loads are small and more appropriately modeled stochastically. We model viral dynamics using continuous-time branching processes to investigate how viral replication error assumptions change predictions on risk of infection and time to infection clearance/detection.

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MS2

Coping with Model Uncertainty in the Analysis of Acute Hiv Infection Datasets

HIV datasets are sparse. For example, sampling occurs infrequently relative to the pace of the infection, sampled viral sequences are few in number or lack linkage informa-

tion, and data for the immune response is sparse relative to the complexity of the immune system. I will describe an approach for dealing with this uncertainty in the context of estimating CTL escape rates. CTLs are immune system cells that kill HIV infected cells depending on the viral genotype, thereby mediating selective pressure from which HIV escapes through mutation. Quantifying the rate of this escape is valuable in understanding the role of CTL response in HIV infection.

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MS2

Multi-Scale Modeling of Immune Response to Influenza Infection

Many systems in engineering and physics such as a rocket system can be represented by differential equations, which can be derived from well-established physics laws and theories. It is unclear whether the biological systems follow a mathematical representation such as differential equations. Fortunately, recent advances in cutting-edge biomedical technologies allow us to generate intensive high-throughput data to gain insights into biological systems. It is badly needed to develop mathematical models and statistical methods to test whether a biological system follows a mathematical representation based on experimental data. In this talk, I will present our recent work in developing statistical methods to identify high-dimensional ordinary differential equation (HD-ODE) models and solve the associated inverse problems for HD-ODE models in modeling immune responses to influenza infection. The time course high-throughput data from both mice and human experiments will be used to illustrate our methodologies.

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MS3

Mechanical Forces Drive Morphogenesis: How the Embryonic Brain Twists

The embryonic chick brain undergoes progressive, rightward torsion, one of the earliest organ-level symmetry-breaking events. Researchers speculated that heart looping affects the brain torsion direction, but direct evidence rarely exists. Our experiments show that the vitelline membrane exerts loads necessary for torsion and that direction of heart looping determines brain torsion direction. A computational model and a physical model are built to interpret these findings, together classifying mechanical origins of brain torsion.

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MS3

Bio-Mechanical Modeling of Tracheal Angioedema by Nonlinear Finite Elasticity

Tracheal angioedema refers to the rapid swelling of tracheal tissue by excess accumulation of fluid from vascular leakage, which can be life threatening if it narrows airway rapidly. We present a bio-mechanical analysis with a swelling dependent natural configuration to reflect the altered tissue volume increment under angioedema. Various localized swelling and far field boundary conditions are studied in order to assess how the interaction between swelling, anisotropy and large deformation affects airway constriction.

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MS3

A Continuum Mechanics Model of Stress Mediated Arterial Growth During Hypertension Using An Eulerian Frame.

In the classical approach to continuum mechanics, one assumes that a material body is deformed from a "stress free" reference configuration into a loaded current configuration. However, a reference configuration is merely a mathematical construct and cannot actually be determined, especially for dynamic physiological processes. We introduce a framework that is formulated entirely in the current configuration and test its effectiveness by showing how well it predicts arterial growth during instantaneous hypertension.

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MS3

Estimating Residual Stresses in Soft Tissues by An Inverse Spectral Technique

A mathematical model is studied to estimate residual stresses in the arterial wall using intravascular ultrasound (IVUS) techniques. A BVP is formulated for the nonlinear, slightly compressible elastic wall, the boundary of which is subjected to a quasi-static blood pressure, and then an idealized model for IVUS is constructed by superimposing small amplitude time harmonic vibrations on large deformations. Using the classical theory of inverse Sturm-Liouville problems and optimization techniques, an inverse spectral algorithm is developed to approximate the residual stresses, given the first few eigenfrequencies of several

induced pressures.

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MS4

Modeling the Melanopsin Phototransduction Cascade

Melanopsin is a recently discovered photopigment found in intrinsically photosensitive retinal ganglion cells (ipRGCs) and is involved in non-image forming vision, such as circadian rhythm entrainment and the pupillary light reflex. We model the activation and inactivation of the melanopsin phototransduction cascade, and compare the model simulations to experimental data. The research was conducted by undergraduates at UMBC and funded by an NSF undergraduate training grant.

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MS4

Collective Cell Migration: Modeling from Initiation to Destination

Collective cell migration is critical in development and pathology. We consider the Drosophila ovary as an experimental system for transition to cell. We use a force balance dynamical system approach to capture cell adhesion, repulsion, chemotaxis, and stochastic motion in the migration. We show that basic forces in 3-dimensions can account for observed apparent rotation of the cluster, as well as reduced migration speed in mutants that reduce the number of migrating cells.

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MS4

Phototransduction in Melanopsin Expressing Retinal Ganglion Cells

Intrinsically photosensitive retinal ganglion cells (ipRGCs) in the mammalian retina express the photopigment melanopsin and constitute a third class of photoreceptors. The ipRGCs contribute primarily to non-image forming vision and the melanopsin-based signaling cascade generates a depolarizing light response. Our goal is to characterize the biochemical pathways that mediate the intrinsic light responses of ipRGCs and mediate its adaptation to light and dopamine.

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MS4

Genetic Regulation of Cell Motility

Morphogens generate distinct cell fates by differences in concentrations. The release, diffusion, uptake, and decay rates of these molecules impact concentration and thereby cellular responses. We propose that the irregular domains of adjacent tissue also alter the local concentration. To examine this, we utilize the well-studied development of the Drosophila ovary. We are characterizing a genetic pathway that promotes cell motility in response to a morphogen and relate pathway activation to tissue architecture.

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MS5

Marine Invertebrate Sperm Chemotaxis: Search Trajectories

In marine invertebrate sperm, chemotaxis guides the sperm towards the egg. The chemoattractant causes changes in intracellular calcium, associated with changes in flagellar waveforms and curvature of path trajectories. We use a fluid-structure interaction model where the calcium concentration is coupled to the forces in the flagellum. Results will be presented to show how trajectories can be modulated by calcium parameters as well as elastic properties of the flagellum.

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MS5

Modeling Tumor and Microenvironment Interactions under Treatment: the Role of the Interstitial Fluid

The interactions between tumor cells and their microenvironment are complex, and this complexity is leveraged when both tumor and stromal cells are exposed to anticancer therapeutic agents. We use fluid-structure interaction methods to systematically explore the role of the interstitial fluid flow and tumor tissue architecture on the extent of drug and biomarker molecule penetration into the tissue.

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MS5

Sperm Altruism and Motility Near Surfaces

As mammalian sperm traverse the oviduct, they undergo significant changes in motility. During this process, sperm are known to bind to the oviductal epithelium and their ability to detach is dependent upon contractions that occur near the time of ovulation. Thus, the impact that surfaces and their motion have upon sperm fertility is significant. Using the method of regularized Stokeslets, we investigate surface interactions and sperm cooperativity to elucidate how epithelial detachment occurs.

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MS5

Swimming Through Highly Heterogeneous, Viscoelastic Media

We present a simple model of a free microswimmer in a highly heterogeneous, viscoelastic medium. An effect of viscoelasticity is modeled by immersing viscoelastic structures into a viscous environment. Varying complexity of those structures allows medium to exhibit different viscoelastic properties. Several tests are performed showing that the model agrees with rheological properties of a medium. Regions of higher structural density can significantly affect a swimming pattern of a microorganism.

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MS6

Novel Characterization of Brain Networks Through Low-Rank Network Decomposition

Small-world networks occur naturally throughout the brain on multiple scales. In this work, we develop a new formalism using a low-rank decomposition of network adjacency matrices to classify neuronal networks. This new procedure scales well with network size and connection density, yielding stable results independent of node indexing. We apply our methodology to recent experimental data on cerebral cortex connectivity, proposing such a network may be categorized into a broader class of networks than small-worlds.

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MS6

Improved Estimation of Neural Correlations Suggests Detailed Interactions in Visual Cortex

How does connectivity impact network dynamics? We address this question by linking network characteristics on two scales. On the global scale we consider the coherence of overall network dynamics. We show that such global coherence in activity can often be predicted from the local structure of the network. To characterize local network structure we use motif cumulants, a measure of the deviation of pathway counts from those expected in a minimal probabilistic network model.

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MS6

Sparsity and Compressed Coding in Sensory Systems

Considering many natural stimuli are sparse, can a sensory system evolve to take advantage of sparsity? We show significant downstream reductions in the numbers of neurons transmitting stimuli in early sensory pathways might be a consequence of sparsity. Our work points to a potential mechanism for transmitting stimuli related to compressed-sensing (CS) data acquisition. Through simulation, we examine the characteristics of networks that optimally encode sparsity and the role of receptive fields in stimulus sampling.

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MS6

Spatiotemporal Dynamics of Neuronal Population Response in the Primary Visual Cortex

We use a large-scale computational model of the primary visual cortex (V1) to study the population responses in V1 as observed in experiments in which monkeys performed visual detection tasks. Our model can well capture spatiotemporal activities measured by voltage-sensitive-dye-based optical imaging in V1. Our computational modeling approach allows us to reveal intrinsic cortical dynamics, separating it from those statistical effects arising from averaging procedures in experiment.

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MS7

Bayesian Support Vector Machines and Supervised Factor Modeling for General Omic Data

A new Bayesian formulation is developed for nonlinear support vector machines (SVMs), based on a Gaussian process and with the SVM hinge loss expressed as a scaled mixture of normals. We then integrate the Bayesian SVM into a factor model, in which feature learning and nonlinear classifier design are performed jointly. Inference is performed with expectation conditional maximization (ECM) and Markov Chain Monte Carlo (MCMC). An extensive set of experiments on multiple types of omics data demonstrate the utility of using a nonlinear Bayesian SVM within supervised feature learning and factor modeling, from the standpoints of prediction accuracy and physiological interpretability.

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MS7

Perfusion Heterogeneity in Tumors As a Challenge for Optimal Nanotherapeutics Delivery

Optimal nanotherapeutics delivery remains elusive because of heterogeneities in vascular perfusion within solid tumors. Using intravital microscopy data previously obtained, we develop a machine-learning framework to determine which perfusion features most affect nanoparticle transport. Further, nanoparticle surface modifications can provide for increased targeting and uptake within tumor tissue. To guide nanoparticle design, we apply computational modeling to simulate tumor perfusion heterogeneity in order to evaluate uptake and distribution as functions of nanoparticle- and tumor-specific characteristics.

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MS7

Dynamics of Living Systems: Wave-Based Mechanisms for Contact Guidance and Collective Migration

Guided cell migration is a key aspect of many physiological processes from the immune response to cancer metastasis. I will describe how simple physical measurements of shape dynamics and motion reveal an underlying wave-like process of the cellular scaffolding that drives persistent migration. We find that wave-like dynamics of the scaffolding also contributes to the ability of cells to recognize and follow surface nanotopography, and allows cells to couple to each other during collective motion.

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MS7

Random Walks, Markov Chains, and Cancer Progression Models from Longitudinal and Autopsy Data

We will describe our models of metastatic cancer progression using Markov chain modeling on a directed graph of nodes that are the various anatomical sites where metastatic tumors can form for a given type of primary cancer. We use metastatic tumor distributions gathered from historical autopsy data, as well as current longitudinal data sets to estimate the transition probabilities from site to site. This creates a systemic network diagram from which we can calculate reduced two-step diagrams using the fact that the systems converge to their steady-state distribution after roughly two steps. The diagrams are used to categorize metastatic sites as 'sponges' or 'spreaders', as well as to run hypothetical therapeutic scenarios based on Monte Carlo simulations of progression. A useful metric which we describe is the notion of metastatic entropy.

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MS8

Modeling and Inverse Problems in Environmental Toxicity

Daphnia magna is a vital species in ongoing investigations into the synergistic toxicity of chemicals. D. magna is a species with a complex life history; females are parthenogenetic and males are only produced in response to environmental stressors. Males can fertilize the females' eggs, transforming them into diapause eggs which are capable of withstanding extreme conditions and hatch when conditions improve. We model D. magna population growth by combining a two-sex age structured partial differential equation model with an ordinary differential equation model to describe their food environment. We then validate this model by performing parameter estimation using structured population data collected from experiments. This work is joint with K. Adoteye (Math), Karissa Cross (Biological Sciences) and a group of toxicologists lead by Gerald LeBlanc.

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MS8

Flocculation Dynamics and Cell Sorting

Flocculation is the process whereby particles in suspension aggregate and fragment and size-structured models are the best framework for modeling and simulation. It arises in many natural, environmental, and medical settings such as wastewater treatment and algal dyanmics. In this talk, we will present recent results in how size-structured models of cell sorting devices can be used to improve sorting efficiency.

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MS8

Estimating the Division Rate for a Growth-fragmentation Equation with Self-similar Kernel

Abstract not available at time of publication.

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MS8

Applied Particle Aggregation for Cell Isolation in the Life Sciences

Among the many applications for particle aggregation, controlled assembly of synthetic beads onto the surface of living cells is of particular industrial, life science, and therefore commercial interest. By fabricating beads with high affinity for cell surface markers, methods for achieving remarkable levels of enrichment from mixed populations are possible. In this presentation, Ill present current and proposed methods for exploiting aggregative physics towards real world applications, and consider where mathematics will play a large role.

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MS9

A Model for the Spatial Transmission of Dengue with Daily Movement between Villages and a City

Dengue is a re-emergent vector-borne disease affecting large portions of the worlds population living in the tropics and subtropics. A discrete-time multi-patch model which takes into account the mobility of people as well as processes of infection, recovery, recruitment, and mortality is considered here. One patch (the city) is connected to all other patches (the villages) in a spoke-like network. Vector control, human treatment and vaccination, and different kinds of mobility are studied.

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MS9

Modeling Hiv Latency and Viral Blips

HIV cannot be eliminated by combination therapy because of latent infection. The latent reservoir consisting of latently infected CD4+ T cells is relatively stable. Many patients also experience transient viral load measurements above the detection limit (the so-called "viral blips") even with suppressive treatment for many years. The mechanisms underlying the emergence of intermittent viral blips and stability of the latent reservoir are not fully understood. In this talk, I will introduce a new model based on the establishment of HIV latency to address this issue. Both deterministic and stochastic simulations of the model show that it is able to generate a stable latent reservoir, intermittent viral blips, as well as low-level viremia persistence. The results provide more insights into the latent reservoir replenishment and long-term HIV dynamics in patients on suppressive combination therapy.

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MS9

Disease Invasion of Community Networks with Environmental Pathogen Movement

Consider a set of communities (patches), connected to one another by a network. When can disease invade this network? Intuitively, this should depend upon both the prop-

erties of the communities, as well as on the network structure. Here we make this dependence explicit for a broad class of disease models with environmental pathogen movement. In particular, the rooted spanning trees of the network and a generalization of the group inverse of the graph Laplacian play fundamental roles in determining the ability of disease to invade.

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MS9

Dynamics of Low and High Pathogenic Avian Influenza in Wild and Domestic Bird Populations

An earlier infection with low pathogenic avian influenza (LPAI) provides a partial immunity towards infection with high pathogenic avian influenza (HPAI). We consider a time-since recovery structured model to study the dynamics of LPAI and HPAI in wild and domestic bird populations. The system has a unique disease-free equilibrium which is locally and globally stable when the reproduction number is less than one. There are unique LPAI-only and HPAI-only equlibria, which are locally asymptotically stable as long as the other pathogen can not invade the equilibrium. There exist a coexistence equilibirum when the invasion number of both pathogens are greater than one. We show that both pathogen can coexist in the form of sustained oscillations.

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MS10

Within-Host Virus Model with Immune Response and Infected Cell Age Structure

There is substantial evidence that the CTL (Cytotoxic T Lymphocyte) immune response plays a crucial role in controlling HIV in infected patients. CTLs recognize pathogen-derived proteins (epitopes) presented on the surface of infected cells to mediate their killing. Recent studies have demonstrated the heterogeneity of epitope presentation and recognition with respect to the infected cell lifecycle, which may impact the efficacy of the immune response. This talk concerns modeling the coupled within-host population dynamics of virus and CTL immune response, paying special attention to the cellular infection-age kinetics of recognition and killing of infected cells by CTLs. In particular, we extend a cellular infection-age structured within-host virus model to include immune response and analyze the resulting dynamics.

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MS10

Modeling Human Papilloma Virus and the Onset of Cervical Cancer

High-risk strains of Human Papillomavirus are the dominant cause of cervical cancers. Incorporating the known biology of viral persistence and the generation of cancerous and pre-cancerous cells, we develop and analyze a model the connection between HPV infection and cervical cancer onset. The model provides a framework for understanding the factors relevant to reducing cancer risk and the role of suppressive drug therapies in long-term treatment.

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MS10

A Basic Model for In-Host TB Infection

Tuberculosis (TB) infection can result in clearance, latent infection or active disease. Mathematical models have been used to provide insight into TB infection and progression. The models to date, however, have been very complex or have not been able to produce all disease outcomes. We present a simple 4-dimensional mathematical model of TB infection in-host. The model includes macrophages, T lymphocytes, TB bacteria and their interactions. The model provides a foundation for future studies on the pathogenesis of drug resistant TB and HIV-TB co-infection.

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MS10

Mechanism Elucidation in Intracellular Signaling Models Via Sensitivity Functions

Many physiological and cellular processes, from G-protein coupled receptor (GPCR) signaling to circadian rhythms, are regulated by oscillatory signals. Although an actively studied area, even the most well-known and commonly studied pathways can have controversy and lack of clarity on circuit architecture. Time-dependent stimulation, using microfluidics technology, has proven valuable in eliciting previously unseen cellular responses, thereby potentially allowing researchers to glean new insights. We discuss the use of sensitivity functions as tools to decipher the underlying mechanisms driving the responses, and to understand the differences in circuitry under constant and time-dependent stimulation patterns. We further discuss the possible information gained from observing other species in the pathway, and offer suggestions to improve future experimental design.

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MS11

Quantification of Iliac Artery Tortuosity and Its Implication for Rotation of Fenestrated Aortic Stent Grafts

Tortuosity is a measure of the deviation of an artery from a straight line, and is an indicator of potential problems during deployment of fenestrated aortic stent grafts, which can have unwanted rotation in severely tortuous arteries. We will present mathematical techniques for tortuosity assessment and iliac artery tortuosity values for typical patients and those for which rotation was an issue, with the goal of establishing criteria to predict when tortuosity will cause graft rotation.

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MS11

A Mechanical and Biochemical Model of Intimal Hyperplastic Lesions

We investigate an axisymmetric model of intimal hyperplasia using hyperelasticity theory. Our model incorporates growth of the intima due to cell proliferation which is driven by the release of cytokines. The growth rate is tied to local stresses and concentration of cytokine. We find that rapid intimal thickening coupled to a quiescent media puts the intima in a state of compression. Our results are compared with intima-media thickness measurements of carotid arteries from clinical studies.

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MS11

Understanding the Role of Cell-substrate Interaction in Cell and Focal Adhesion Shapes

Mechanical interaction between a cell and its underlying substrate have important implications in many contexts, and it has been shown experimentally that that the material properties of the substrate affect cellular response. We present a two-dimensional mathematical model and finite element simulations of a biological cell interacting with a deformable substrate and use this model to gain a better understanding of how the mechanical interaction between the cell and substrate affects cell shape and focal adhesion (FA) dynamics during cell spreading. The cell is treated as a hypoelastic actively-deforming continuum and the substrate is modeled as a linearly elastic continuum. The active deformation, captured by the addition of an active rate of deformation tensor, models local cytoskeletal reorganization. FAs connecting the cell and the substrate are modeled as a collection of discrete elastic springs, which can be dynamically added and removed. We use this model to investigate how substrate elasticity, cell elasticity, FA strength, and FA spacing affect cell shapes during spreading. We also investigate how cellular active deformation must be coupled to FA forces and intracellular stresses in order to obtain experimentally observed cell spread areas and observed tractions exerted by the cell onto the substrate.

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MS11

Modeling the Growth of an Atherosclerotic Lesion

Atherosclerosis is a vascular disease driven by inflammatory processes. Atherogenesis can be viewed as an inflammatory instability of a reaction-diffusion-chemotactic (RDC) system on a fixed domain while modeling atherosclerotic lesion growth requires coupling the RDC system to the momentum balance system for the mechanical response of the affected tissue. This talk presents a model of this process and presents numerical simulations of a free-boundary problem modeling lesion growth.

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MS12

Collective Effects and Correlations in Semidilute Bacterial Suspensions

To understand the non-trivial correlations emerging from collective swimming, a simple model is introduced where a bacterium is represented as a force dipole subject to two types of interactions: hydrodynamic and excluded volume (collisions). This model allows for efficient direct simulations confirming a striking experimental observation: correlations are independent of concentration and swimming speed, past the concentration threshold for collective motion. The effects of the particle shape, size, and dipole moment will also be presented.

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MS12

Remarks on Modeling and Identification in Bacterial Chemotaxis

We discuss various topics related to the modeling and identification of bacterial chemotaxis, including the use of advection-diffusion and other PDE's to match microfluidics-generated population behavior, and the inference of signaling dynamics to match single-cell tracking data. Mathematically, the first topic involves the careful modeling of pathways and shallow gradient approximations (following work of Grunbaum, Othmer, and Erban), and the second topic requires the development of tools for the identification of time-varying parameters in nonhomogeneous Poisson processes that model motor events (such as tumbling) as a function of the phosphorylation states of certain enzymes. We present new results on these topics, including a model-based approach to the latter identification problem, and discuss our results in view of new experimental data.

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MS12

Relating the Chemotactic Sensitivity with Intracellular Signaling and Cell Movement

Chemotaxis of single cells has been extensively studied and a great deal on intracellular signaling and cell movement is known. However, systematic methods to embed such information into continuum PDE models for cell population dynamics are still in their infancy. In this talk, I will present our recent results on relating the chemotaxis sensitivity in the PatlakKellerSegel (PKS) model with the detailed biochemistry of intracellular signaling for run-and-tumble bacteria. Our general formulas are useful in explaining relations of single cell behavior and population dynamics. We show that the PKS model is valid when the external signal changes slowly, but inadequate when the signal changes fast. The general theory can also be applied to collective behavior of other individuals that move using a similar strategy.

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MS12

Global Asymptotic Stability of Constant Equilibrium States of a Repulsive Chemotaxis Model with Logarithmic Sensitivity

In contrast to diffusion (random diffusion without orientation), chemotaxis is the biased movement of cells/particles toward the region that contains higher concentration of beneficial or lower concentration of unfavorable chemicals. The former often refers to the attractive chemotaxis and latter to the repulsive chemotaxis. Chemotaxis has been advocated as a leading mechanism to account for the morphogenesis and self-organization of a variety of biological coherent structures such as aggregates, fruiting bodies, clusters, spirals, spots, rings, labyrinthine patterns and stripes, which have been observed in experiments. In this talk, I will present recent results on the rigorous analysis of a partial differential equation model arising from repulsive chemotaxis, which is a system of hyperbolic balance laws consisting of nonlinear and coupled parabolic and hyperbolic type PDEs. In particular, global wellposedness, large-time asymptotic behavior of classical solutions to such a model are obtained. The long-time behavior result shows that constant equilibrium states are globally stable, which indicates that chemorepulsion problem with non-diffusible chemical signal and logarithmic chemotactic sensitivity exhibits strong tendency against pattern formation. The results are consistent with general results for classical repulsive chemotaxis models.

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MS13

Flow Through a Two-Chambered Zebrafish Heart with Trabeculae

Trabeculae form in developing zebrafish hearts for Re on the order of 0.1; effects of trabeculae in this flow is not well understood. Dynamic processes, such as vortex formation, are important in the generation of shear at the endothelial surface layer and strains at the epithelial layer, which aid in proper morphology and functionality. In this study, CFD is used to quantify the effects of Re and idealized trabeculae height on the resulting flows.

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MS13

The Effects of Perturbations on Lamprey Swimming

The lamprey is a basal vertebrate and a model organism for neurophysiology and locomotion studies. Here a 2D, integrative, multi-scale model of the lamprey's anguilliform (eel-like) swimming is driven by neural activation and muscle kinematics coupled to body interactions with fluid surroundings and implemented using the immersed boundary method. Effects on swimming speed and cost (metabolic work) by nonlinear dependencies associated with muscle force development combined with perturbations to the neural activation are presented.

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MS13

Hydrodynamic Contributions to Amoeboid Cell Motility

In this research, we develop a computational model of crawling *Physarum polycephalum* based on the Immersed Boundary Method. Our model incorporates the effects of cell cytoplasm, the internal cytoskeleton and adhesions to the substrate. Of particular interest are stresses generated by flow and how transmission of stresses to the substrate is coordinated. We attempt to characterize conditions necessary to generate directed motion. Cytoplasmic flows and traction stresses are compared to experimentally measured values in Physarum.

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MS13

Population Scale Effects of Macrophytes on Plankton Mobility

Small-scale interactions between water and vegetation can have a significant, complex effect on water flow. Using a two-dimensional hydrodynamic model, we represent macrophytes as a simple, flexible and deforming porous layer, varying the bending stiffnesses and porosities of the plants, as well as background flow speeds and type of flow. Studying velocities, shear stress, and mixing, we show that small-scale physical-biological interactions can have major and important implications for plankton patchiness, movement, and ultimate destiny.

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MS14

Path-integrals and large deviations in a stochastic hybrid neural network

We construct a path-integral representation of solutions to a stochastic hybrid system describing the dynamics of synaptically coupled neuronal populations. The state of each local population is described in terms of two stochastic variables, a continuous synaptic variable and a discrete activity variable. The spike-driven dynamical equations for the synaptic currents are only valid between stochastic jumps in spiking activity, which are described by a neural master equation. We use the path-integral representation to derive a large deviation variational principle for a stochastic hybrid neural network. We illustrate the theory by considering the optimal paths of escape from a metastable state in a bistable neural network.

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MS14

Vasculature Adaptation and Optimization in Embryonic Zebrafish Brain

During the development of vasculature in the midbrain of embryonic zebrafishes, both angiogenesis and vessel pruning are observed. The vessel pruning occurred preferentially at loop-forming segments, leading to gradual reduction in the vasculature complexity. An shear-stress-driven adaptation model of blood vessels, which naturally optimizes the vessel network, is employed to predict the vessel pruning. The successful prediction suggests that vessel pruning is a consequence of the adaptation process and makes the vasculature more efficient.

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MS14

Theoretical Modeling of Nonlinear Dendritic Integration

We address the question of how a neuron integrates excitatory (E) and inhibitory (I) inputs from different dendritic sites. For an idealized neuron with an unbranched dendrite, a conductance-based cable model is derived and its asymptotic solutions are constructed. The solutions reveal the underlying mechanisms of a dendritic integration rule discovered in a recent experiment. We then extend our analysis to the multi-branch case and confirm our analysis through numerical simulation of a realistic neuron.

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MS14

Analytical Evaluation of Targeting Performances at Short and Long Distances in a Stochastic Model for Neural Arborization

We investigate the behavior of a simplified neural growth model that branches with uniform probability and is subject to a total length constraint. Treating all possible tree instantiations as outcomes drawn from a discrete probability distribution, we compute the expected number of active tree branches as a function of distance. We show analytically that both the rising and decaying part of the resulting curve are respectively described exactly and approximated by geometrical series.

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MS15

The Dependence of the Existence of Positive Steady States on the Rate Coefficients for Deficiency-One Mass Action Systems

It is well-known that there exists a unique positive steady state in each of the positive stoichiometric classes for single linkage class weakly reversible (WR) deficiency-one mass action systems. The existence result does not remain valid in general if we omit the weak reversibility assumption. In this talk, we charaterise those single linkage class non-WR defeiciency-one mass action systems for which the existence of positive steady states does not depend on the rate coefficients.

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MS15

Degree Two Polynomials for Saddle Node Bifurcations in Mass Action Networks

Bistability has been recognized an important feature of dynamical systems originating in Biology and it is often established numerically (via a saddle-node bifurcation). However, parameter uncertainty complicates numerical analysis. Hence techniques allowing the analytic computation of parameters where a given system exhibits bistability are desirable. We present a condition involving only polynomials of degree ≤ 2 that allows to determine state and parameter vectors where a mass action system generically undergoes a saddle-node bifurcation.

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MS15

Structural Identifiability of Biological Models

Identifiability concerns finding which unknown parameters of a model can be quantified from given input-output data. Many biological models are unidentifiable, which means that parameters can take on an infinite number of values and yet yield the same input-output data. We study the identifiability properties of several types of models, arising in Systems Biology and Chemical Reaction Networks, and demonstrate how to obtain identifiable reparametrizations of these models when they are unidentifiable.

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MS15

A Global Convergence Result for Processive Multisite Phosphorylation Systems

Multisite phosphorylation plays an important role in intracellular signaling. There has been much recent work aimed at understanding the dynamics of such systems when the phosphorylation/dephosphorylation mechanism is distributive, that is, when the binding of a substrate and an enzyme molecule results in addition or removal of a single phosphate group and repeated binding therefore is required for multisite phosphorylation. In particular, such systems admit bistability. Here we analyze a different class of multisite systems, in which the binding of a substrate and an enzyme molecule results in addition or removal of phosphate groups at all phosphorylation sites. That is, we consider systems in which the mechanism is processive, rather than distributive. We show that in contrast with distributive systems, processive systems modeled with mass-action kinetics do not admit bistability and, moreover, exhibit rigid dynamics: each invariant set contains a unique equilibrium, which is a global attractor. Additionally, we obtain a monomial parametrization of the steady states. Our proofs rely on a technique of Johnston for using "translated" networks to study systems with "toric steady states", recently given sign conditions for injectivity of polynomial maps, and a result from monotone systems theory due to Angeli and Sontag.

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MS16

Data Assimilation Methods and Inverse Problem for Protein Polymerization

Data assimilation methods are particular methods that exploiting some available data give us an estimation of parameters or state variables. In this presentation, we will introduce several data assimilation methods and their application to protein aggregation, a chain reaction which is one of the causes of neurodegenerative diseases called amyloid diseases (among which are Alzheimers, Huntingtons,

Parkinsons etc). Moving from Lifshitz-Slyozov equation, we define a model for protein polymerization. We couple the model and observations to define an inverse problem. The aim is to apply data assimilation methods on this inverse problem to obtain an estimation of kinetic coefficients and/or cluster concentrations, with application on real data.

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MS16

Limited Measurement Domains: Robustness of Parameter Estimation in Flocculation Dynamics

While incorporating the Smoluchowski coagulation equation to model aggregation in size structured populations, the actual physical structures we study can exist in clusters smaller than the lower limit and larger than the upper limit of experimental devices. With the motivation of identifying an aggregation kernel under real-world experimental limitations, we aim to rigorously study the impact of the limited measurement domain on the robustness of our parameter estimation inverse problem.

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MS16

Impact of Ellipsoid Geometry and Deformation on Flocculation Dynamics

Fragmentation is an important yet poorly understood aspect of flocculation dynamics. Simulations of fragmentation events can be simplified by approximating the floc as a solid ellipsoid. The force on the surface of such an ellipsoid can have a strong dependence on its geometry, further compounded by deformation due to the flow. We present results on the deformation of ellipsoidal flocs in laminar flow.

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MS16

A General Structured Population Model with the Application to Amphibians Infected with Chytridiomycosis

The disease Chytridiomycosis occurs when the skin of an amphibian is infected by the chytrid fungus Batrachochytrium dendrobatidi (Bd). The rapid and widespread growth of Chytridiomycosis has been associated with major population declines and extinctions in many frog species. Studies show that the inoculation of anti-Bd bacterial species Janthinobacterium lividum (Jl) could reduce Bd infection on amphibians. We first develop a new and general class of structured metapopulation models with wide range of application including amphibian dynamics and associated diseases. This modeling approach is then extended to investigate amphibians to understand the effect of the disease Bd and the symbiont Jl on their population dynamics and provide useful insights to biologists in the control of Chytridiomycosis under various scenarios.

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MS17

Merging Population Genetics, Mosquito Behaviour and Epidemiology to Predicting the Success of the Use of GM Mosquitoes for Malaria Control

Transgenic mosquitoes are a potential tool for the control or eradication of insect-vectored diseases. For malaria, one possible strategy relies on the introduction of malaria-refractory transgenes into wild Anopheles mosquito populations that would limit their capacity to transmit the disease. This could be done with or without a gene-drive that could facilitate the spread of the allele of interest. By merging population genetics, epidemiology and mosquito life-history traits, it is possible to explore the importance of the gene-drive, the eventual role of mosquito mating preferences as well as the impact of the cost and efficacy of refractoriness on its spread in the mosquito population. As the aim of such approach is not only a modification of the mosquito population but a significant decrease of malaria prevalence in the human population, it is essential to determine how such releases could affect the long-term prevalence of malaria in humans. Those different aspects are going to be discussed in the current context of the fight against malaria.

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MS17

The Effect of IPT on the Spread of Drug Resistant Malaria Parasite When Regions are Connected

The use of IPT is an increasingly popular preventive strategy aimed at reducing malaria incidence in vulnerable individuals. We seek to understand how IPT can affect the spread of antimalarial drug resistance when there is movement between neighboring low and high transmission areas. We expanded a previously published model to include movement between neighboring high and low transmission areas. Our results suggest that population movement results in resistance spreading fastest in high transmission

areas. The more complete the antimalarial resistance, the faster the resistance spread through a population.

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MS17

Ipt and the Spread of Drug Resistant Malaria

Intermittent Preventive Treatment (IPT) is a malaria control strategy in which vulnerable asymptomatic individuals are given a full curative dose of an antimalarial medication at specified intervals, regardless of whether they are infected with malaria or not. A mathematical model is developed to explore the effect of IPT use on the malaria prevalence and control under different scenarios. The model includes both drug-sensitive and drug-resistant strains of the parasite as well as interactions between human hosts and mosquitoes. The basic reproduction numbers for both strains as well as the invasion reproduction number by the resistant strain are computed and used to examine the role of IPT in the development of resistant infections. Sensitivity and uncertainty analysis is carried out to examine the influence of model parameters in the model outcomes.

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MS17

Application of P. Falcipalrum Gametocyte Sex Ratios Via Competitive and Non-Competitive Strategies: The Evolutionary Implications

A mathematical model that simulates the within-mosquito dynamics of *Plasmodium falciparum* in an Anopheles mosquito is used to investigate optimal gametocyte sex ratios under varying fecundity. Gametocytes are the sexual forms of the *Plasmodium* malaria parasite and understanding mechanisms that determine the ratio of male gametocytes to female gametocytes has engendered considerable interest among researchers. Under unbiased random mating and incomplete fertilization the model illustrate that optimal gametocyte sex ratios vary from a highly female-biased to a slight male-biased sex ratio under a non-competitive strategy. When two distinct fitness optimization strategies for for *P. falciparum* with varying fecundity was analyzed, initial results indicate that the non-competitive strategy is the winning strategy.

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MS18

An Application of Mathematics to Osteoarthritis Related Inflammation

The degenerative joint disease osteoarthritis (OA) has traditionally been viewed as a consequence of aging and "wear and tear." However, the most recent research indicates that inflammation, as related to the innate immune response, is fundamental in the development and progression of OA. The goal of this talk is to describe mathematical approaches to developing a theoretical foundation for recent discoveries in this area of biological research, and for understanding the connections between OA and inflammation.

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MS18

Success, Failure, and Spreading Speeds for Invasions on Spatial Gradients

We present a model that describes the spatial spread of a species along a habitat gradient. We demonstrate that the species may succeed or fail in local invasion depending on the species' growth function and dispersal kernel. We show how a species can escape a region of poor quality habitat by climbing a resource gradient to good quality habitat where it spreads at a constant spreading speed. Joint work with William Fagan and Kimberly Meyer.

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MS18

Modeling and Analysis of Glioma Tumor Growth

Glioblastoma multiforme is the most common and most deadly primary brain tumor in adults. Gliomas are characterized by highly diffusive growth patterns, thus reaction-diffusion equations are often used in modeling. To give insight on the mechanisms most responsible for tumor growth and the difficult task of forecasting future tumor behavior, numerical and analytical results from various models, including ones with density-dependent diffusion, are compared to experimental data.

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MS18

The Effects of Cross-diffusion on an SIR Model

During the outbreak of infectious diseases, susceptible individuals naturally tend to avoid infective individuals. We use a two-dimensional reaction-diffusion model, adapted from the Shigesada-Kawasaki-Teramoto (1979) model, to describe the effects of cross-diffusion on an SIR model.

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MS19

Actin-myosin Spatial Patterns from a Simplified Isotropic Viscoelastic Model

F-actin networks are involved in cell mechanical processes ranging from motility to endocytosis. The mesoscale architecture of assemblies of individual F-actin polymers that gives rise to micrometer-scale rheological properties is poorly understood, despite numerous in vivo and vitro studies. In vitro networks have been shown to organize into spatial patterns when spatially confined, including dense spherical shells inside spherical emulsion droplets. Here we develop a simplified model of an isotropic, compressible, viscoelastic material continually assembling and disassembling. We demonstrate that spherical shells emerge naturally when the strain relaxation rate (corresponding to internal network reorganization) is slower than the disassembly rate (corresponding to F-actin depolymerization). These patterns are consistent with recent experiments, including a collapse of shells to a central high-density focus of F-actin when either assembly or disassembly is reduced with drugs. Our results demonstrate how complex spatio-temporal patterns can emerge without spatially-distributed force generation, polar alignment of F-actin polymers, or spatially non-uniform regulation of F-actin by upstream biochemical networks.

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MS19

Exploring Motility of Breast Cancer Cells Using a 3D Individual Cell Based Model

Experiments have demonstrated that white blood cells are directly involved in the invasion of breast tumor cells into surrounding tissues and blood vessels. The white blood cells interact with tumor cells via a short-ranged chemical signaling loop involving two signalling molecules. We developed a 3D individual cell based computational model to study these interactions and to understand the observed streaming motility pattern. The cells are simulated as freely moving deformable ellipsoids and the signalling molecule concentrations are estimated using reaction-diffusion equations. The movement and deformation of cells are calculated from equations of motion accounting for all forces acting on each cell. This simplified model is able to reproduce results from both in vitro and in vivo experiments. The model suggests that the removal of the signalling molecules is essential to produce the observed ratio of 3 invasive tumor cells per 1 invasive white blood cell. A preliminary exploration of the parameter space indicates that the ratio between tumor cells and iwhite blood cells is robust to changes in most model parameters, supporting the experimental results. An exception to this robustness is that changes in the decay and secretion rates of the signalling molecules can alter and even eliminate the invasion of tumor cells.

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MS19

Insights into Cytoplasmic Rheology Gained from Modeling Cellular Blebbing

Blebbing occurs when the cytoskeleton detaches from the cell membrane, resulting in the pressure-driven flow of cytosol towards the area of detachment and local expansion of the cell membrane. Recent experiments involving blebbing cells have led to conflicting hypotheses regarding the timescale of intracellular pressure propagation. The interpretation of one set of experiments supports a poroelastic cytoplasmic model which leads to slow pressure equilibration when compared to the timescale of bleb expansion. A different study concludes that pressure equilibrates faster than the timescale of bleb expansion. To address this, a dynamic computational model of the cell was developed that includes mechanics of and the interactions between the intracellular fluid, the actin cortex, the cell membrane, and the cytoskeleton. The model results quantify the relative importance of cytoskeletal elasticity and drag in bleb expansion dynamics. This study also shows that recent multi-bleb experimental results can be explained by the combination of cytoskeletal poroelasticity with either dynamic membrane-cortex adhesion or cortical reformation.

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MS19

The Physics of Collective Cell Migration in Wound Healing and Cancer Metastasis

Multicellular organisms require groups of cells to function together as a unit. A common scenario involves the collective movement of cells. For example, when your skin gets cut, one of the first processes is re-epithelialization where epidermal cells crawl over the wounded region. And, in cancer, tumor cells will often move as a group to detach from the primary tumor and invade distal regions of the body. In this presentation, I will describe the work that we have been doing to develop a multiscale model for collective cell migration. This model is based in the fundamental biophysics of a single cell. We show that a combination of directed cell motility, dipole-distributed forces, and adhesion to neighboring cells and the environment is sufficient to explain in vitro wound healing dynamics and gives insight into the biophysical changes that occur when cancer cells become metastatic. This model provides testable predictions that we are now testing with experiments.

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MS20

Impact of Single-Neuron Dynamics on Transfer of Correlations from Common Input

One source of spike train correlations in the nervous system is common input, an inevitable consequence of the ubiquity of coding by populations. The details of how input correlations map onto output spike correlations is surprisingly complex, depending on single-neuron dynamics in subtle ways. Much progress has been made in untangling this relationship in Type I and Type II excitable neurons, in both simplified phase oscillator and conductance-based models. In this talk, we apply these techniques to novel patterns of excitability that arise in the presence of calcium currents.

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MS20

Integrate-and-Fire Model of Insect Olfaction

When a locust detects an odor, the stimulus triggers a series of synchronous oscillations of the neurons in the antenna lobe. These oscillations are followed by slow dynamical modulation of the firing rates which continue after the stimulus has been turned off. I model this behavior by using an Integrate-and-Fire neuronal network with excitatory and inhibitory neurons. The inhibitory response of both types of neurons contains a fast and slow component. The fast component, together with the excitation, creates the initial oscillations while the slow component suppresses them and aids in the creation of the slow patters that follow. During the initial oscillations the stimulus can be identified by determining which excitatory neurons participate consistently in every cycle of the oscillations.

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MS20

Reduction Methods for Spiking Networks

We consider a simple spiking LIF neuron model driven by excitatory conductance input, and highlight a dimension reduction method to capture the firing rate dynamics. We further consider a QIF population with adaptation and recurrent (all-to-all) excitatory coupling, where an analogous reduction method can be applied with augmentation. Based on the reduction, a linear stability analysis method is applied to capture some of the features of the simulations.

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MS20

The Essential Role of Phase Delayed Inhibition in Decoding Synchronized Oscillations within the Brain

The widespread presence of synchronized neuronal oscillations within the brain suggests that a mechanism must exist that is capable of decoding such activity. Two realistic designs for such a decoder include: 1) a read-out neuron with a high spike threshold, or 2) a phase-delayed inhibition network motif. Despite requiring a more elaborate network architecture, phase-delayed inhibition has been observed in multiple systems, suggesting that it may provide inherent advantages over simply imposing a high spike threshold. We use a computational and mathematical approach to investigate the efficacy of the phase-delayed inhibition motif in detecting synchronized oscillations, showing that phase-delayed inhibition is capable of detecting synchrony far more robustly than a high spike threshold detector. Furthermore, we show that in a system with noisy encoders where stimuli are encoded through synchrony, phase-delayed inhibition enables the creation of a decoder that can respond both reliably and specifically to a stimulus, while a high spike threshold does not.

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MS21

The Use of Physiological Model of Menstrual Cycle Regulation in Women's Health: Fertility and

Contraception

The biology of female menstrual cycle hormonal regulation is complex and not completely understood. The system makes an excellent case study for mathematical modeling due to intrinsic nonlinearities, feedback mechanisms and delays. Several dynamical models with varying complexity and biological plausibility have been proposed. We provide an industrial perspective for how these models can and should be used to inform clinical decisions for therapies targeting contraception, fertility, and endometriosis.

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MS21

The Role of Insulin and Androgen Dynamics in Female Hormone Dysregulation

Although the physiological role of insulin and androgens in follicle development remains unclear, excess concentrations are commonly associated with ovulatory defects. We incorporate insulin and androgen dynamics into a mathematical model of folliculogenesis, which describes hormone production and pituitary-ovarian feedback through successive growth stages. Changes in model periodicity and gonadotropin/hormone profiles under various biological circumstances are used to characterize the physiological versus pathological influences of insulin and androgens on ovulation.

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MS21

Multiple Cycles and Bifurcation in Models of Hormonal Control of the Menstrual Cycle

Two models for hormonal control of the menstrual cycle are presented using the same system of differential equations but based on different data sets . For the best-fit parameter sets, simulations for the two models agree well with the data but one model also has a stable periodic solution representing an abnormal, nonovulatory menstrual cycle. Differences in model behavior are explained by studying hysteresis curves in bifurcation diagrams with respect to sensitive model parameters.

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MS21

A Differential Equation Model for the Bovine Estrous Cycle

Based on the models for the human menstrual cycle by Selgrade and coworkers, a fully coupled feedback model for the bovine estrous cycle has been developed. It has been used for an analysis of follicular wave patterns and for the simulation of synchronization studies. In this talk, we will present the model and its dynamical properties. Open questions such as the administration of GnRH and an improved modeling of follicular development will be discussed.

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MS22

An Algebraic Framework for Describing and Studying Binary Enzymatic Networks

We present a framework to describe and reason about enzymatic networks. The initial motivation for this construct was to extend examples from the literature into the following theorem: a binary enzymatic network that is futile and cascaded is persistent, i.e. molecular species do not tend to extinction. The framework provides mathematically sound and biochemically applicable definitions for the notions of futile enzymatic cycles and enzymatic cascades, and several prerequisite concepts. The framework could be used to prove more results, or even to help assess the plausibility of models of enzymatic networks during their design.

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MS22

Correspondence of Regular and Generalized Mass Action Systems

In this talk, we investigate systems where graph-based correspondence of dynamics for mass action systems may not be made directly, but for which correspondence may be made to a "generalized" mass action system. The constructed generalized mass action system contains different monomials than implied by the chemistry of the system, but has a "well-structured" reaction graph. We will discuss some of the newest results regarding the algorithmic construction of such generalized mass action systems.

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MS22

Atoms of Multistationarity in Chemical Reaction Networks

Multistationarity is a prerequisite for a reaction network to act as a biochemical switch. Theoretical tools that help rule out multistationarity include the Jacobian criterion of Craciun and Feinberg. We provide results that are helpful in establishing multistationarity of certain networks. The key result is that if a multistationary network N is "embedded" in a larger network G then G is also multistationary. The partial ordering resulting from the embedding property yields minimal (with respect to number of chemical species and reactions) multistationary networks. We also provide results which identify the smallest such minimal networks.

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MS22

Exploiting Reaction Network Structure for Parameter Identification of Biochemical Switches

One key challenge in Systems Biology is the identification of kinetic models from limited quantitative data. In this work we illustrate the potential of Chemical Reaction Network Theory (CRNT) for the parameter identification of kinetic models. We introduce a method for inverse bifurcation of bistable biochemical reaction networks, that exploits inherent structural properties of bistable switches to infer the kinetic parameters from dose response curves. Uniqueness and identifiability properties of the associated inverse problem are analyzed.

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MS23

Real-Time Model Calibration and Prediction Testing with the GPU and Dynamic Clamp

Electrical activity of anterior pituitary cells is heterogeneous, motivating model fitting to individual cells. We use the parallel computational power of the GPU to find parameters of a biophysical model with similar bifurcation structure to live individual cells. The optimization is iteratively improved by making model predictions that induce a qualitative changes in electrical activity, testing the predictions with dynamic clamp on the same cell, then adding the results to the set of optimization constraints.

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MS23

Hypothalamic Vasopressin Neurons: Signal Processing in An Asynchronous Bursting Population

Vasopressin acts as an antidiuretic hormone, as part of the homeostatic system that maintains osmotic pressure. Experiments show a robust linear relationship between osmotic pressure and vasopressin secretion despite very nonlinear properties of spike generation and secretion in the neurons, and highly heterogeneous spiking activity. Here we develop a previous model of the spiking and secretion mechanisms to examine how the heterogeneous population might coordinate a robust signal response using local interneuronal (dendritic) communication.

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MS23

Leveraging Mathematical Models to Understand Population Variability in Response to Cardiac Drugs

Mathematical models of heart cells and tissues are sufficiently advanced that the models can predict mechanisms underlying pro-arrhythmic or anti-arrhythmic effects of drugs. However, these models are not presently adequate for understanding variability across a population, i.e. why a drug my be effective in one patient but ineffective in another patient. I will discuss novel computational approaches my laboratory has developed that can quantify and predict differences between individuals in the response to cardiac drugs

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MS23

Paracrine Regulation of Glucagon and Somatostain Secretion

Pancreatic islets are composed of α-, β-, and δ-cells. These cells secrete the hormones glucagon, insulin, and somatostatin, respectively. Together, these hormones regulate glucose homeostasis in the body. While β-cells are coupled through gap junctions, individual α- and δ-cells are heterogenous. We investigate the paracrine interacts between these cells, which gives synchronous oscillations of insulin and somatostain, and anti-synchronous oscillations of insulin and glucagon at high glucose levels.

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MS24

Epidemiological and Economic Benefits of Targeted

Tuberculosis Screening in a Correctional Facility of New River Health District

Objective: The objective of this study is to conduct cost-effectiveness analysis of pre-screening inmates for tuberculosis compared to no pre-screening in a correctional facility in Southwest Virginia. Background: Correctional facilities represent a relatively higher risk for tuberculosis transmission in the United States because they have close living quarters, overcrowding, and poor ventilation, thereby enhancing the risk of tuberculosis acquisition and transmission. Methods: We conducted cost effectiveness analysis to evaluate pre-screening measures for tuberculosis compared to the baseline scenario of no pre-screening. We developed a dynamic model to understand and analyze the transmission dynamics of tuberculosis in a correctional facility and its associated costs over a time horizon of 5 years, from the perspective of the correctional facility and the local health department. Data from a tuberculosis outbreak in 2011 at a correctional facility located in Southwest Virginia is incorporated to calibrate the dynamic model. Results: We used the ratio of 68 to 200 out of 100,000 inmates will develop active tuberculosis while incarcerated when conducting analysis for the baseline of no pre-screening. Based on preliminary results, the incremental cost-effectiveness ratio of tuberculosis pre-screening is estimated at $-15,461 per disability adjusted life year averted (cost saving) from the perspective of the correctional facility and the local health department. Conclusion: Our findings indicate that tuberculosis pre-screening is a cost-saving intervention; thereby, we recommend adoption of tuberculosis pre-screening programs in correctional facilities.

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MS24

A Simple Epidemic Model with Nosocomial Transmission

The SARS epidemic of 2002-3 drew attention to nosocomial disease transmission, as many of the disease cases were transmitted through hospital staff and visitors. Various types of models have been proposed to describe this, including metapopulation models. We formulate and analyze a simple compartmental model with heterogeneous mixing to describe nosocomial transmission and determine its reproduction number and the final size relations.

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MS24

Demographic Transition and the Dynamics of Measles in China

Industrialization and demographic transition generate non-stationary dynamics in human populations that can impact the transmission and persistence of infectious disease. By catalytic transmission model, we show that demographic transition and reduced prevalence has driven a shift in the age distribution of susceptibility to measles in China. The force of infection of measles has declined dramatically in the industrialized eastern provinces in the last decade; while central and western provinces exhibit dynamics consistent with endemic persistence.

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MS24

Modeling SIS Disease Dynamics on Random Contact Networks

Contact networks represent persons by nodes and contacts by edges. It is a more realistic model of disease related human contacts than the random mixing model, which assumes that every pair of individuals have identical contact rate. An effective degree SIS epidemic model was developed before, and was shown to have different disease thresholds than an SIR model. This contradicts with the prediction of classic disease models that SIR and SIS models should have the same disease threshold. But this effective degree model is too complex to derive a closed formula for the disease threshold. In this talk, I will introduce a simplified SIS model on random contact networks, which agrees with stochastic simulations and is mathematically tractable. The model yields a disease threshold formula that bears a clear biological meaning: for the disease to spread, the average number of transmissible neighbours times the average number of times a neighbour can be infected must be greater than unity. The threshold converges to that of the SIR model under the homogeneous mixing limit.

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MS25

Models of Neurovascular Coupling and Cerebral Autoreglation

Our research group has developed a parallel numerical model describing neurovascular coupling. NVUs are coupled through a space filling H-tree simulating a vascular tree and spatially embedded in cerebral tissue. The model regulates bloodflow in response to neuronal activity in a 2-dimensional tissue slice of width and depth of the order of millimetres culminating in the dynamic simulation of several million cells. The model thus allows us to study a number of important pathological scenarios.

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MS25

Assessing the Impact of Structural Organization of the Renal Medulla on Oxygen Distribution Using a Mathematical Model

A theoretical model is presented to analyze the impact on oxygen distribution of the heterogeneous organization of the rat medulla revealed in anatomical studies. Model equations are based on transmural transport and conservation of water and solutes (NaCl, urea, O_2, HbO_2, Hb), and are solved to steady state. Results suggest that the structural organization of the renal medulla produces significant axial and radial PO_2 gradients, and impacts the effectiveness of the medullary urine concentrating mecha-

nism.

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MS25

Can Pre-Glomerular Oxygen Transport Be Used to Investigate Renal Anatomy?

There is a close spatial association of arteries and veins in the pre-glomerular vasculature, which facilitates oxygen shunting and protects the kidney from hyperoxia. However this anatomical structure may lead to hypoxia. We have developed a mathematical model of oxygen transport in the paired pre-glomerular branched vasculature. Here we demonstrate how differences in transit times and shapes of pulses of oxygen and labelled haemoglobin, due to shunting, could be used to explore this pre-glomerular anatomy.

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MS25

Development of Hypoxia in a Model of Renal Blood Flow Control and Oxygen Consumption

Hypoxia is an important pathway in the development of acute kidney injury during cardiopulmonary bypass surgery. Using a model of renal hemodynamics we assess the degree to which hypoxia develops under reduced hematocrit, temperature, and systemic pressure that are commonly induced in such surgery. Oxygenation is determined by renal blood flow and the metabolic work of sodium reabsorption. Results suggest that although oxygen supply and consumption both decrease bellow physiologic levels, fractional extraction increases significantly.

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MS26

Computational Design of Megadalton-Scale Nucleic Acid Nanoassemblies

Programmed self-assembly of nucleic acids offers the unique opportunity to engineer complex megadalton-scale macromolecular architectures with atomic-level accuracy. The sequence specificity of DNA additionally renders these nanoassemblies spatially addressable structural scaffolds to host secondary molecules such as light-harvesting dyes and chemically active compounds. These properties may be exploited to rationally design, for example, biomimetic light-harvesting constructs to replicate aspects of bacterial photosynthesis. Here, I present our computational design tool CanDo (http://cando-dna-origami.org) that quantitatively predicts the 3D solution structure of megadalton-scale DNA-based assemblies based on underlying DNA sequence, as well as their emergent light-harvesting properties when decorated with dyes and porphyrins.

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MS26

The Structural Glycobiology of HIV: Insights from Molecular Simulations and Implications for the Design of Virucidal Lectins

The HIV envelope-glycoproteins are heavily glycosylated to avoid immune recognition, creating both challenges to the effective inhibition of viral-cell recognition and unique opportunities; for example, carbohydrate-binding proteins have been shown to have the potential to act as potent virucides. The development of detailed computational models that explain the relative affinities of distinct oligosaccharides, provide insight into mechanisms of multi-valent binding, and provide a foundation for the rational design of improved inhibitors will be presented.

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MS26

3D Continuum Modeling of Ion Permeation in Ion Channel Systems

As it is hard to apply all-atomic model to simulate the whole process of ion permeation in ion channel, we use continuum electrodiffusion description for ion flow in the channel system. Electrodiffusion process exists in many apparently different physical objects such as electrolyte cell, nanofluidic device, charged porous media, and ion channel in biology. Real 3D ion channel is particularly difficult to simulate due to the multiscale nature of the transport process and the complex geometry/boundary of the channel protein system. For this reason, there are so far only a few software publicly available in this important area of biology. We will present a software platform for ion channel simulations. The platform includes three parts: (1) finite element solver for the Poisson-Nernst-Planck equations and their improved forms, (2) molecular meshing that is required for finite element method. We recently developed a novel and robust molecular surface mesh generation tool TMSmesh that can handle complex and arbitrarily large biomolecular system. (3) a visual system, VCMM, for molecule, mesh and simulation data visualization and analysis. The platform is applied to compute properties such as current-voltage characteristics (curves) and conductance of a few channel systems, and the calculations are compared with Brownian Dynamics simulation and experimental results.

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MS26

Monte Carlo Solution of Biochemical Electrostatics Problems

Electrostatic forces and the electrostatic properties of molecules in solution are among the most important issues in understanding the structure and function of large biomolecules. The use of implicit-solvent models, such as the Poisson-Boltzmann equation (PBE), have been used with great success as a way of computationally deriving electrostatics properties such molecules. We discuss how to solve an elliptic system of partial differential equations (PDEs) involving the Poisson and the PBEs using path-integral based probabilistic, Feynman-Kac, representations. This leads to a Monte Carlo method for the solution of this system which is specified with a stochastic process, and a score function. We use several techniques to simplify the Monte Carlo method and the stochastic process used in the simulation, such as the walk-on-spheres (WOS) algorithm, and an auxiliary sphere technique to handle internal boundary conditions. We then specify some optimizations using the error (bias) and variance to balance the CPU time. We show that our approach is as accurate as widely used deterministic codes, but has many desirable properties that these methods do not. In addition, the currently optimized codes consume comparable CPU times to the widely used deterministic codes. Thus, we have an very clear example where a Monte Carlo calculation of a low-dimensional PDE is as fast or faster than deterministic techniques at similar accuracy levels.

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MS27

Near Wall Motion of a Model Swimmer in a Viscoelastic Fluid

Microorganisms interacting in viscoelastic fluids are ubiquitous in nature; this includes bacteria colonizing in viscoelastic mucus in human and animal bodies, bacteria in biofilms grown on natural and manmade surfaces. Here is this work, we perform a three-dimensional direct numerical simulation of an archetypal low-Reynolds-number swimmer, squirmer, near a surface and investigate the role of viscoelasticity of the background fluid on the swimming speed and trajectory of the swimmer near the surface.

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MS27

Flagellar Kinematics in Complex Fluids: Viscous and Elastic Effects

The motility behavior of microorganisms can be significantly affected by the rheology of their fluidic environment. Here, we experimentally investigate the effects of fluid elasticity on the swimming behavior of the microscopic alga Chlamydomonas reinhardtii and on the kinematics of its flagella. We find that the flagellar beating frequency and wave speed are both enhanced by fluid elasticity. Interestingly, the swimming speeds during the alga power and recovery strokes are enhanced by fluid elasticity for Deborah numbers larger than unity, $De > 1$. Despite such enhancements, however, the alga net forward speed is hindered by fluid elasticity by as much as 30% compared to Newtonian fluids of similar shear viscosities. We use slender body theory and Principal Component Analysis (PCA) to analyse ciliary waveforms and elucidate the role of fluid elasticity and viscous dissipation in regulating the kinematics of the swimming process.

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MS27

Finite Length Undulatory Swimmers: Whether to Kick or to Burrow in a Viscoelastic Fluid

We explore finite length undulatory swimmers in viscoelastic fluids. The worm is modeled as an inextensible infinitely thin sheet in 2 dimensions and the swimming is driven using a prescribed target curvature. We look at front-back asymmetries in the prescribed stroke pattern and consider the effect on swimming speed and efficiency. The importance of passive dynamics, where swimmers are given prescribed torques rather than prescribed shapes, is explored. We show that kickers can get a larger boost from viscoelasticity than burrowers.

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MS27

Lyme Disease and Microorganism Swimming in

Complex Fluids

Lyme disease is caused by infection of the mammalian host by the highly invasive spirochete, Borrelia burgdorferi. These bacteria easily invade and colonize the dermis, joints, connective tissue, heart, and central nervous system. The motility of this organism is, therefore, crucial to the pathogenesis of the disease. I will describe experiments that we have been doing to measure the biophysical parameters of motility of these bacteria in realistic environments, such as matrices that mimic the ECM. These experiments show a number of interesting behaviors that are not predicted by recent theories of swimming in non-Newtonian environments. I will then describe the models and simulations that we have been sing to describe the motility of this fascinating organism in complex environments. Using our data, we have also developed a mathematical model to elucidate pathogen-host interactions during early Lyme disease, which explains the spatiotemporal dynamics of the characteristic first sign of the disease, a large (5 cm diameter) rash, known as an erythema migrans (or EM). The model predicts that the bacterial replication and dissemination rates are the primary factors controlling the speed that the rash spreads, whereas the rate that active macrophages are cleared from the dermis is the principle determinant of rash morphology. In addition, the model supports the clinical observations that antibiotic treatment quickly clears spirochetes from the dermis and that the rash appearance is not indicative of the efficacy of the treatment. The quantitative agreement between our results and clinical data suggest that this model could be used to develop more efficient drug treatments and may form a basis for modelling pathogen-host interactions in other emerging infectious diseases.

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MS28

Shilnikov Cornerstone Bifurcation Generates a Family of Mechanisms Governing Dynamics of Central Pattern Generators

The cornerstone Shilnikov bifurcation generates a family of mechanisms that determines temporal characteristics of endogenously bursting, spiking, and silent neurons. We described a model of insect locomotion. The model gait is controlled by the burst duration and interburst interval of protractor and retractor interneurons. The transition from tetrapod to tripod gait is governed by the duty cycle of endogenously silent retractor interneurons, which fire in response to endogenously bursting protractor interneurons.

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MS28

Using Experimental Phase Response Curves to Characterize Inter-Leg Coupling

Walking movements result from a complex interplay of central pattern generating networks (CPGs), local sensory feedback about movements and forces generated in the legs and coordinating signals from neighboring limbs. Currently, we use a combined experimental and computational approach to investigate the effect of specific front leg sensors onto the middle leg CPGs to gain a deeper insight into the inter-connection of the CPGs of all legs and into the processing of inter-leg sensory signals.

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MS28

Multiple Rhythms from One Network: Phase Plane and Stochastic Analyses of Rhythmic Activity in Turtle Motor Circuits

We analyze a central pattern generators ability to produce differing motor patterns from a single pool of neurons under different tonic drives, focusing on a particular motoneurons response to different phasic synaptic inputs. We study the impact of these phasic inputs on motoneuron phase space, associated trajectories and show how these yield sufficient conditions for reproduction of observed rhythms. We also present preliminary results from stochastic analysis to examine the role of strong synaptic conductances.

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MS28

Dynamical Architectures for Control of Rhythmic Behavior

How do rhythmic motor systems achieve both robustness to perturbations and sensitivity to variable operating conditions? Do limit cycle (LC) oscillators and chain reflexes (CR) capture two extremes along a continuum of central pattern generation models? We investigate the consequences of different dynamical architectures for incorporating sensory input in motor control, and quantitatively evaluate the advantages of intermediate architectures, such as stable heteroclinic channels, which combine features of both LC and CR dynamics.

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MS29

Therapeutic Implications from a Multiscale Model of Blood Clot Degradation

We develop a multiscale model of blood clot degradation to study safer, more effective treatments for stroke patients. With a microscale model of a single fibrin fiber, we study how individual activator and inhibitor molecules affect the degradation of the fiber. Data from this microscale model are used in a macroscale model of a full blood clot, where we study the effect of different treatment strategies on clot degradation.

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MS29

A Model-Based Comparison of Clinical and Biological Determinants for Anticoagulation Therapy

We combine temporal models of coagulation and fibrinolytic pathways with warfarin pharmacokinetics and pharmacodynamics to study anticoagulation therapy. We compare two modeling frameworks to determine treatment efficacy: a traditional clinical assessment based on a simulated prothrombin time test and a biological assessment influenced by platelet activation and simplified chemical/cellular transport dynamics. We then discuss the roles of these assessment methods in the development and success of individualized treatment strategies.

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MS29

Structural Hierarchy Governs Nonlinear Mechanics of Fibrin Networks and Transport of Blood Clotting Factors

When a blood vessel ruptures, a hemostatic clot, consisting mainly of platelets and fibrin, is formed to restrict the loss of blood. Salutary blood clotting is highly regulated, but a pathological clot (thrombus) may form within a vessel and restrict blood flow to organs or clot pieces (emboli) can detach and be carried to the lungs, causing a life-threatening complication called pulmonary embolism. Fibrin network plays an important role in determining thrombus mechanical properties. It is responsible for thrombus integrity and redistribution of various mechanical loads acting on the thrombus due to blood flow and vessel deformations. Additionally, the structure of the network affects movement of blood clotting factors through the clot. This study demonstrates that structural changes in fibrin networks exposed to external load strongly correlate with networks mechanics. It is also shown that permeability of the fibrin network and protein diffusivity are important factors determining the transport of blood proteins inside the thrombus. The obtained results combining microfluidic experiments and thrombus hemodynamics model suggests that a fibrin network formed at early stages of thrombus initiation can prevent normally asymptomatic thrombi from developing into pathological clots.

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MS29

Fibrin Polymerization in Flow: Gelation and Post Gelation Dynamics

Blood clots are composed of platelets and a gel of fibrin fibers. The amount and structure of the fibrin fibers depend on conditions during their formation. In this presentation, I will discuss a 2-D advection-diffusion model for fibrin polymerization in flow that includes gelation and post gelation dynamics. Hindered diffusion and a Brinkman resistance term dependent on fiber properties, including branch point density and volume faction, supply feedback in the system.

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MS30

Recent Developments, Connections and Open Problems in Chemical Reaction Network Theory

I'll give a brief overview of some recent developments in chemical reaction network theory, namely the study of the structure-dynamics relationship for chemical reaction networks (CRNs). The talk will outline the nature of conclusions which may be drawn about a CRN based primarily on network structure, and some of the challenges remaining: these include theoretical challenges, but also questions regarding the implementation of theory as algorithms. I will also discuss some connections between claims for mass action kinetics and for more general kinetics.

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MS30

Persistence and the Global Attractor Conjecture

A positive trajectory of a dynamical system is called persistent if, in the long run, it does not approach the boundary of the positive orthant. In biological applications, the persistence property is critical in deciding if a species in an ecosystem will become extinct, an infection will die off, or a chemical species will be completely consumed by a reaction network. We describe some classes of dynamical systems for which all positive trajectories are persistent. We also describe connections to the global attractor conjecture, which says that a large class of mass-action systems (called complex balanced or toric dynamical systems) have a global attractor within any invariant subspace.

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MS30

Monotonicity of Chemical Reaction Networks with Respect to Non-Simplicial Cones

The theory of monotone flows has been applied to numerous chemical reaction networks in recent years. A dynamical system is said to be monotone if states preserve a partial ordering as they evolve with time. Monotonicity restricts the possible asymptotics of dynamical systems: stable periodic orbits cannot exist in a monotone dynamical system, and it is frequently possible to draw stronger conclusions, such as generic convergence to equilibria. To date, most applications of the theory of monotone flows to chemical reaction networks focus on networks that are either cooperative, or can be made cooperative by applying a similarity transform to the state space. This talk will explore networks that cannot be made cooperative, yet are still monotone with respect to an ordering defined by a non-simplicial cone. The problem of identifying a suitable cone for a given network will be discussed, along with the consequences for the dynamics.

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MS30

Sign Vectors in Chemical Reaction Network Theory

Abstract not available at time of publication.

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MS31

Estimating the Functional Connectivity in Networks of Neurons

We will discuss the role of chaotic interplay among voltage gated neural dynamics and intracellular Calcium dynamics. In particular we have analyzed the issues that arise in determining unknown parameters in the dynamical equations of such models when presented with observed data. Neither voltage data nor Calcium concentration data alone suffices to estimate properties of the model; two measurements are required. We show that both voltage and Ca measurements suffice or measurements based on the waveform of the time course of voltage will suffice. This has strong implications for experiment on neurons where both types of dynamics are present.

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MS31

Using Mathematical Models to Determine the Source of Heterogeneity in Cellular Calcium Dynamics

Cell responses to stimuli are commonly heterogeneous. We describe a model-based technique for determining the source of the heterogeneity in the calcium response of pituitary lactotrophs to a calcium-mobilizing agonist. This method samples specific parameters to produce various responses, and then compares scatter plots of features of the response to features from experimental traces to determine the likely sources of response variability. This technique is applicable to any situation in which the heterogeneous biological response is described by a mathematical model.

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MS31

Heterogeneity As a Consequence of Homeostasis

A fundamental question in neuroscience is how neurons develop, control, and maintain their electrical signaling properties in spite of ongoing protein turnover and activity perturbations. I will introduce some recent modelling work that has tied together experimental data with longstanding questions about the inherent variability of neuronal properties. Interestingly, the model predicts pathological behavior that can arise as a consequence of homeostasis rather than a failure of it.

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MS31

Inference of Network Structure from Spikes and Time Series

We discuss recent usage of data assimilation techniques to track and infer structure from networks of excitable cells. We emphasize methods that are statistical in nature in the sense of avoiding arbitrary thresholds, and that can be applied in real time to deal with nonstationary systems.

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MS32

Contact and Transmission in Epidemiological Models

The mechanisms of contact leading to the transmission of pathogens from one host to another in a population shape the dynamics of an epidemic. Despite major modeling efforts at the population level in epidemiology; the mechanisms of contact and transmission remain poorly understood and their modeling remain typically rooted in models describing mixing of particles in homogeneous baths. Here, we discuss how a combination of theoretical and experimental approaches can be used to start reformulating the fundamental definitions and formulations of contact and transmission between hosts in a population.

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MS32

Economic Evaluation of the Fungal Meningitis Outbreak Response in New River Valley: Local Health Department and Clinical Perspectives

The objective of this study is to conduct an economic evaluation of the fungal meningitis outbreak response in New River Valley of Virginia from the local public health department and clinical perspectives. The multi-state fungal meningitis outbreak started during September 2012 in Tennessee. The immediate cause of the outbreak was injection of contaminated lots of methylprednisolone acetate used in epidural steroid injections. Roanoke and New River Valley were the epicenter of this outbreak in Virginia, with two clinical centers having administered the contaminated injections to their patients. New River Health District and local hospitals deployed their resources to control the regional impact of the outbreak, starting in October 2012. Public health personnel, in collaboration with clinicians in local hospitals, followed up the exposed patients for 6 months, and provided treatment including lab tests and hospitalizations. The health department continued the outbreak investigation until March 2013 to ascertain that all possible cases were identified and treated. None of the followed-up patients met the case definition, as defined by CDC. Based on preliminary analysis, the local health department expenditure is estimated to be $30,493 and 73.5 years of disability adjusted life years are averted among the patients, for an incremental cost-effectiveness ratio of $415 per disability adjusted life year averted. The estimated incremental cost effectiveness ratio assists the local health department to prioritize and allocate limited public health resources. We are currently extending the analysis to include the clinical perspective.

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MS32

Mathematical Modeling of Cholera

Cholera was one of the most feared diseases in the 19th century, and remains a serious public health concern today. It can be transmitted to humans directly by person-to-person contact or indirectly through ingestion of contaminated water. Basic cholera models that include both direct and indirect transmission and assume homogeneous mixing in the host population will be reviewed. Detailed models that incorporate spatial heterogeneity will be applied to understand cholera transmission and to evaluate disease control strategies.

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MS32

Modeling Cholera in Heterogeneous Environments

We present some recent work in mathematical modeling of cholera, a severe water-borne infectious disease. Particularly, we discuss the impacts of spatial heterogeneity and seasonal variation on the transmission dynamics of cholera, using both mathematical analysis and numerical simulation. Based on a deterministic modeling framework that involves systems of ODEs and PDEs, we establish results of disease extinction and persistence for each model, and compare the threshold dynamics in homogeneous and heterogeneous settings.

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MS33

Convergence Properties of Gauss-Newton Methods, Well-Posedness of Parameter Estimation Problems and the Reliability of Parameter Estimates

Parameter estimation from measurement data is crucial for model validation. After computing of the estimates the question arises about their reliability. It appears that reliability of the estimates is connected to a convergence rate of Gauss-Newton methods which present good local convergence in so-called small residual problems. We show that bad performance of Gauss-Newton in large residual problems is an advantage rather than a disadvantage of the method, since it indicates ill-posedness of problems.

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MS33

Parameter Estimation for Large-Scale Biological Systems

As scientists continue to make discoveries in the biological sciences, the dynamical systems they are studying continue to grow in size and complexity. These increases make model fitting and parameter estimation more difficult. Hence, the effectiveness and efficiency of such techniques are crucial. This presentation shares a new parameter estimation technique designed to address some of the issues presented by large-scale biological systems by taking advantage of the sparsity often present in such systems.

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MS33

Removing Irrelevant Parameters from Complex Biological Models

Parameter inference in biological sytems often results in estimates with huge uncertainties. I discuss how these irrelevant parameter combinations can be systematically removed to reveal relevant combinations that govern the collective system behavior and can be accurately inferred from data. Using an information geometric approach, I recast the model reduction problem as a manifold approximation problem. The coarse-grained models vividly illustrate the emergent control mechanisms (e.g. feedback loops) that govern the system's behavior.

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MS33

Beyond Acceptable Parameter Fits

Biological time series contain enormous, but hidden information that needs to be extracted with computational means. This extraction is difficult, due to noise, large numbers of parameters, and computational issues. Furthermore, the typical criterion of squared residual errors is often insufficient, especially if the best-suited functional forms for describing the biological system are not known. The structural uncertainty complicates any estimation, but can be ameliorated if the right types of time series data are available.

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MS34

Effect of Intraocular Pressure and Arterial Blood Pressure on Oxygen Saturation Levels in the Retina: a Theoretical Model

Impaired oxygen delivery to the retina has been shown to contribute to the retinal cell death characteristic of glaucoma. A mathematical model is used to predict retinal oxygen saturation as intraocular pressure (IOP) and mean arterial pressure (MAP) are varied. Model predictions suggest that oximetry data from patients are not sufficient for distinguishing between the factors that alter saturation levels, since nearly identical venous saturation levels are predicted for various combinations of MAP and IOP.

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MS34

Computational Modeling of Oxygen and ATP Transport in Skeletal Muscle Capillary Networks of Normal and Pre-Diabetic Rats

In skeletal muscle, capillaries are responsible for delivering oxygen and are involved in regulating the oxygen supply to meet tissue needs. A key mechanism in this regulation is oxygen-dependent release by red blood cells of the signaling molecule ATP, leading to changes in upstream arteriolar resistance and hence blood flow. We present an experiment-based model of oxygen and ATP transport in 3D capillary networks showing how oxygen delivery and RBC ATP-based regulation are disturbed in pre-diabetes.

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MS34

Green's Function Methods for Simulating Solute Transport in the Microcirculation

Delivery of oxygen and other solutes to tissue is an essential function of the microcirculation, and is critically dependent on the spatial arrangement of microvessels. For numerical simulations involving realistic three-dimensional vascular network geometries, Greens function methods are more computationally efficient than finite-difference or finite-element methods, and are also advantageous with regard to the imposition of appropriate boundary conditions. Steady-state and time-dependent formulations will be presented and applications to several tissue types will be discussed.

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MS35

Nonlinear Poisson-Nernst-Planck Equations for Ion Flux Through Confined Geometries

The mathematical modelling and simulation of ion transport trough biological and synthetic channels is a challenging problem since at least two major effects have to be taken into account: the electrostatic interaction of ions and

the effects due to size exclusion in narrow regions. We investigate an important modification of the Poisson-Nernst-Planck (PNP) equations due to size exclusion, which is derived from a self-consisted random walk. Next we discuss the stationary solutions as well as the computation of conductance. The need of incorporating nonlinear mobilities in high density situations is demonstrated in an investigation of conductance as a function of bath concentrations, which does not lead to obvious saturation effects in the case of linear mobility.

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MS35

New Effective Finite Element Algorithms for Solving Local and Nonlocal Poisson-Boltzmann Equations for Biomolecules in Ionic Solvent

Calculation of electrostatic potential energy for biomolecule (such as protein and DNA) in ionic solvent is a fundamental task in computational biology. To reflect the polarization correlations among water molecules, nonlocal dielectric models were studied in the last thirty years, but only limited to the case of pure water solvent due to modeling and algorithmic difficulties. We recently overcome such difficulties and proposed a new nonlocal dielectric model for protein in ionic solvent, together with a fast finite element solver and an effective program package. In this talk, I will give these new progresses a short review. Specifically, a new nonlocal and nonlinear Poisson-Boltzmann Equation (PBE) model will be discussed in details. Since our nonlocal PBE model includes the classic local PBE model as a special case, our new finite element program package works efficiently and effectively not only for our nonlocal PBE model but also for the local PBE model. This project is a joined work with Prof. L. Ridgway Scott at the University of Chicago under the support by NSF grants (DMS-0921004, DMS-1226259, and DMS-1226019) and the UWM Research Growth Initiative.

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MS35

Fluctuation and Fidelity Control of Single Transcriptional Machine

Polymerases catalyze gene replication and transcription. We investigated how polymerases achieve high fidelity efficiently by stepwise nucleotide selection. We noticed that early selections outperform the late ones in error reduction, while initial screening seems indispensable for maintaining speed. We studied T7 RNA polymerase in atomistic simulations, and found that substantial nucleotide selection happens prior to full insertion of the nucleotide for Watson-Crick base pairing. Our studies provide a kinetic framework along with molecular mechanisms.

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MS35

Fast Pseudo-Time Simulations of the Nonlinear Poisson-Boltzmann (NPB) Equation

Recently, we have developed a pseudo-time approach for solving the NPB equation. In the operator splitting framework, an analytical integration is conducted to suppress the nonlinear instability, and central differences are designed for both sharp and diffused molecular surfaces. Various time splitting schemes that reduce 3D linear systems into 1D ones, such as ADI, LOD, and AOS, have been examined for unconditional stability, accuracy, and efficiency so that a fast NPB solver can be built for biomolecular simulations of large proteins.

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MS36

Swimming Through Heterogeneous Networks

I will present results for swimmers moving near similar-size microstructural heterogeneities. First, spherical obstructions are used to deduce physical principles linking the swimmer flow field, forces on obstructions, and changes in swimming velocities. Then single rod-like obstructions are studied which are similar to the filaments of networks. Using these results, we deduce the effect of a network of filaments. Notably, swimming properties such as the variance of the swimming speed reflect the density and orientation correlations of the microstructure, and hence swimming properties can be used as probes of microstructure.

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MS36

An Active Polar Nematic Model of Microtubule/motor-Protein Assemblies

We develop a multiscale theory for a class of "bioactive' materials consisting of microtubules and motor-proteins. Brownian dynamics simulations are used to study microscopic organization and identifies two sources of active destabilizing stress: polarity-sorting and crosslink relaxation. A Doi-Onsager theory captures polarity sorting, and the hydrodynamic flows generated by active stresses. In simulating experiments of active flows on immersed surfaces, the model exhibits turbulent-like flows and generation and annihilation of disclination defects.

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MS36

An Immersed Boundary Method for Two-fluid Mixtures

We present an Immersed Boundary method for interactions between elastic boundaries and mixtures of two fluids. A penalty method is used to enforce the condition that both fluids' velocities agree with that of the elastic boundaries. The method is applied to several problems: Taylor's swimming sheet problem for a mixture of two viscous fluids, peristaltic pumping of a mixture of two viscous fluids, with and without immersed particles, and peristaltic pumping of a mixture of a viscous fluid and a viscoelastic fluid. Numerical results demonstrate that the method converges and show its capability to handle a number of flow problems of substantial current interest.

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MS36

Computational Models of Cilia and Flagella in a Brinkman Fluid

The interaction between dynamic elastic structures and their surrounding fluid is important for sperm navigation and cilia beating within airways. We study a generalized Euler elastica immersed in a Brinkman fluid, a viscous fluid filled with a network of proteins. Regularized Greens functions for Brinkman flow are used to investigate emergent dynamics with preferred kinematics. Results are presented for swimming speeds, synchronization, and efficiency of flagella with planar waveforms in a Brinkman fluid.

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MS37

Linear Currents Can Be Pacemaker Currents

Regenerative currents necessary for production of oscillatory activity are inward voltage-gated currents. I will show that voltage-dependence is not required. A linear current with negative conductance plus a voltage-gated recovery current are sufficient. We will discuss conditions that these currents need to satisfy for oscillations to be produced, and will provide biological examples of oscillations generated by such linear inward currents. The stabilizing role that hyperpolarization-activated inward currents may play will also be discussed.

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MS37

Robustness and Multifunctionality of Reduced CPG Models

CPGs stably produce bursting patterns underling vital rhythmic behaviors. We developed analytical and computational tools reducing the problem of robustness and existence of rhythmic patterns to analysis of attractors in return maps for phase lags between bursters. We identify organizing centers determining CPG outputs and analyze their bifurcations as network circuitry varies. We study sustainability of networks by revealing statistics of rhythms switching due to random perturbations. Our findings are applicable for most oscillatory networks.

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MS37

Differential Effects of Conductances on Pyloric CPG Output

Central pattern generators are neuronal circuits that control rhythmic activities such as breathing and chewing. The output of such circuits can be characterized with relative ease, making them good candidates for studying regulation of neuronal activity at the network and single-cell levels. Our recent work characterizes the effect of specific conductances on the activity of the pacemaker kernel in the pyloric circuit of the crustacean stomatogastric ganglion through a series of computational and electrophysiological studies.

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MS37

Identifying and Explaining Three Time Scale Oscillations

CPGs may exhibit behavior, including bursting, involving multiple distinct time scales. Our goal is to understand bursting dynamics in three-time-scale systems, motivated by a model from respiratory CPG neuron. Using geometric singular perturbation theory, we explain the mechanisms underlying some forms of bursting dynamics in a three-

time-scale model. To elucidate which characteristics truly represent three-time-scale features, we investigate certain reductions to two time scales and the parameter dependence of solution features in the three-time-scale framework.

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MS38

Translational Modeling and Optimal Concurrent Treatment in Oncology

Neutropenia caused by the indiscriminate nature of anticancer drugs is a dose-limiting consequence of chemotherapy which necessitates treatment adaptation. To avoid therapy interruption, granulocyte colony-stimulating factor (G-CSF) is administered during chemotherapy. This talk will outline the development of physiologically-based mathematical models of myelopoiesis in conjunction with pharmacokinetic and pharmacodynamic models of zalypsis and filgrastim, and address their use in the optimisation of chemotherapeutic regimens with G-CSF.

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MS38

Systems Pharmacology: Revolutionizing Health Care One Equation at a Time

Similar challenges and questions arise in both the mathematical and pharmaceutical sciences. Unfortunately, differences in culture and approach sometime blur our common goal: Improving the health and well being of patients. This talk will discuss opportunities within the developmental pipeline where significant contributions can be made by classically trained mathematicians. We will address the unique challenges that pharmaceutical companies face within a highly regulated world and specific areas of greatest need. Novel and symbiotic research opportunities await those with the tools and vision for exploration in this interface where a systems approach to pharmacology is increasingly necessary.

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MS39

Elimination of Intermediate Species in the Stochastic Reaction Networks

Biochemical reactions often proceed through the formation of intermediate species. These species are transient species, such as the substrate-enzyme complex appearing in Michaelis-Menten kinetics. For the sake of simplicity the intermediates are often ignored in the description of a reaction network, especially when they happen to be more unstable than the other species and they are degraded at a fast rate. It is not clear, however, whether this simplification can have consequences on the reliability of the model. We focus on stochastically modeled reaction networks and provide a rigorous asymptotic result for the elimination of the eventual intermediate species from the model. In our settings the intermediate species can only appear alone and with unitary stoichiometric coefficient in any reaction involving them. We define a suitable reduced system and we prove that the complete system tends to the reduced one in finite dimensional distribution when the rates of consumption of the intermediate species tend to zero. Further we show that our reduced system coincide with one obtained before in the deterministic settings, where the the number of equilibrium points were studied. Moreover, we extend our results to the situation when the non-intermediate species are described by a single scaled system. We only add the assumption that the rates of the intermediate consumption tend to infinity fast enough compared to the rates of their production.

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MS39

Perturbations of the Lotka-Volterra System

We explore certain large perturbations of the Lotka-Volterra system, and show that they retain persistence, and even periodicity. This is an exploration of how persistence is affected by a reaction network not being endotactic.

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MS39

Bistability in the Dual Futile Cyle

The idea has been around for some years that the system consisting of two successive phosphorylation/dephosphorylation loops exhibits bistability and on the level of heuristic and numerical investigations this can be seen as well-established. After surveying the existing results I will present a purely analytical proof (obtained together with Juliette Hell) that there exist parameter values for which this system has two stable stationary solutions. The methods used are bifurcation theory and geometric singular perturbation theory. I will then go on to discuss possible generalizations to a larger number of loops and to more complicated systems such as those modelling the MAP kinase cascade.

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MS39

Reaction-Diffusion Equations With Periodic Behavior

We consider the Lotka-Volterra model and the Ivanova reaction. The ODE equations have explicit periodic solutions and equilibrium points. With equal diffusion rates, we give conditions for a solution to converge to a spatially homogeneous periodic solution.

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MS40

On a Diffusive Predator-prey Model with Nonlinear Harvesting

In this talk, we study the dynamics of a diffusive Leslie-Gower model with a nonlinear harvesting term on the prey. We analyze the existence of positive equilibria and their dynamical behaviors. In particular, we consider the model with a weak harvesting term and find the conditions for the local and global asymptotic stability of the interior equilibrium. The global stability is established by considering a proper Lyapunov function. In contrast, the model with strong harvesting term has two interior equilibriums and bistability may occur for this system. We also give the conditions of Turing instability and perform a series of numerical simulations and find that the model exhibits complex patterns.

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MS40

Evolutionary Dynamics of a Population Model with Component Allee Effects

We investigate the evolutionary outcomes of a single species prey population subject to component Allee effects within the framework of a continuous strategy evolutionary game theory (EGT) model. Our model assumes a single trait creates a phenotypic trade-off between carrying capacity and predator evasion ability following a Gaussian distribution. This assumption contributes to one of our interesting findings that evolution prevents extinction even when the population is subject to strong Allee effects. However, the extinction equilibrium can be an ESS under some special distributions of anti-predation phenotypes. The ratio of variation in competition and anti-predation phenotypes play an important role in determining the global dynamics of our EGT model: (a) evolution may suppress strong Allee effects for large values of this ratio; (b) evolution may preserve strong Allee effects for small values of this ratio; and (c) intermediate values of this ratio can result in multiple ESSs.

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MS40

An Application of Optimal Control Theory to a Simple Age-of-Infection Sir Model

Abstract not available at time of publication.

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MS41

Form-Function Relationship in E. coli Chemotaxis

Cell-to-cell variations in protein abundance in clonal cell populations are ubiquitous in living systems. Because protein composition determines responses in individual cells, it stands to reason that the variations themselves are subject to selective pressures. However, the functional role of these cell-to-cell differences is not well understood. One way to tackle questions regarding relationships between form and function is to perturb the form (e.g., change the protein abundances) and observe the resulting changes in some function. We take on the form-function relationship from the inverse perspective, asking instead what specific constraints on cell-to-cell variations in protein abundance are imposed by a given functional phenotype [1]. We develop a maximum entropy based approach to posing questions of this type and illustrate the method by application to the well-characterized chemotactic response in *Escherichia coli*. We find that full determination of observed cell-to-cell variations in protein abundances is not inherent in chemotaxis itself but, in fact, appears to be jointly imposed by the chemotaxis program in conjunction with other factors (e.g., the protein synthesis machinery and/or additional non-chemotactic cell functions, such as cell metabolism). These results illustrate the power of maximum entropy as a tool for the investigation of relationships between biological form and function. [1] Sayak Mukherjee, Sang-Cheol Seok, Veronica J. Vieland, and Jayajit Das, Proceedings of National Academy of Sciences **110** 18531 (2013).

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MS41

From Single Molecule Experiments to Coupled Molecules

Molecular motors convert chemical energy, often stored in the form of ATP, into mechanical energy, a vital activity for living cells. In particular, kinesin and dynein are two molecular motors that convey cargo, such as vesicles and organelles, along microtubules to where they are needed in the cell. This is especially important in neurons which can be up to a meter in length and where a breakdown in motor function has been implicated as a factor in neurodegenerative diseases. Since the early 1990's, experimentalists have been manipulating single motor molecules in vitro using laser traps. This has allowed detailed mechanical information to be gathered from isolated motors, at least in these non-physiological experimental conditions. In living cells, however, a single motor does not move a single cargo. Multiple motors, possibly both kinesin and dynein each biased towards opposite directions, are attached to a single cargo transporting it along the microtubule. A number of questions arise. How do different motors with opposing biases transport the cargo? How are cargos transported to the appropriate locations within the cells? Are there important regulatory proteins which affect this transport process? In this talk, we will discuss data emerging from these multi-motor/single cargo experiments and how information from single molecule experiments can be incorporated into the multi-motor analysis. In addition, we will discuss how these experiments can inform us about the underlying mechanisms which drive this multi-motor transport phenomena using a combination of stochastic models and statistical inference.

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MS41

Estimating Velocity for Processive Motor Proteins with Random Detachment

Processive motor proteins are ATP-powered biological nanomachines that drive many forms of movement in living organisms. For example, kinesin and cytoplasmic dynein motors transport payloads, such as organelles or vesicles, through the cytoplasm of eukaryotic cells. The existence of eukaryotic organisms depends on these tiny motors because the passive process of diffusion is not sufficient to transport large and/or massive payloads through the crowded cytoplasm in a timely fashion. A motor protein overcomes these difficulties by hydrolyzing ATP in order to tow a cargo rapidly and in a directed path along a suitable substrate. An understanding of these motors could lead to important biomedical applications, e.g., anti-tumor technologies; treatments for neurodegenerative diseases; devices for blood testing and genetic screening; and treatments for diseases caused by motor protein defects. We show that, for a wide range of models, the empirical velocity of processive motor proteins has a limiting Pearson type VII distribution with finite mean but infinite variance. We develop maximum likelihood inference for this Pearson type VII distribution. In two simulation studies, we compare the performance of our MLE with the performance of standard Students t-based inference. The studies show that incorrectly assuming normality (1) can lead to imprecise inference regarding motor velocity in the one-sample case, and (2) can significantly reduce power in the two-sample case. These results should be of interest to experimentalists who wish to engineer motors possessing specific functional characteristics.

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MS41

Superresolution Microscopy As a Quantitative Tool

Protein-protein interaction is the basis for all of communication and information transfer in biology. Nonetheless, protein complexes –the basic interaction subunit– are difficult to image in living cells because of their size (tens of nm). Superresolution imaging methods are now commonly used to generate high resolution images of biological features about 10-100nm in size. We describe a strategy for turning superresolution imaging data into a quantitative tool to enumerate proteins in a complex.

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MS42

A Computational Method for Nearly Singular Integrals

We will describe a realtively simple method for computing singular or nearly singular integrals on a closed curve in 2D or a closed surface in 3D. This method can be used for Stokes flow, e.g., if values of velocity and pressure are needed at regular grid points. In work with Anita Layton, we have used this approach for a moving elastic interface in 2D Stokes flow. We have also devised a second-order accurate method for Navier-Stokes flow coupled with an interface, in which the velocity is decomposed into a Stokes velocity and a more regular part. The advantage is that the interaction of the interface with Stokes flow is much simpler to deal with than the full Navier-Stokes equations. Partially implicit motion of the interface can be used in either case to improve the time step.

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MS42

A Treecode-Accelerated Boundary Integral PoissonBoltzmann Solver for Electrostatics of Solvated Biomolecules

We present a treecode-accelerated boundary integral (TABI) solver for electrostatics of solvated biomolecules described by the linear Poisson-Boltzmann equation. The method employs a well-conditioned boundary integral formulation for the electrostatic potential and its normal derivative on the molecular surface.. The surface is triangulated and the integral equations are discretized by centroid collocation. The linear system is solved by GMRES iteration and the matrix-vector product is carried out by a Cartesian treecode which reduces the cost from $O(N^2)$ to $O(N \log N)$, where N is the number of faces in the triangulation. We find that the TABI solver exhibits good serial and parallel performance combined with relatively

simple implementation, efficient memory usage, and geometric adaptability.

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MS42

On a Parallel Adaptive Fast Multipole Poisson-Boltzmann Solver

In this talk, I will present the mathematical analysis, numerical algorithms, and parallel implementation details of the Adaptive Fast Multipole Poisson-Boltzmann (AFMPB) solver. The package is available under open source license agreement.

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MS42

Surface-Tension Molecular Surfaces for Deployment in Boundary Element Electrostatic Calculations

Molecular surface generators that define the surface by a rolling probe inevitably produce regions with cusps and points, and are not suitable for BEM applications. The SMART algorithm was developed in our laboratory to avoid these issues with a guaranteed continuous surface normal. As an alternative to the rolling-probe approach, we have begun to explore physics-based surfaces whose results will be discussed, along with a new BEM implementation developed to handle large macromolecules.

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MS43

Physiological Modeling in Hypertension and Heart Failure

In this talk, we present the application of a fluid mechanics model in drug development. The model is a cardiovascular circulation model which has enabled decisions on compounds in development. The circulation model integrates systemic, pulmonary and cardiac function, and is fit for the purpose of assessing questions arising in heart failure and hypertension drug development. In this presentation, we provide a description of the circulation model, and demonstrate its utility through some examples.

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MS43

A Coupled Model of the Left Ventricle and the Systemic Arteries

A three-dimensional finite-strain model of a human left ventricle is coupled with a one-dimensional physiologically-based structured-tree model of the systemic arteries by matching the pressure and flow rate at the aortic root. The governing equations, which also incorporate fluid-structure interaction and active contraction of the myocardium, are solved using a combined immersed-boundary finite-element method, and a Lax–Wendroff scheme. The effects of changes in vascular compliance and rarefaction on blood pressure and flow are studied.

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MS43

Comparison of Inflow Boundary Conditions for Ventriculo-Arterial Coupling in 3D and 1D Fluid-Structure Interaction Models

Each cardiac cycle the heart contracts and ejects blood into the systemic circulation. Coupled via the aortic

root, cardiac output into the systemic circulation is governed by both ventricular contractility and haemodynamic impedance of the systemic vasculature. Following a reduced-order coupling approach, a 0D model of cardiac contraction was implemented in 3D and 1D fluid-structure interaction frameworks. Using such models permits the examination of pressure wave propagation under altered physiological states of the heart.

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MS43

Pulsatile Flow in the Entire Coronary Arterial Tree

The hemodynamic analysis, based on the experimental measurements, plays an important role in the study of coronary circulation given millions of blood vessels in the vasculature. Here, I will show a mathematical model of pulsatile blood flow in the entire coronary arterial tree that is reconstructed from the measured morphometric data. The pathological states (i.e., left ventricular hypotrophy and congestive heart failure) are studied in relation to changes in model parameters and tree structures.

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MS44

Modeling Interindividual Differences in Spontaneous Internal Desynchrony Patterns

Using a physiological model of a sleep-wake regulatory network, we investigated the transition from typical human sleep patterns to spontaneous internal desynchrony. The model describes the neurotransmitter-mediated interactions among neuronal populations that promote wake, REM sleep and non-REM sleep, and the circadian pacemaker in the SCN. Model analysis suggests that similar mechanisms underlie different desynchronized behaviors, and that synchronization of sleep and circadian rhythms may depend on SCN modulation of REM sleep-promoting centers.

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MS44

A Mathematical Model of the Wake/NonREM/REM States

We propose a mathematical model for REM/NonREM dynamics with sleep/wake cycling that illustrates several features observed in humans during sleep. These include first falling into the NonREM stage, oscillating between it and the REM stage during the sleep period, and having four or five REM bouts which become longer as the night progresses. This model is motivated by one presented by previous authors and is constructed using known neuronal groups involved with sleep and wake.

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MS44

Spiking Neuron Vs. Neural Mass Models in the Context of Sleep-Regulatory Circuits

Neural populations can be abstracted in different ways. Neural mass models assign macroscopic state variables to each neural population, whereas spiking neuron models simulate the dynamics of individual neurons. Both types of models are widely used, but it is not always clear under what conditions the two agree when it comes to predicting dynamics of real physiological systems. Here, we consider this problem in the context of sleep-regulatory circuits.

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MS44

Modeling the Effects of Temperature on Sleep Patterns

Several studies have been done on human patients that suggest that different temperatures, such as room temperature, core body temperature, and distal skin temperature, have an important effect on sleep patterns, such as length and frequency of REM cycles. A mathematical model is created to investigate the effects of temperature on the

REM/NonREM dynamics. Our model was based on previous well established and accepted models of sleep dynamics and thermoregulation models.

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MS45

Disentangling Protein Fitness Requirements Using Computational Mutagenesis

Although methods in comparative sequence analysis can measure conservation within a protein family, purely sequence-based methods cannot elucidate the reasons underlying conservation. To deconvolve the multiple roles of amino acids in protein fitness, we have adapted computational protein design algorithms for efficient large-scale mutagenesis, and compare this to alternative in silico modeling approaches. Our method is applied to a G-protein heterotrimer, and provides insight on amino-acid involvement in structural stability, and ligand- or protein-binding interactions.

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MS45

A Mechanistic Model of the Bacterial Flagellar Motor

The bacterial flagellar motor (BFM) drives swimming in many bacterial species. Using structural information from recent experiments, we propose a mechanism for the BFMs conversion of transmembrane ion potential into torque. We also address how the motor reverses the torque direction, allowing bacteria to reorient during chemotaxis. Additionally, we suggest a "mechanical homology" between the BFM and the only other known protein motor driven by a transmembrane ion potential: the Fo motor of ATP synthase.

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MS45

Decoding Information in Cell Shape

Shape is an indicator of cell health. But how is the information in shape decoded? We hypothesize that decoding occurs by modulation of signaling through changes in plasma membrane curvature. Using analytical approaches and numerical simulations, we studied how elongation of cell shape affects plasma membrane signaling. Mathematical analyses reveal transient accumulation of activated receptors at regions of higher curvature with increasing cell eccentricity. In this talk, I will discuss the applicability of reaction-diffusion formulations in understanding the role of cell shape.

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MS45

Conserved Enhancer Function When Sequence Is Not Conserved: Adventures with Cis-Regulatory Logic

The blastoderm stage of *Drosophila* development affords unique advantages for the study of transcriptional control. The embryo can be used as a microarray in which the response of reporters to transcription factors can be quantitatively monitored at cellular resolution. With this data, we have constructed quantitative and predictive models of transcriptional control that shed light on the apparent paradox that conserved gene expression can be driven by highly diverged regulatory sequence.

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MS46

From Within-Host to Between-Host Dynamics. Systems Biology of Epidemiology

This talk explores an alternate mechanistic formulation of epidemiological dynamics based upon studying the influence of within-host dynamics in environmental transmission. A basic propagation number is calculated from the host-pathogen interaction; such quantification takes into account antigenic diversity and antigenic variation, and could guide public health policy.

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MS46

Modeling Drug Resistance in Metastatic Cancers

The development of drug resistance is a major challenge in the treatment of cancer. In this talk we will overview our recent results on studying the role of cell density and mutations on the dynamics of drug resistance in metastatic cancers. This is a joint work with Jim Greene, Orit Lavi, and Michael Gottesman.

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MS46

The Impact of Decay in BedNet Efficacy over Time on Malaria Transmission

Insecticide-treated nets (ITNs) are at the forefront of malaria control programs. The potential impact of ITNs on reducing malaria transmission is limited due to inconsistent or improper use, as well as decay in effectiveness. We develop a mathematical model for malaria spread that captures the decrease in ITN effectiveness. We perform uncertainty and sensitivity analyses to identify and rank parameters that play a critical role in malaria transmission. These analyses show that the basic reproduction number R0, and the infectious human population are most sensitive to bed-net coverage and the biting rate of mosquitoes. We consider the case in which ITN efficacy is constant over time as well as the case in which ITN efficacy decays over time.

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MS46

Vector Dynamics and Its Impact on the Vector Borne Disease-Malaria

Mathematical models have extended our understanding of the biology and transmission dynamics of the vector borne disease malaria, dating back to the models of Sir Ronald Ross and George Macdonald. However, most models either treat the mosquito population density as a constant or do not model the reproductive gains that accrue to the mosquito's population as a result of its lifestyle, feeding and reproductive habits, as well as its interaction with the human population. The interaction between mosquitoes and humans introduce high variability in the mosquito population density and this variability affects both the mosquito population and the disease dynamics. Using a mathematical model, I will highlight how the lifestyle of the *Anopheles* mosquito and the interaction between the mosquito and humans affect malaria transmission dynamics and introduce complexities not previously observed in unforced continuous time models. Implications for disease control will also be discussed.

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MS47

A New Mathematical Model for Hepatitis C Infection: Derivation, Analysis and Implications

The hepatitis C virus was first identified in 1989 and mathematical models for HCV infection followed within a decade. Since then, many models have been proposed. Biological knowledge regarding HCV has also progressed recently and we use this to derive a new model of HCV infection. We analyse the steady states and bifurcations in this model and show how the solutions differ from those of other models. We then consider the implications for HCV treatment.

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MS47

Mathematical Modeling of Malignant Brain Tumor with T11 Target Structure As a Potent Immune Stimulator.

T11 Target structure, a membrane glycoprotein isolated from sheep erythrocytes, reverses the immune suppressed state of brain tumor induced animals by boosting the functional status of the immune cells. This study aims at aiding in the design of more efficacious brain tumor therapies with T11 target structure as a potent immune stimulator. We propose a mathematical model for brain tumor (glioma) and the immune system (microglial cells, cytotoxic T lymphocytes, TGF-β, IFN-γ) interactions, which aims in designing efficacious brain tumor therapy. The system undergoes sensitivity analysis, that determines which state variables are sensitive to the given parameters and the parameters are estimated from the published data. Computer simulations were used for model verification, which highlight the importance of T11 target structure in brain tumor therapy.

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MS47

Parameter Subset Selection and Generalized Sensitivities for a Model of Erythropoiesis

We present a model for erythropoiesis involving structured population models for the various cell stages involved. Since the model involves around 30 parameters and only limited data are available, it is necessary to investigate which parameters can be estimated with reasonable accuracy and how the collection of data can be improved within the given limitations. We show how recently devel-

oped methods for parameter subset selection and generalized sensitivity analysis can be applied.

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MS47

Deconvolution of Isotope Signals Mixed from Sampling Bundles of Multiple Hairs

Hair records temporal information of body chemical signals, including stable isotopes. Multiple hairs are typically combined into a bundle to obtain enough material for analysis by segmentation. We developed a mathematical model to describe signal averaging from combining multiple hairs for analysis and an inverse method to estimate the original signal from measurements. The inverse method provides a refined interpretation of an oxygen stable isotope chronology from hair of an unidentified murder victim.

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MS48

Competitive Geometric Evolution of Lipid Bilayers and Pores

We discuss the competitive geometric evolution of co-existing complex structures in amphiphilic mixtures, modeled by the functionalized Cahn-Hilliard (FCH) equation. The system supports lipid bilayers, filamentous pores, micelles, and complex network structures. We analyze the geometric evolution laws of bilayers and pores, respectively, the mechanism under which they compete, and the possibility of co-existence.

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MS48

Continuum Models of Membrane Protein Insertion and Stability

Experimental and computational studies have shown that cellular membranes deform to stabilize the inclusion of transmembrane (TM) proteins harboring charge. Recent analysis suggests that membrane bending helps to expose charged and polar residues to the aqueous environment and polar head groups. We previously used elasticity theory to identify membrane distortions that minimize the insertion of charged TM peptides into the membrane. Here, we extend our work to consider the energetics of ion and small peptide penetration into the membrane as well as large protein complexes. First, we show that our continuum method accurately reproduces energy profiles and membrane shapes generated from molecular simulations of bare ion permeation at a fraction of the computational cost. Importantly, we find that the energetics of membrane deformation strongly depend on membrane patch size both for ions and peptides. Finally, we present experimental and theoretical analysis that suggests that the antibacterial protein RegIIIa, a C-type lectin, forms channel like complexes that disrupt cellular homeostasis by inserting into membranes containing anionic lipids. We believe that our work presents a novel, computationally efficient method to simulate the effects of small molecules, peptides and large complexes with the membrane.

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MS48

On Minimizers of the Bending Energy of Two-Phase Biomembranes

We consider the problem to find the shape of multiphase biomembranes, modeled as closed surfaces enclosing a fixed volume and having fixed surface area. The surface energy is assumed to be the sum of two terms: the Canham-Helfrich energy, in which the bending rigidities and spontaneous curvatures depend on the phase, and a line tension penalization for the phases interface. By restricting attention to axisymmetric surfaces and phase distributions, we prove existence of a global minimizer. This is a joint work with Rustum Choksi (McGill University, Montreal) and Marco Morandotti (Instituto Superior Tecnico, Lisbona).

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MS48

Periodic Migration in a Physical Model of Cells on Micropatterns

We extend a model for the morphology and dynamics of a crawling eukaryotic cell to describe cells on micropatterned substrates. This model couples cell morphology, adhesion, and cytoskeletal flow in response to active stresses induced by actin and myosin. We propose that protrusive stresses are only generated where the cell adheres, leading to the cell's effective confinement to the pattern. Consistent with experimental results, simulated cells exhibit a

broad range of behaviors, including steady motion, turning, bipedal motion, and periodic migration, in which the cell crawls persistently in one direction before reversing periodically. We show that periodic motion emerges naturally from the coupling of cell polarization to cell shape by reducing the model to a simplified one-dimensional form that can be understood analytically. Additionally, we will discuss a turning instability arising from our model applying onto a free moving cell without interaction with the micropatterned substrates. Some attempts have made to test how the instability depends on the parameters in the model numerically. For a much simplified model, we do find that surface tension is a key factor to stabilize the cell turning.

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MS49

Topological Tools for Detecting Hidden Geometric Structure in Neural Data

Experimental neuroscience is undergoing a period of rapid progress in the collection of neural activity and connectivity data. This promises to allow more direct testing of a variety of theoretical ideas, and thus advance our understanding of "how the brain works." Detecting meaningful structure in neural data, however, remains a significant challenge. A major obstacle is that these data often measure quantities that are related to more "fundamental" variables by an unknown nonlinear transformation. This transformation obscures the underlying structure, diminishing the power of traditional linear algebra-flavored tools. Methods from computational topology, however, are often capable of detecting the hidden structure. We adapt these methods for the analysis of correlation matrices, and illustrate their use for testing the "coding space" hypothesis on neural data.

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MS49

Topological Distances on DNA Knots and Links

Topoisomerases and recombinases are two classes of proteins which can knot circular DNA. Type II topoisomerases are proteins which cut one double-stranded DNA segment, allowing a second DNA segment to pass through before resealing the break. This is mathematically modeled by changing a crossing. Recombinases break two segments of DNA, exchanging the DNA ends before resealing the breaks. This action can be mathematically modeled by smoothing a crossing. Distances between knots have been defined based upon the minimum number of times these proteins must act to convert one knot into another knot. Methods for calculating these distances will be discussed. Applications and ways to visualize and analyze these distances via graphs and KnotPlot will be discussed.

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MS49

The Topological Structure of the Mitochondrial Dna from Trypanosomes

Trypanosomatid parasites are the cause of disease and death in many third world countries. One of the most unusual features of these organisms is the 3 dimensional organization of their mitochondrial DNA into maxi and minicircles. Here we investigate the effects of the confinement on the topology of the network using a simplified model where randomly oriented minicircles are placed on the plane with their centers on the vertices of the simple square lattice.

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MS49

Modeling Dna Packing with Confined Equilateral Random Polygons

We introduce and study a model of equilateral random polygons confined in a sphere. DNA packed in a virus head motivates this model. The difference between the biologically observed topological characteristics and benchmark data created by our model reveals the bias of DNA packed in the viral capsids and possibly lead to a better understanding of the DNA packing mechanism.

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MS50

Build-Up and Neural Competition in a Model of Auditory Streaming

A two-population rate model is built to study the perceptual organization of tones in the auditory cortex. When repetitive sequences of tones alternating between two frequencies are presented, the system's dynamics switches between two distinct states: (1) a coherent, galloping-like single stream ("integration"), and (2) two separate streams of constant pitch tones ("segregation"). The model accounts for the dynamics observed for such stimuli, in single unit recordings in monkey primary auditory cortex. The underlying mechanism for the build-up of the stream segregation is also investigated.

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MS50

Modelling the Emergence and Dynamics of Percep-

tual Organisation in Auditory Streaming

Auditory perception solves the problem of associating causes with sound events by switching between alternative solutions. I present a model of auditory scene analysis at the core of which is a process that seeks to discover predictable patterns in the ongoing sound sequence. Representations are created on the fly, and maintained, strengthened or weakened depending on predictive success and conflict with other representations. Auditory perceptual organisation emerges spontaneously through the competition between these representations.

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MS50

Bistable Auditory Perception: Neural Competition with Periodic Input

Spontaneous switches in perception occur for auditory stimuli where high A and low B tones are repeated in ABA- sequences [van Noorden 1975, Pressnitzer and Hupé 2006]. We extend a classical neural competition model to include periodic onset-like inputs and capture the parametric organisation of percepts reported in the psychoacoustics literature. We use the model to carry out a comparison study between bistability in auditory perception and other sensory modalities.

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MS50

Diagnosing Excitation-inhibition Balance using Psychophysics

Excitation-inhibition imbalance is a potential cause of mental illness such as Autism. It is useful to understand how such a perturbation may be manifested in psychophysical tests, such as perceptual rivalry. Here, I will discuss recent experimental and theoretical work that makes this connection explicit.

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MS51

Delay-Differential Equations in Cardiac Electrophysiology Models

In the heart, period-2 behavior of electrical responses, referred to as alternans, often gives rise to more complicated arrhythmias. To date, alternans has been generated mathematically from coupled nonlinear ODE/PDE systems. We use the fact that delays arise naturally in non-instantaneous cellular processes to suggest an alternative approach using delay-differential equations (DDEs), which are known to promote complex dynamics. We analyze the dynamical behaviors of our DDE system and discuss the implications of our findings.

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MS51

Experimentally-based Modified Cable Equation That Reproduces Alternans Measured in Cardiac Tissue

We incorporate a data-based model to regulate gap junction conductance by transjunction potentials into the cable equation. This modification results in a dynamic decrease of gap-junction conductance during the action potential (AP) plateau, which lowers coupling at high membrane potentials without altering AP restitution dynamics and conduction velocities. Inclusion of a voltage-dependent gap-junction conductance in the cable equation allows spatial alternans to develop in realistic tissue sizes without altering other predictions from the cable equation.

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MS51

Effects of Intracellular Sodium Accumulation on Cardiac Reentry Dynamics

The morphology and duration of cardiac action potentials is controlled partly by ionic currents that depend on intracellular sodium concentration. We demonstrate how the dynamics of cardiac reentry vary with intracellular sodium accumulation and how this plays a special role in simulated chronic atrial fibrillation.

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MS51

The Role of Feedback and Heart Rate Variability on Cardiac Rhythm Stability

Cardiac dynamics is usually analyzed under the assumption of periodic stimulation, i.e. in the presence of feedback. However, under physiological conditions, the heart rate exhibits substantial variations in time, known as heart rate variability (HRV), which introduces deviations from periodic stimulation. We incorporated HRV into pacing protocols, both with and without feedback, and investigated the role of HRV and feedback on rhythm stability using numerical simulations of an ionic model of the cardiac action potential.

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MS52

Stochastic Dynamics in Signal Transduction, Stem Cells, and Development Patterning

Abstract not available at time of publication.

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MS52

Mathematical Models for Stem Cell Interactions

Abstract not available at time of publication.

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MS52

Computation of Transition State and Its Applications in System Biology

Abstract not available at time of publication.

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MS52

Numerical Studies on Cell Lineage Models

Multistage cell lineages, typically comprising of a stem cell stage and several subsequent progenitor cell stages (also referred to as transit-amplifying or TA cells), underlie the production of different terminally differentiated (TD) cell types within a tissue. Genetic studies and tissue culture experiments have shown that control of stem and progenitor cell proliferation and differentiation, which ultimately control the TD cell number, is mediated by secreted morphogens through feedback regulation. In this talk, I shall present our recent work on using numerical simulations of advection-reaction-diffusion model to study the formation and regeneration of intestinal crypts, which is based on our early model on tissue stratification patterning of the olfactory epithelium of the mouse. This is a joint work with Tian Jiang (University of Notre Dame), Lei Zhang (Peking University), and Qing Nie (University of California, Irvine).

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MS53

Mathematical Model of Community-Acquired and Hospital-Acquired Methicillin-Resistant Staphylococcus Aureus Transmission in Hospital Settings

In this paper a deterministic model to quantifying the interactions of community-acquired and hospital-acquired methicillin-resistant staphylococcus aureus transmission in a hospital settings is developed. The model include environmental contaminants and isolation of colonized and infected patients. The reproduction number is determined and sensitivity analysis is carried out to determine the impact of model parameters to various outputs. The results of the stochastic version of the deterministic model is discussed.

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MS53

Optimizing Vaccine Allocation for Influenza

The emergence of the 2009 H1N1 influenza A strain and delays in production of vaccine against it illustrate the importance of optimizing vaccine allocation. We have developed computational optimization models to determine optimal vaccination strategies with regard to multiple objective functions: e.g. deaths, years of life lost, economic costs. Looking at single objectives, we have found that vaccinating children, who transmit most, is robustly selected as the optimal allocation. I will discuss ongoing extensions to this work to incorporate multiple objectives and uncertainty.

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MS53

Malaria Vaccine Efficacy in a Region with Naturally Acquired Immunity

The advent of malaria vaccines raises the question of how effective vaccination will be in regions with naturally acquired immunity (NAI). Our malaria model incorporating vaccination and NAI suggests that disproportionately treating non-immune individuals increases the likelihood of subthreshold endemic equilibria, a dangerous scenario that increases the risk for malaria epidemics and renders vaccination ineffective. Additionally, optimal control theory suggests that efforts to vaccinate should increase as the level of NAI in a population decreases.

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MS53

A Two-Patch Avian Influenza Model

Abstract not available at time of publication.

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MS54

Optimizing Hiv Treatment In a Resource Limited Settings

Antiretroviral drugs have a clinical benefit of substantially reducing infectiousness thus making them potentially an important strategy in the fight against AIDS. Recent advances in drug therapy have seen the use of antiretroviral medications as a prophylaxis. In this study, we constructed a compartmental heterosexual transmission model based on the dynamics of HIV in heterosexual population in Sub-Sahara. The model classifies the male and female populations by risk (low, medium and high) according to their sexual preferences. Data from South Africa was used to parameterize the model. For a finite amount of drugs we implemented a numerical optimization algorithm to find optimal allocation of the drugs that minimizes objective functions such as Total Number of Deaths and Total Number of Infections. Preliminary results suggest that, the priority should be given to the high-risk females during drug allocations to minimize the number of deaths or infection per year

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MS54

The Impact of Spatial Arrangements on Intervention Strategies in Epidemic Models

The role of spatial arrangements in a metapopulation on the spread and optimal intervention strategies of a cholera epidemic is investigated. We consider how human and pathogen movement affects the optimal vaccination strategy. For each patch, the model has an SIR system of differential equations coupled with an equation modeling the concentration of Vibrio cholerae in an aquatic reservoir. The model will be used to compare two basic spatial arrangements of populations along a water source. The work is motivated by the recent cholera outbreak in Haiti. Optimal control results are found numerically.

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MS54

Optimal Control and Analysis of a Coupled Ode/pde Immuno-Epidemiological Model

Optimal control can be used to design intervention strategies for the management of infectious diseases, and has been applied in immunological and epidemiological models separately. We formulate an immuno-epidemiological model of coupled within-host model of ODEs and between-host model of ODE and PDE. Existence and uniqueness of solution to the between-host model is established, and an explicit expression for the basic reproduction number of the between-host model is derived. Stability of disease-free and endemic equilibria of the between-host model is investigated. An optimal control problem with drug-treatment control on the within-host system is formulated and analyzed. Numerical simulations based on the forward-backward sweep method are obtained.

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MS54

Inferring Equation Models from Agent-Based Model Data

Abstract not available at time of publication.

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MS55

Numerical Simulations of Fluctuating Vesicles in Linear Flow

In this talk, we present the fluctuation dynamics of a 2D vesicle in extensional flow. In the quasi-circular limit, we derive a Langevin type SDEs. We then simulate a vesicle dynamics using an immersed boundary method, and achieve good agreement with the theoretical predictions for the equilibrium deformation correlations. Preliminary results show that thermal noise can change the characteristic wavelength of the wrinkles, and prevent the rotation of a tilted vesicle in extensional flow.

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MS55

Electromechanics of Bilayer Membrane: Forces and Fast Algorithms

Lipid bilayers appear ubiquitously in living systems. Defining and computing the forces on lipid membranes is critical to understanding how these systems operate. In this talk, the electrostatic potential energy for membrane-protein interactions is defined and used to compute the dielectric boundary force via the shape derivative. We then describe a fast algorithm for minimizing the electromechanical energy of vesicles using a spherical harmonic parameterization of the membrane surface. We conclude with examples and numerical results.

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MS55

Three Dimensional Vesicle Electrohydrodynamics:

A Numerical Investigation

The dynamics of three-dimensional vesicles when exposed to electric fields is complex. There is a nonlinear relationship between the material parameters and the shape of the vesicle. This talk will present a numerical method developed to investigate the electrohydrodynamics of three-dimensional vesicles is presented. This represents a first step towards modeling the electroporation of vesicles in a general, fully three-dimensional framework. Here, the numerical method will be outlined and an investigation of vesicle dynamics will be shown.

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MS55

A Continuum Model for Simulating Bilipid Membrane Deformation During Vesicle Drying

Bilipid membranes are of interest due to their similar dynamics to certain cells under flow and the ability to manufacture them in a lab. Modeled as a homogeneous, continuum material, the deformation of a vesicle undergoing drying is studied. The level set method is modified to explicitly capture the curvature in order to avoid stability issues when calculating curvature derivatives. The results will guide lyopreservation approaches, where cell drying is used as a storage technique.

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MS56

Flexibility-Rigidity Index for Protein Flexibility Analysis

We introduce a simple method, flexibility-rigidity index (FRI), to analyze macromolecular flexibility and rigidity in atomic detail. The FRI measures the topological connectivity of protein atoms or residues and characterizes the geometric compactness of the protein structure. The FRI bypasses matrix diagonalization, which underpins most other flexibility analysis methods and FRIs computational complexity is of O(N2) at most, where N is the number of atoms, in contrast to O(N3) for Hamiltonian based methods.

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MS56

Knotting in Open Chains, Closed Chains, and Proteins

Some proteins are now classified as being knotted. However, proteins have free ends and knotting, mathematically, is only defined for closed curves. Defining knotting in open chains (like proteins) is tricky and ambiguous. We show one definition of open knotting and search for knotted arcs within knotted open chains, closed chains, and proteins. This is joint work with Ken Millett, Andrzej Stasiak, and Joanna Sułkowska.

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MS56

Unlinking of Supercoiled DNA Catenanes by Type IIA Topoisomerases

It was found recently that DNA catenanes, formed during replication of circular plasmids, become positively (+) supercoiled, and the unlinking of such catenanes by type IIA topoisomerases proceeds much more efficiently than the unlinking of negatively (-) supercoiled catenanes. In an attempt to explain this striking finding we studied, by computer simulation, conformational properties of supercoiled DNA catenanes. Although the simulation showed that conformational properties of (+) and (-) supercoiled replication catenanes are very different, these properties per se do not give any advantage to (+) supercoiled over (-) supercoiled DNA catenanes for unlinking. An advantage became evident, however, when we took into account the established features of the enzymatic reaction catalyzed by the topoisomerases. The enzymes create a sharp DNA bend in the first bound DNA segment and allow for the transport of the second segment only from inside the bend to its outside. We showed that in (-) supercoiled DNA catenanes this protein-bound bent segment becomes nearly inaccessible for segments of the other linked DNA molecule, inhibiting the unlinking.

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MS56

Invariant Manifold and Persistent Homology for Biomolecules.

We introduce molecular nonlinear dynamics (MND) as a theoretical framework for describing protein folding. We unveil the existence of intrinsically low dimensional manifolds (ILDMs) in the chaotic dynamics of folded proteins. We reveal that the transition from disordered to ordered conformations in protein folding increases the transverse stability of the ILDM, which yields some the best quantification of protein uncertainty or protein thermal factors. Persistent homology is employed to characterize protein folding pathways and protein flexibility. The predicted cutoff distance is highly consistent with the numerical results from our ILDM model and other state-of-art methods.

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MS57

Fluid-Composite Structure Interaction in Hemody-

namics

The speaker will talk about modeling and simulation of FSI between an incomprensible, viscous fluid and a composite structure. Examples include FSI between blood flow and arterial walls, which are composed of several layers, each with different mechanical characteristics, and FSI between blood flow, arterial walls, and vascular devices called stents. A stable loosely coupled scheme will be introduced, and numerical results, showing novel features of this class of FSI problem, will be discussed.

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MS57

Transport in the Embryonic Lung II

Numerous studies have led to the identification of genes and morphogens that play important roles in lung branching morphogenesis. However the mechanism by which these signaling molecules regulate lung branching is not fully understood. It is also known that physical processes such as transport of morphogens could drive biological responses during development. Thus, in this study, we utilize a computational model to investigate the role of solute transport in lung morphogenesis.

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MS57

Transport in the Embryonic Lung I

Airway peristalsis (AP) begins as soon as the smooth muscle forms, and persists until birth. We analyze a model of the fluid-structure interactions between embryonic tissues and lumen fluid resulting from peristaltic waves that partially occlude the airway. We conclude that AP has a strong effect on flow sensing away from the tip and on transport of morphogens. These effects may be the intermediate mechanisms for the enhancement of branching seen in occluded embryonic lungs.

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MS57

Role of the Pericardium in the Tubular Hearts of Tunicates

Tubular hearts of tunicates have a stiff, outer pericardium that encloses a layer of myocardium which contracts to drive fluid flow through the tube. Most models of heart function have not included the pericardium or its possible contributions to the fluid flow produced by myocardial contractions. Here I present both experimental and model evidence that the pericardium fulfills an important mechanical role in the tunicate hearts ability to produce fluid flow through the circulatory system.

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MS58

Integration of Information over Multiple Timescales in a Large-scale Model of the Cortex

Models of the neural mechanisms of decision-making typically focus on local circuits operating within a single functionally-defined cortical area. To move beyond this, we study the dynamics of distributed decision-making in an anatomically-constrained model of multiple interacting areas in the macaque cortex. The anatomical constraints produce a hierarchical architecture where cortical areas are optimized to integrate information over different timescales. We investigate how such dynamical heterogeneity can be combined to allow flexible decision-making.

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MS58

Network Symmetry and Binocular Rivalry Experiments

This talk discusses a generalized network model for rivalry proposed by Hugh Wilson. The application shows how symmetry-breaking Hopf bifurcation can lead to rigid phase-shift synchrony in periodic solutions of coupled systems of differential equations that in turn can predict percepts in a variety of binocular rivalry experiments.

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MS58

Noise and Adaptation in Multistable Perception: A Case Study with Tristable Visual Plaids

We study the dynamics of perceptual switching in ambiguous visual scenes that admit more than two interpretations to gain insight into the dynamics of perceptual multistability and their underlying neural mechanisms. We focus on a classical paradigmatic stimulus, the visual plaids, consisting of two superimposed drifting gratings with transparent intersections. For visual plaids, tristable perception is

experienced: one coherent percept (the gratings move together as a single pattern) and two transparent percepts (the gratings slide across one another) with alternating depth order. In order to decipher the complex mechanisms of tristable perception, we gathered a large amount of psychophysical data on tristable plaids and developed a firing-rate model based on mutual inhibition and adaptation that involves stochastic dynamics of multiple-attractor systems. The model can account for the dynamical properties (transition probabilities, distributions of percept durations, etc) observed in the experiments. Noise and adaptation have been shown to both play a role in the dynamics of bistable perception. Here, tristable perception allows us to specify the role of noise and adaptation in our model. Noise is critical when considering the time of a switch. However, adaptation mechanisms are critical when considering perceptual choice (in tristable perception, each time a percept ends, there is a possible choice between two new percepts).

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MS58

Networks That Learn the Timing of Event Sequences

We discuss a neuronal network model capable of learning the timing of a sequence of events, each of which lasts milliseconds to seconds. Short term facilitation is a second-timescale accumulation process that controls switching between events. Long term plasticity allows the network to learn event timings quickly and accurately. Time scale separations, between the plasticity processes and neuronal activity dynamics, allow us to describe how long term plasticity parameters should depend upon short term facilitation parameters for the network to be able to learn **any** sequence of timings.

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MS59

Intramural Forecasting of Cardiac Electrical Dynamics Using Data Assimilation

As a first step in reconstructing the three-dimensional propagation and breakup of electrical waves, a data-assimilation system is coupled to a simple model of cardiac electrical dynamics. Data assimilation is a technique–common in numerical weather prediction–for combining observations with a numerical model to derive an improved estimate of the state of a dynamical system. Here an ensemble Kalman filter is used on synthetic data for both 1D and 3D models.

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MS59

Microscale Modeling of Cardiac Tissue

Focal activity in localized regions of cardiac tissue with poor, heterogeneous gap junction coupling can lead to long conduction delays, isolated wavefront breakthrough sites, and reentry as the wavefront propagates into healthy surrounding tissue. In this study we use two-dimensional, microstructural computer models of ventricular monolayers (1 cm x 1 cm) to investigate the effect of modulating sodium and calcium currents on the formation of breakthrough sites and the development of sustained reentry.

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MS59

Predicting Arrhythmias with a Nonlinear Cardiac Fiber Model

A dynamical model of a cardiac fiber was developed to help investigate the relationship between premature beats and ventricular fibrillation (VF), a lethal cardiac arrhythmia. When tested with canine ventricular data, the model was shown to predict which patterns of premature beats were more likely to produce VF *in vitro*. In addition, model-predicted spatial changes in action potential duration were positively correlated with the observed values.

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MS59

Compositionality Results for Cardiac Cell Dynamics

We show that the 13-variable Markovian sodium-channel component of the 67-variable Iyer Mazhari Winslow cardiac cell model can be replaced by an approximately equivalent 2-variable Hodgkin-Huxley-type abstraction. This substitution of (approximately) equals for equals is safe in the sense that the approximation error between the sodium channel models does not get amplified by the feedback-loop context in which the components are placed. The proof entails automatic computation of Lyapunov-like functions that characterize input-to-output stability of dynamical systems.

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MS60

Spatial-Temporal Regulation of the First Embryonic Development Decision

Abstract not available at time of publication.

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MS60

Analysis and Simulations of a Three Dimensional Model of Cell Signal Transduction

We consider a model of cell singnal transduction in a spherical cell. Signal molecule production is restricted to specific areas of the cell. We use asymptotic analysis to construct an system of ordinary differential equations which approximate the full partial differential equation. We then consider the effect of adding in a delay to the production of signal molecules and analyze the resulting Hopf bifurcation.

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MS60

Time to Mutation Acquisition in Stem Cell Driven Cancers

Abstract not available at time of publication.

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MS60

Mathematical Modeling of Proliferation Kinetics of Cancer Stem Cells

Abstract not available at time of publication.

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MS61

Detailed Viral Kinetics During Liver Transplantation Indicates that the Liver Plays a Role in HCV Clearance

While the liver is widely accepted as the main site for hepatitis C virus (HCV) production, its role in the clearance of circulating HCV remains unknown. By analyzing and modeling HCV kinetics during liver transplantation we were able to shed light on the function of the liver in clearing free virus from the circulation. In vitro experiments in HCV-infected hepatocytes support in part our findings.

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MS61

Silibinin As a Drug for Hepatitis C in Patients with Compromised Liver

Hepatitis C patients with compromised liver and those awaiting liver transplant rarely respond to standard therapy. Silibinin lowered viral load in such patients in two pilot clinical trials. We use treatment data from these studies to understand the mode of action, efficacy and compare these between the two cohorts. We also aim at describing Hepatitis C viral kinetics in patients treated with Silibinin, according to severity of liver disease, from the two clinical trials.

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MS61

Role of Methamphetamine in Transmission Dynamics of HIV in MSM Population

Methamphetamine is an addictive stimulant that releases high levels of neurotransmitter dopamine. The use of methamphetamine have shown to increase libido and reduces inhibition. As a result, methamphetamine is commonly used among men who have sex with men to to initiate, enhance, and prolong sexual encounters. This, in turns, promotes high risk sexual behavior in this community of methamphetamine users which increases the risk of acquiring an STD. Furthermore, studies have shown that the use of methamphetamine is associated with more frequent risky sexual behaviors among HIV positive men when compared with HIV negative men. This study seeks

to evaluate the dynamics of the methamphetamine abuse and HIV incidence through the stability analysis. The reproduction number of the system is identified. All parameters are approximated and the system is explored by simulations. The implications of preventative measures will be discussed.

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MS62

Developing Fit-for-purpose Physiological Models in Drug Discovery and Development - A Framework for Qualification Best Practices

Physiological models are used in drug discovery and development programs to enable decisions such as dose selection, risk assessment, or competitive strategy. We have developed a framework for the qualification of physiological models, which employ statistical or other techniques to explain variability from various sources. The adoption and application of this framework will support the goals of effective physiological model development, communication, and increased acceptance of physiological models for enabling critical decisions.

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MS62

A Sensitivity Based Statistical Approach to Parameter Selection and Uncertainty Quantification

We discuss both global and local sensitivity analysis in the context of statistical approaches (requiring a good statistical model as well an adequate mathematical model) to assessing and quantifying the effect of known and unknown parameters in complex systems. We use recently developed parameter subset techniques to investigate the impact of estimated parameters on the corresponding selection scores and uncertainty. These ideas are presented in the context of an in-host model for HIV-1 infection dynamics developed and validated with patient data.

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MS62

Application of Modelling and Simulation in Oncology: Physiologically-based Pharmacokinetics and Dynamics Examples

A physiologically-based model applicable for oncological questions in drug development was developed by use of the systems biology platform including PK-Sim and MoBi.

It includes representation of all relevant processes and its typical variability for small molecules and biologics at a physiological level.

By means of different examples it will be demonstrated that such models are able to represent the pharmacokinetics and related tumor growth dynamics in preclinical species and to provide useful insight into scenarios relevant for the clinic including exploration and separation of variability and uncertainty by the model process.

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MS62

Leveraging Visualization and Probabilistic Thinking to Get Consensus on an Assay Level Target for a Cancer Drug

Quantitative thresholds can support effective clinical oncology program decisions. Such thresholds are often derived from preclinical and (sparse) clinical data. Here, nonlinear mixed-effect modeling allowed integration of variability and uncertainty in data, and enabled simulations identifying an biochemical assay level (threshold) predictive of clinical efficacy. A kernel-based probabilistic model integrating these simulations captured the necessary phenomena. The model allowed non-mathematical visualization enabling effective collaboration with the development team on the complex, multi-dimensional, probabilistic data.

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MS63

Chemical Insights, Matrix Approximations, and Boundary-Integral Equations

Abstract not available at time of publication.

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MS63

Geometry of Surfaces in the Protein Images and the Graph Algorithms

Abstract not available at time of publication.

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MS63

Protein Modeling from Intermediate-Resolution Density Maps Using Geometric Skeletons

This talk will present our continuing work on protein modeling from density maps that are captured at intermediate resolutions (6-10Å), which have become increasingly available for imaging macromolecular complexes. Our work computes and makes use of the geometric skeleton of the density map to automate several model-building tasks, including detecting secondary structure elements, identifying their topology on the backbone, and flexibly fitting probe structures into the map. The algorithms are distributed in our open-source tool, Gorgon.

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MS63

Accurate Electrostatics in 3D Classical Dft

Abstract not available at time of publication.

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MS64

Surface Tension in Human Lungs: Modeling and Experiments

Naturally produced surfactant, which lowers surface tension is required for normal human lung function. Premature babies born before surfactant production begins, are at risk for respiratory distress, and often require surfactant replacement therapy. For 20 years mathematicians and scientists have sought to model the complicated flow of fluid lining the passageways and alveoli of the lungs. New experiments allow us to visualize a simplified system that includes a thin film of glycerol and a surface layer of surfactant. This talk will describe what we can learn from such experiments, how the results compare to a commonly accepted model, and how we might modify the experiments to better capture dynamics in the lungs.

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MS64

Fluid Dynamics of the Tracks of Tears

In humans, tears are used to wash away irritants, lubricate the eye, and express emotion. The chemical makeup of tears, as well as their mechanical properties, also varies. In addition to changes in chemical properties, the path that the tear exists the eye can change from the corner of the eye to directly over the lid and eyelashes. In this presentation, we use high-speed video to construct simple models of the dynamics of different tears.

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MS64

Modeling and Simulation of Biofilm Flows

Biofilms are ubiquitous in nature. It consists of bacteria, polysacharrides, water and nutrient. Bacteria are live organisms while polysacharrides, also known as EPS, are biopolymers that cross-link into a resilient network encasing the bacteria. In this talk, we will report our efforts in developing a hydrodynamic theory to study the viscoelasticity of the EPS and how they interact with the live bacteria and the host solvent matrix. Different bacterial phenotypes and quorum sensing effect will be considered in the model. 3-D numerical simulation will be carried to benchmark the model with some available experiments.

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MS64

Biofilm Pattern Formation Within Microfluidic Chambers

Recently, many biological phenomena involving complex mechanical and biochemical interactions of multiple components have been successfully modeled using a multiphase framework, including tumorigenesis, cell motility, and developmental processes. In this talk, I will present a two-dimensional multiphase model of the biofilm formation by *Xylella fastidiosa*, the causative agent of Pierce's Disease. Numerical simulations of this model demonstrate the regular spatial patterning observed in microfluidic experiments representing an artificial plant xylem.

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MS65

Optimal Control in PDE/DE Model for an Anthrax Epizootic

Anthrax is a fatal, infectious disease which occurs in many animal species, particularly land mammals. It is a cause of population decline in several national parks worldwide such as in bison at northern Canada in 1993. Due to the ability for anthrax spores to survive in soil for a long time even under harsh conditions, clearing anthrax spores from the environment is practically impossible. As infected animals die, their carcasses contribute bacteria in the surrounding environment. Proper disposal of the carcasses and effectively controlling new infections are feasible ways to help control the disease. In this talk, I will present some preliminary results of these measures of controlling the spread of the disease.

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MS65

Habitat and Abundance Modeling of West Nile Virus Vector

Mosquito-borne disease incidence is particularly influenced by climate through two main pathways. First, climate dictates the habitat available for breeding, immature development, and adult resting. Second, fluctuations in temperature and precipitation drive pathogen and mosquito development as well as changes in availability of breeding habitat. As a result of these associations researchers can predict where mosquitoes and mosquitoes-borne diseases are likely to occur and, using dynamic simulation models, researchers can estimate mosquito abundance for specified locations (i.e., climates). Such estimations facilitate our understanding of disease dynamics and spread. Using the mosquito-borne West Nile Virus disease as a case study, I will discuss how spatial and temporal models can be used to understand emerging diseases and where they fall short in our ability to predict new invasions.

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MS65

Parameter Estimation and Model Discrepancy with Application to the Life Sciences

In this presentation we consider the problem of parameter estimation for systems governed by ordinary and delay differential equations and discuss the impact of modeling errors which are an important source of model discrepancy. We present an approach based on assuming the model is defined as a dynamical system with uncertain disturbances. This approach can be used to develop prior knowledge about model discrepancy in order to improve

the models predictive usefulness.

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MS65

Basic Reproductive Ratios in Ecosystems and Disease Models

In this talk, we will discuss the basic reproductive ratios in ecosystems and disease models. In general, for a periodic differential system with time delay, it is difficult to obtain explicit formula for the basic reproductive ratio in terms of model parameters. We will provide a novel technique in finding approximate formulas for basic reproductive ratios in various ecosystems and disease models.

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MS66

Probability of Extinction in Stochastic Models of Populations and Infectious Diseases: Importance of Time and Location

Multitype branching process theory is used to estimate the probability of population or disease extinction in multipatch, multi-group, and multi-stage models. The success of a species invasion or of a disease outbreak often depends on the conditions of the environment at a specific time and location. Applications of the theory are discussed in terms of several zoonotic diseases.

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MS66

How Fish Ecology Affects the Effectiveness of Marine Protected Areas

MPAs (Marine Protected Areas) are regions where fishing is restricted or prohibited. As a fisheries management tool, their purpose is to protect overharvested species and their habitats. Assume that the fish population consists of a predator and a prey. One system of nonlinear ODEs describes the predator-prey interaction in the MPA where fishing is prohibited. A similar but different system describes the interaction of predator and prey in the Fishing Grounds where fishing is allowed. Now assume that both predator and prey can move between MPA and Fishing Ground, in a way that mimics Fick's albeit in an ODE context. How does the resulting coupled model, consisting of 4 nonlinear ODEs behave? I will show that the coupling tends to stabilize the system. In the special case that the prey is immobilized, but the predator can move, I will outline a proof showing global stability based on the construction of a Lyapunov function, in conjunction with Lasalle's invariance principle. I will also discuss when diffusion is equalizing.

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MS66

Optimal Control Applied to Hospital-Acquired and Community-Acquired Methicillin-Resistant Staphylococcus Aureus Strains in Hospitals

Optimal control are applied to a deterministic mathematical model to characterize the factors contributing to the replacement of hospital-acquired Methicillin-resistant Staphylococcus aureus (MRSA) with community-acquired MRSA, and quantify the effectiveness of three interventions aimed at limiting the spread of CA-MRSA in health care settings. Adjoint equations and the characterization of the optimal control strategies are established, and various numerical simulations are provided to illustrate the results.

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MS66

Optimal Control of Continuous Systems with Impulse Controls

Impulse control problems, in which a continuously evolving state is modified by discrete control actions, have applications in epidemiology, medicine, and ecology. In this paper we present a simple method for solving impulse control problems for systems of differential equations. In particular, we show how impulse control problems can be reformulated and solved as discrete optimal control problems. The method is illustrated with two examples.

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MS67

Combined Parameter and State Estimation in Ensemble Kalman Filters

Ensemble Kalman filtering techniques have traditionally been developed to perform state estimation for nonlinear dynamical systems with fixed parameters. However, in many biological applications, there is often uncertainty in the model parameter values. We propose a method for estimating the system parameters along with the states in an ensemble Kalman filter framework. The effectiveness of the resulting algorithm is demonstrated in estimating the maximum reaction rates and affinity constants of Michaelis-Menten flux expressions in a model for skeletal

muscle metabolism.

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MS67

Model Calibration in Systems Biology: Making the Most of Limited Data

The field of Systems Biology was developed in response to experimental advances that allow system-level observations of intracellular networks. While such high-throughput assays provide valuable insight into cellular processes, they typically fall short of providing sufficient data to calibrate mechanistic models of intracellular dynamics. This talk will relate our experience with modelling in metabolism and signal transduction, highlighting the tools we used to gain insight from models that were calibrated against limited data.

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MS67

Patient Specific Modelling of the Endocrine HPA-Axis and Its Relation to Depression: Ultradian and Circadian Oscillations

Correlation between depression and a recently defined index characterizing the hypothalamus-pituitary-adrenal (HPA) axis is established. A novel capturing circadian as well as ultradian oscillations of hormone concentrations related to the HPA-axis is suggested. Three parameters related to depression are identified and estimated based on data from 29 subjects using non-linear mixed effects modelling and statistical hypothesis testing. These parameters represent underlying physiological mechanisms of the HPA-axis and may be used for diagnosing and understanding depression.

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MS67

Uncertainty Quantification in ODE Modeling of Immune Response

Our team has utilized Bayesian inference for quantifying the uncertainty in parameter estimation for several models of host immune response to bacterial and viral infection. Due to the scarcity of data we have supplemented the likelihood function with heuristic criteria designed to impose restrictions on the qualitative behavior of modeled systems. I will discuss our experience with the feasibility and utility of ensemble modeling, including the use of parallel tempering for speeding up convergence.

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MS68

A Multicell Model to Investigate How Vasculogenesis Is Disrupted in Cerebral Cavernous Malformations

Abstract not available at time of publication.

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MS68

Diffusion in Soft Matter: Theory, Modeling, and Simulations

This lecture highlights anomalous diffusion of particles in soft matter in general, and in lung airway fluids in particular. We present particle path data from experiments, discuss models that are consistent with the data, and predictive simulations of models that have been fitted to the data. Relevance to pulmonary medicine will be presented.

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MS68

Homeostatic Mechanisms in Biochemical Systems

We will discuss the structure of homeostatic mechanisms in a variety of metabolic systems including folate metabolism, methylation reactions, and detoxification by glutathione in the liver. These mechanisms are designed to allow cells to regulate crucial functions in the face of large fluctuations in inputs due to meals. From a mathematical point of view, the question is how these mechanisms dampen stochastic fluctuations as they propagate through the biochemical network.

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MS68

Mathematical Understanding of Cancer Virotherapy

Abstract not available at time of publication.

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MS69

The Way Cells Talk: Modeling and Simulations of Ion Transport

Ion channels are fundamental components that conduct ionic exchanges through cellular membranes, thus they are critical in many biological process such as change of action potentials, signaling and interactions with extracellular microenvironment. In this talk I will first briefly overview the methodologies and models of ion channels, then focus a specific ionic transport, the proton transport through cellular membranes. A multi scale and multi physic model is proposed based on a total energy functional, from which the governing equations of proton dynamics and electrostatics are derived. A set of highly accurate and efficient numerical algorithms are developed to perform the simulations. A specific application of proton transport could be a better understanding of abnormal acidity in tumor microenvironment.

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MS69

Ions in Channels: Natural Nanovalves

Ions in channel proteins are the ultimate multiscale device. They are natural nanovalves in which a handful of atoms control many processes crucial to life by controlling macroscopic flows of ions. Statistical mechanics was not designed with interacting systems in mind, let alone systems in which atoms control macroscopic flows and living machines. Variational mechanics (of dissipative flowing systems like complex fluids) is needed to engineer the nanovalves of life, in my opinion.

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MS69

A Energy-Preserving Scheme for Pnp Equations

In this talk, we present a finite difference scheme that satisfies the energy dissipation law of the Poisson-Nerst-Planck equation exactly. We formulate the chemical potential differently and show that the energy-preserving scheme comes out of the new formulation. Numerical results comparing the energy-preserving scheme with the standard scheme will be shown.

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MS69

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MS70

Neuromuscular Pumping in Jellyfish Bells

A current question in jellyfish propulsion is how the underlying neuromuscular organization of their bell allows for maneuvering. Using an immersed boundary framework, we will examine the neuromechanics of swimming by incorporating neural and muscles models into a model of the elastic jellyfish bell. We then use this model to understand how variability in the electrophysiology allows for complicated swimming behavior, such as steering. We will compare the results of the simulations with experiment.

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MS70

The Effects of In Phase and Out of Phase Pulsations in Groups of Upside-down Jellyfish, Cassiopea sp

Upside-down jellyfish of the genus Cassiopea use bell contractions to generate feeding currents. These jellyfish typically situate themselves on the bottom of the ocean floor in groups. Little is known about the costs and advantages of the different pulsation modes within a group and how these trade-offs are related to the size of the individual jellyfish. In this study, the effects of synchronous and asynchronous pulsations are investigated using particle image velocimetry.

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MS70

The Metachronal Limb Stroke Pattern in Crustacean Swimming

Crayfish and other long-tailed crustaceans swim by rhythmically moving four or five pairs of limbs. Despite variations in limb size and stroke frequency, movements of ipsilateral limbs always maintain a tail-to-head metachronal rhythm with an approximate quarter-period inter-limb phase-difference. Relatively few studies have examined the fluid dynamics of metachronal limb stroke for the range of Reynolds numbers under which crustaceans operate. Here, we use a computational fluid dynamics model to address this issue.

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MS70

Experiments and Modeling Study of Low Reynolds Number Flows Generated by a Processing Nodal Cilia

Theoretical study and experiments are developed to emulate dynamics biological interest such as primary cilia in developing embryos, where primary cilia are the main agent for the embryonic forms of nutrient circulation. Experiments are performed using high viscosity silicon oil with magnetically actuated precessing rod in a table-top setup. Stereoscopic Lagrangian tracking show quantified long-time agreement with an appropriately imaged slender body theory to enforce the no-slip condition at the floor. In contrast, breaking symmetry by a bent rod creates additional flow components which destroy quantitative short time agreement with the theory while maintaining its qualitative features including the creation of large scale Lagrangian tori.

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MS71

The Influence of Neurochemistry

Mathematical models in neuroscience often treat individual neurons as nodes in networks and biochemistry appears, if at all, as some intermediate variables by which the neurons communicate with each other. In fact, many neurons change brain function not by communicating in one-to-one fashion with other neurons, but instead by projecting changes in biochemistry over long distances. This biochemical network is of crucial importance for brain function and it influences and is influenced by the more traditional electrophysiological networks.

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MS71

How Precise Can We Make a Biophysical Neural Integrator?

Recently, Boerlin et al 2013 derived a recurrent network of leaky-integrate-and-fire neurons with instantaneous synaptic dynamics that can perform a variety of computations. Although this framework is flexible in that the derived network can perform any linear computation, it is important to ask whether the framework generalizes to more realistic synaptic and spike-generating dynamics. Here, we show that this framework can indeed be extended to include slow, alpha function synaptic dynamics and Hodgkin-Huxley-like spike-generating currents.

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MS71

The Effects of Long-Range Coupling on Neural Activity in the Crayfish Swimmeret System

The crayfish swimmeret system exhibits a stable stroke pattern during forward swimming, where the limbs move in a back to front metachronal wave with a delay of approximately 25%. A chain of nearest neighbor coupled oscillators indicates that the network topology of the crayfish neural circuit promotes the robust generation of this pattern (Zhang et al.). We extend this modeling work to consider the influence of the long-range connections that are present in this system.

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MS71

Interaction of Two Distinct Timescales in Computational a Model of in-Vitro Sigh Generation

Augmented breaths, or sighs, increase air intake and a lack of sighing is associated with sudden infant death syndrome. Since sighs operate on significantly slower time scale than eupnoea, it is still debated if they are produced by the same network of neurons or by distinct sub-networks. We developed a mathematical model that proposes that sighs and eupnoea are generated by the two neural sub-networks. The model accounts for dynamics of sigh and eupnoea and reproduces several in-vitro experiments.

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MS72

Large Reduction of Defibrillation Threshold Using a Four-Electrode System

In this talk we propose a new shock protocol that is based on a four electrode system instead of the of standard procedure based with only two electrodes. The model is tested using one-dimensional ring with bidomain properties and with the Beeler-Reuter model for the active properties of the membrane. Three different shock types are tested: monophasic and two types of biphasic shock. The results are compared with those obtained with standard two electrode protocol. Substantial reduction in defibrillation threshold is achieved with respect to the standard protocol.

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MS72

Unification of Electrical Restitution Dynamics and Ion Channel Dynamics in the Control of Cardiac Rhythm - An Eigenmode Approach

The characterization of action potential dynamics in cardiac tissue has traditionally followed two parallel tracks: use of the dependence of action potential duration and wave propagation speed on the preceding diastolic interval (called electrical restitution theory), and use of intricate ion channel models. In our work, we unify these two approaches by applying eigenmode theory to the mapping of perturbations of both sets of dynamical variables from one action potential to the next. This link between the two approaches provides us with an important foundation on which we can discuss in a rigorous manner how drugs and electrical interventions impact the onset and control of fibrillation in the heart.

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MS72

Local Termination of Cardiac Alternans Using Isostable Response Curve Techniques

Phase reduction methods have been tremendously useful for understanding the dynamics of nonlinear oscillators, but have been difficult to extend to excitable systems with stable fixed points, such as those that commonly describe individual cardiac cells. Here, we extend the notion of phase reduction to include excitable media, and use this reduction to formulate an energy-optimal control strategy for terminating cardiac alternans in a high-dimensional model

of cardiac cellular activity.

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MS73

Exact Protein Distributions for Stochastic Models of Gene Expression

In this talk, I will discuss approaches developed by my group for obtaining analytical results for protein distributions in stochastic models of gene expression. We invoke the partitioning property of Poisson processes to develop a mapping that significantly simplifies the analysis of such models. Using this mapping, we derive exact analytical results for steady-state and time-dependent protein distributions for the basic 2-stage model of gene expression. Considering extensions of the basic model, we obtain exact protein steady-state distributions for models that include the effects of post-transcriptional and post-translational regulation. Finally, I will introduce a model which includes the interplay between bursting and feedback regulation and discuss insights gained from analyzing the corresponding steady-state protein distribution.

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MS73

An Optimal Control Framework for Stochastic Gene Regulatory Networks

Modeling stochasticity in gene regulation is an important and complex problem in molecular systems biology due to probabilistic nature of gene regulation. This talk will introduce a stochastic modeling framework for gene regulatory networks which is an extension of the Boolean modeling approach. This framework incorporates propensity parameters for activation and degradation and is able to capture the cell-to-cell variability. In this setting, optimal control problems can be studied using methods from control theory for Markov decision processes for the purpose of developing optimal intervention strategies. These control methods will then be applied to the p53-mdm2 complex.

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MS73

Extrinsic Noise and Cell-Cycle Dependence of Genetic Oscillators

Understanding the effect of noise and the cell cycle on gene networks is fundamental in developing accurate models. Typically, comparing experimental data and simulations only takes into account individual trajectories, but not the lineage and the corresponding variability and correlation. Here we show that a model that includes extrinsic noise can capture the variability seen in a synthetic gene oscillator. Furthermore, we show that it is sufficient to model extrinsic noise as cell-to-cell variability at cell division.

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MS74

Optimal Control in Models of Management Involving Trees and Forest Resources

Two applications of optimal control are presented in examples of managing populations related trees and forest products. One example is a discrete model of gypsy moth populations affecting tree defoliation. The other example is a system of ordinary differential equations modeling the harvesting (lethal and non-lethal) for forest products.

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MS74

Modeling of Transgenic Or Sterile Mosquitoes in Fighting Vertor-Borne Diseases

To prevent the transmission of malaria or other mosquito-borne diseases, an effective weapon is to use genetically-altered (transgenic) mosquitoes or mosquitoes carrying genetically-modified bacteria, that are resistant to the infection, to replace the wild mosquitoes, or to release sterile mosquitoes to reduce the wild mosquito population. To study the impact of these mosquitoes mixing with wild mosquitoes on the diseases transmission and different strategies in releasing sterile mosquitoes, we formulate simple continuous- or discrete-time mathematical models of interactive wild and transgenic or sterile mosquitoes. We present fundamental analysis of the model equations, and demonstrate the rich dynamical features of the models by numerical examples.

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MS74

An Ecological Model for Producers and Scroungers in a Spatial Habitat

We describe the dynamics of a producer-scrounger system in a spatial habitat using a partial differential equation model. Both species are assumed to increase logistically and to move randomly in their environment. Producers can obtain the resource directly from the environment, whereas scroungers must steal it from nearby producers. When possible, parameter combinations which allow producers

and/or scroungers to persist either alone or together are distinguished from those in which they cannot.

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MS74

The Role of Avian Stage-structure in the Transmission and Control of West Nile Virus

The seasonal occurrence of West Nile Virus in humans has been associated with the end of the avian nesting season. Newly hatched nestlings are more vulnerable to mosquitoes than older birds. While total avian population size increases throughout the season, nestling abundance declines at the end of the brooding season. This temporal variation in host stage abundance may play an important role in structuring WNV transmission. We develop and analyze a stage-structured differential equation model for WNV and investigate the impact of vector preference for specific host life stages on the timing of WNV activity as well as implications for public health interventions.

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MS75

Identifiability and Parameter Estimation in Modeling Disease Dynamics

Connecting differential equation models with data to yield predictive results requires a variety of parameter estimation, identifiability, and uncertainty quantification techniques. Identifiability analysis addresses the question of whether it is possible to uniquely recover the model parameters from a given set of data. In this talk, I will discuss some recent work using and developing identifiability methods based on tools from computational differential algebra and systems theory, and present several clinical and public health applications to problems in human disease, including cholera and other infectious disease transmission processes.

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MS75

Identifiability of High-Dimensional Models

The structure of a complex system ultimately determines whether key unknown parameters can be unambiguously quantified from experimental observations. Although many identifiability techniques have been proposed to examine model structures before parameter estimation, we have never gained the capability to explore the territory of high-dimensional problems due to various limitations in existing methods. Here we develop the very first graphical approach to analyze the identifiability of high-dimensional systems that are governed by dynamic laws. We apply this method to several real model structures, and show how model topology and experimental inputs and outputs affect the identifiability. The proposed method provides a basis to systematically examine and refine the structures of a wide range of complex dynamic systems.

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MS75

Identifiability and Parameter Estimation in Systems Biology and Drug Development

Due to the high complexity of biological data it is difficult to disentangle cellular processes relying only on intuitive interpretation of measurements. A Systems Biology approach, that combines quantitative experimental data with dynamic mathematical modeling promises to yield deeper insights into these processes and makes a more rational drug design possible. Nevertheless, with growing complexity and increasing amount of quantitative experimental data, building realistic and reliable mathematical models can become a challenging task: unknown model parameters need to be estimated from the experimental data and uncertainties in model predictions has to be considered realistically. I will present a case study (Raue et al., Bioinformatics 2014) using three current approaches for identifiability analysis for an application from cell biology (Raia et al., Cancer Research 2011). The approaches are conceptually different and are developed independently. The results of the three approaches are in agreement but have different strength and weaknesses. For the estimation of unknown model parameters, the performance of different optimization algorithms is compared systematically (Raue et al., PLOS ONE 2013). The results show that deterministic derivative-based optimization employing the sensitivity equations in combination with a multi-start strategy based on Latin hypercube sampling outperforms the other methods by orders of magnitude in accuracy and speed.

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MS75

Identifiability of Linear State Space Models

Dynamical systems models described by linear systems of ordinary differential equations are ubiquitous in applied mathematics and mathematical biology. Such a model is said to be identifiable if the parameters of the model can be uniquely determined from given input and output data. I will discuss recent progress on developing precise combinatorial methods to determine if a system is identifiable. Joint work with Nicolette Meshkat and Adam Mahdi.

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MS76

Modeling Cartilage Tissue Engineering in Cell-

Seeded Scaffolds

Chondrocytes or stem cells can be used to regenerate cartilage extracellular matrix via tissue engineering approaches in which cells are seeded into porous scaffold materials. In such systems, cell-mediated biosynthesis results in regeneration and accumulation of extracellular matrix constituents concurrent with scaffold degradation. Continuum models are presented for such systems and quantify the effects of evolving porosity on functional outcomes. Both tissue-scale mixture models and microscopic models with individual cells will be presented.

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MS76

Let There be Force: Modeling Cell-ECM Interactions

Extracellular matrix (ECM), a fibrous material that forms a network in a tissue, significantly affects many aspects of cellular behavior, including cell movement and proliferation. Transgenic mouse tumor studies indicate that excess collagen, a major component of ECM, enhances tumor formation and invasiveness. Moreover, cell interactions with the collagen matrix result in aligned fibers that facilitate cell invasion. However, the underlying mechanisms are unclear since the properties of ECM are complex, with diverse topographies and mechanical properties depending on various biophysical parameters. We have developed a three-dimensional elastic computational fiber network model, and parameterized it with in vitro collagen tensile experiments. Using this model, we simulate mechanical testing of fiber networks and examine the mechanical properties of fiber networks with varying density, alignment, and crosslinking. The computational model and simulation results can fill in the gap between microscopic single collagen fiber studies and macroscopic collagen gel studies. This model is the first step toward a fully biomechanical cell-matrix interaction model for changes in matrix organization during cell migration and tumor invasion.

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MS76

Mathematical Modeling of Renal Hemodynamics

We have developed a mathematical model of the rat kidney's blood flow control, and used that model to study the individual contributions of two autoregulatory mechanisms. The model represents an afferent arteriole, glomerular filtration, and a segment of a short-loop nephron. The afferent arteriole exhibits the an autoregulatory mechanism called the myogenic response, such that it responds to transmural pressure elevation with constriction, and to pressure reduction with dilation. Another autoregaulatory mechanism is the tubuloglomerular feedback (TGF): The tubule model predicts tubular fluid and Cl- transport. Macula densa Cl- concentration is sensed as the signal for TGF, which acts to constrict or dilate the afferent arteriole. In other words, TGF contributes to hemodynamics control by adjusting single nephron glomerular filtration rate according to the chloride concentration sensed downstream. With this configuration, the model afferent arteriole maintains stable glomerular filtration rate within a physiologic range of perfusion pressure (80-180 mmHg). The contribution of TGF to overall autoregulation is significant only within a narrow band of perfusion pressure values (80-110 mmHg).

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MS76

Kinetic Monte Carlo Simulations of Multicellular Aggregate Self-Assembly in Biofabrication

We present a three-dimensional lattice model to study self-assembly and fusion of multicellular aggregate systems by using kinetic Monte Carlo (KMC) simulations. This model is developed to describe and predict the time evolution of postprinting morphological structure formation during tissue or organ maturation in a novel biofabrication process (or technology) known as bioprinting. In this new technology, live multicellular aggregates as bio-ink are used to make tissue or organ constructs via the layer-by-layer deposition technique in biocompatible hydrogels; the printed bio-constructs embedded in the hydrogels are then placed in bioreactors to undergo the self-assembly process to form the desired functional tissue or organ products. Here we implement our model with an efficient KMC algorithm to simulate the making of a set of tissues/organs in several designer's geometries like a ring, a sheet and a tube, which can involve a large number of cells and various other support materials like agarose constructs etc. We also study the process of cell sorting/migration within the cellular aggregates formed by multiple types of cells with different adhesivities.

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MS77

Pnp Equations with Steric Effects: A Model of Ion Flow Through Channels

Abstract not available at time of publication.

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MS77

Computer Simulation of Voltage Sensitive Calcium Ion Channels in a Dendritic Spine

Abstract not available at time of publication.

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MS77

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS77

A Model of Tissue Electrodiffusion and Osmosis and Its Application to Cortical Spreading Depression

We propose a PDE model of tissue-level electrodiffusive and osmotic phenomena. An important feature of this model is that it satisfies an energy inequality. This model will be applied to the study of cortical spreading depression, a pathophysiological phenomenon in the brain that is thought to underlie migraine aura and other pathologies.

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MS78

Roles of Droplets and Bubbles in Pathogen Transmission Through Air

Pathogen-bearing droplet creation from contaminated fluids results from the interplay between interfacial flow dynamics and pathogens. Such interplay leads to various modes of formation and ejection of contaminated droplets into the air, thus shaping infectious disease transmission indoors. Particular mechanisms of fluid breakup leading to the creation of pathogen-bearing droplets from bursting bubbles and violent expirations will be discussed.

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MS78

Fluid Flow Through Many Bristled Wings

The smallest flying insects are roughly 1mm in length and at this scale viscous effects are significant. Interestingly, these insects commonly possess wings with long bristles on the fringes, and the physiological importance of the bristles remains a mystery. Depending on the Reynolds number and the local environment, bristled wings could act either as leaky sieves or solid paddles. We used the immersed boundary method to investigate the aerodynamic role of bristles in insect flight.

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MS78

Clap and Fling Interaction of Bristled Wings in Tiny Insect Flight

The flapping flight of the smallest insects that fly at Reynolds numbers (Re) on the order of 10 is often characterized by a 'clap and fling' of the wings. The effect of a bristled wing characteristic of these insects is investigated using 2D numerical simulations based on a porous version of the immersed boundary method. A comparison of the aerodynamic forces generated between solid and porous wings undergoing wing-wing interaction will be presented.

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MS78

Microscale Gas Transport in Insect Respiratory Systems

Insects and some other terrestrial arthropods breathe using a complex network of tracheal tubes. Air is drawn in through sets of openings called spiracles, and follows a branching path down to the tracheoles, which deliver oxygen directly to the cells for respiration. These tracheal networks have recently been found to consist of essentially inelastic but locally (in time and space) collapsible tubes. Mathematical modeling and meshfree computations are presented to describe this transport paradigm.

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MS79

Stochastic Switching: Mathematical Surprises and Biological Insight

Motivated by several biological questions, we consider ODEs with stochastically switching right-hand sides and PDEs with stochastically switching boundary conditions. In a variety of situations, we prove that the system exhibits surprising behavior. In this talk, we will highlight some of the most interesting results and describe their implications both for the mathematical study of stochastic hybrid systems and for the motivating biological problems.

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MS79

Multi-Motor Transport in Neurons: Moving Beyond Tug-of-War

Transport in neurons is intrinsically bidirectional, with each movement modality carried out by molecular motors in either the kinesin (anterograde) or the dynein (retrograde) families. Because all motors are present at a given time there must be competition and/or cooperation among motors that simultaneously bind a single vesicle to nearby microtubules. It has been assumed for much of the last decade that the competition must resolve itself though some kind of tug-of-war; but recent evidence shows conclusively that this is not the case in vivo. In this talk, we will see a few biological mechanisms (and associated mathematical models) that may lead to resolving theory with experimental observations. Joint work with Will Hancock (Penn State), John Fricks (Penn State), and Pete Kramer (RPI).

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MS79

Spontaneous Neural Activity Caused by Ion Channel Fluctuations

The membrane voltage of a neuron is modeled with a piecewise deterministic stochastic process. The membrane voltage changes deterministically while the population of open ion channels, which allow current to flow across the membrane, is constant. Ion channels open and close randomly, and the transition rates depend on voltage, making the process nonlinear. In the limit of infinite transition rates, the process becomes deterministic. The deterministic process is the well known Morris-Lecar model. Under certain conditions, the deterministic process has one stable fixed point and is excitable. An excitable event, called an action potential, is a single large transient spike in voltage that eventually returns to the stable steady state. I will discuss recent development of large deviation theory to study noise induced action potentials.

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MS79

Measuring Edge Importance for Random Processes on Networks

Many neural systems can be represented as a Markov process on a graph. We derived a new measure of the contribution of individual edges in the graph to the accuracy of an approximate process on the graph. We apply this measure to the Hodgkin-Huxley system and extend it for a broad class of random graph models. These results shed new light on the contributions of different ion channel transitions to the variability of neural systems.

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MS80

A Mathematical and Computational Structured-Tree Model of the Pulmonary Circulation

A multiscale mathematical and computational model of the pulmonary circulation is presented and used to analyse both arterial and venous pressure and flow. This work is a major advance over previous studies using structured trees to model vascular beds, e.g. Olufsen et al. (2012), which only address the arterial circulation. For the first three generations of vessels within the pulmonary circulation, the geometry is specified from patient-specific measurements obtained using magnetic resonance imaging (MRI). Blood flow and pressure in the larger arteries and veins are predicted using a nonlinear, cross-sectional-area-averaged system of equations for a Newtonian fluid in an elastic tube. The inflow to the main pulmonary artery is obtained from MRI measurements, while pressure entering the left atrium from the main pulmonary vein is kept constant at the normal mean value of 2 mmHg. Each terminal vessel in the network of 'large' arteries is connected to its corresponding terminal vein via a network of vessels representing the vascular bed of smaller arteries and veins. We develop and implement an algorithm to calculate the admittance of each vascular bed, using bifurcating structured trees and recursion. The structured-tree models take into account the geometry and material properties of the 'smaller' arteries and veins of radii ¿ 50 microns. We study the effects on flow and pressure associated with three classes of pulmonary hypertension expressed via stiffening of larger and smaller vessels, and vascular rarefaction. The results of simulating these pathological conditions are in agreement with clinical observations, showing that the model has potential for assisting with diagnosis and treatment of circulatory diseases within the lung. References: Olufsen, M.S., Hill, N.A., Vaughan, G.D.A., Sainsbury, C. & Johnson, M. (2012) Rarefaction and blood pressure in systemic and pulmonary arteries. J Fluid Mech 705:280-305

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MS80

Individualized Pulmonary Arterial Blood Flow Analysis

We propose an individualized pulmonary arterial blood flow analysis coupled to the lumped windkessel model of heart circulation and mechanics. The pulmonary arterial vasculature is from image segmentation of a mouse simplified as 1D centerline embedded in 3D with cross-sectional radius. We reveal the changes in blood flow patterns and right ventricular adaptation from vascular remodeling and rarefaction, which are consequences of pulmonary hypertension.

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MS80

Analysis of Cardiovascular Dynamics in Pulmonary Hypertensive C57BL6/J Mice

Data on RV pressure and volume, and systemic arterial pressure obtained before, during, and after inferior vena cava occlusion are analyzed using a mathematical model of realistic ventricular mechanics coupled with a simple model of pulmonary and systemic vascular systems. Model analysis suggests monotonic increase in PVR and PA elastance, consistent with prior experimental measurements. Model findings indicate a compensatory remodeling phase of RV precedes pathological remodeling that concludes with heart failure in pulmonary hypertension.

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MS81

Rare Events for Genetic Networks: Studying Interactions Between Meta-Stability and Time-Delays

The dynamics of gene networks are sometimes non-trivially influenced by events that happen on relatively short time scales. To study the impact of such events on gene networks it is not sufficient to study the steady state behavior. Instead, transient behaviors become very important. However, it is difficult to study relevant transient events numerically because they are rare, and the majority of the simulation time is spent sampling events that are not of interest. Therefore, theoretical methods for reliably sampling relevant transient methods for gene networks are required. In the absence of time delays, Langevin equations have proved to be a very important theoretical tool for the study of genetic networks. However, in models of gene networks that include transcriptional delay, such theoretical tools do not currently exist. In this talk, we present a proof of the weak convergence of time-delayed birth death processes to a class of functional Langevin equations. We further prove that as the system size approaches infinity, both these descriptions converge to the mean field limit. Finally, we obtain quantitative estimates on the distance between the birth-death process and the approximating Langevin process. This lays a rigorous groundwork for studying the dynamics of time-delayed birth-death processes by using functional stochastic differential equations.

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MS81

Impact of Stochastic Transcriptional Delay on Gene Networks

Abstract not available at time of publication.

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MS81

Queueing Approaches to Multisite Enzyme Kinetics

Queueing theory was developed long ago to understand the stochastic dynamics of discrete elements processed by a finite number of servers. Researchers have been developing a new biological queueing theory to describe how processing bottlenecks can strongly influence the dynamics of cellular systems. We now present a biological queueing theory for enzymes that can bind multiple substrates simultaneously, as with the *E. coli* protease ClpXP.

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MS81

First-Passage Time Calculations for Gene Net-

works: Implications for Phage Lambda Lysis Time

The inherent stochastic nature of biochemical processes can drive differences in gene expression between otherwise identical cells. While cell-to-cell variability in gene expression has received much attention, randomness in timing of events has been less studied. We investigate event timing at the single-cell level in a simple system, the lytic pathway of the bacterial virus phage lambda. In genetically identical single-cells, lysis occurs on average at 65 mins, with a standard deviation of 3.5 mins. Interestingly, mutations in the lysis protein, holin, alters both the lysis time mean and variance. Mathematically, lysis time is formulated as the first-passage time for cellular holin levels to cross a critical threshold. Analytical expressions for the first-passage time moments reveal how different model parameters modulate lysis time moments, and these predictions are verified with experiments. Finally, our analysis reveals regulatory motifs that enhance the robustness of lysis timing to cellular noise.

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PP1

Network Bursting in Inhibitory Neural Circuits

We study the rhythmogenesis of oscillatory patterns emerging in network motifs composed of inhibitory-coupled parabolic bursters represented by the Plant model of Aplysia-15 nerve cells. Such motifs are the building blocks of larger neural networks including central pattern generators controlling swim locomotion of sea slug Melibe leonine.

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PP1

Test Criterion for Finding the Global Minimum of a Function Using Exclusion Algorithm

The problem of finding the global minimum of a vector function is very common in science, economics and engineering. One of the most notable approaches to find the global minimum of a function is that based on interval analysis. In this area, the exclusion algorithms (EAs) are a well-known tool for finding the global minimum of a function over a compact domain. There are several choices for the minimization condition In this paper, we introduce a new exclusion test and analyze the efficiency and computational complexity of exclusion algorithms based on this approach.We consider Lipschitz functions and give a new minimization condition for the exclusion algorithm. Then we study the convergence and complexity of the method.

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PP1

Staying in Shape: Patterns in Radial Symmetry Provide Protein Structural Stability and Functionality

Toroidal WD40 repeat proteins, such as the beta subunit of heterotrimeric G-proteins, are important in cell signaling. Each repeating unit has about 40 amino acids, comprised of a trademark trpytophan and aspartate. With conventional comparative sequence analysis techniques, the strong signal from these signature positions can mask the importance of less conserved ones. We discuss how computational mutagenesis can overcome these limitations, explaining both the fundamental features of WD40 stability and the advantages of symmetry.

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PP1

Modeling the Deformation of Proteins: from Coarse-Grained to Continuum

There has been much research in the area of mathematically modeling of protein complexes using coarse-grained models or continuum models. We are proposing a new approach that will combine the potential energy found in elastic network model or residual based coarse-grained models, and stress/strain components to produce a stiffness matrix. This matrix will have the proteins anisotropic properties encoded within it. The computed anisotropic elastic moduli will be then used for simulating the deformation of protein-complexes.

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PP1

Demographics and Modeling of Multisite HPV Infection and Transmission

The Human Papillomavirus (HPV) infects the epithelial layer at several anatomical sites in the human body (anogenital and oral/nasalpharyngeal), and certain HPV genotypes can lead to the development of cancer. We present a statistical analysis characterizing HPV trends in the National Health and Nutrition Examination Survey (NHANES), with an emphasis on demographic differences in multiple site concurrent and type-concordant infection. Based on this data, we develop an ODE model of multisite HPV infection and transmission.

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PP1

Binocular Rivalry Waves in Directionally Selective Neural Fields

Binocular rivalry is the phenomenon that occurs when an observer is presented with two different conflicting images in the two eyes and the visual perception switches back and forth between the two images. We have analyzed this by constructing traveling wave solutions to a system of integro-differential equations describing the network activity of a population of directionally selective neurons. We have shown that waves travel faster in the direction of stimulus motion than against it.

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PP1

Modeling Interactions Between Two Major Southeastern U.S. Sea Turtle Nest Predators and Their Effects on Nest Depredation Rates

This project is investigating intraguild predation between two major sea turtle nest predators, North American raccoons and Atlantic ghost crabs. In addition, ghost crab predation assists raccoons in finding nests, thereby facilitating secondary nest depredation (i.e., facilitative predation). Our objectives are to characterize the dynamic interactions between intraguild predators and their effects on prey through the use of an ODE model and determine the role that facilitative predation has in influencing nest densities.

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PP1

Intrinsic Mechanisms for Pattern Generation in Three-Node Networks

Bursting patterns can be qualified and modeled using low-dimensional models. We show that, depending on intrinsic mechanisms of release, escape, and post-inhibitory rebound, reciprocally inhibitory Fitzhugh-Nagumo type networks can produce a range of phase-locked states such as anti-phase bursting, propagating waves, and peristaltic patterns with recurrently phase-varying lags. Phase-lag return maps identify phase states, with rhythm switching and attractor robustness revealed using external inhibition. Our qualification promotes the use of simplified modeling for CPG circuitries.

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PP1

Modeling the Dynamics of Opioid Abuse

We extend previous models of the population-level dynamics of drug abuse to describe opioid abuse. In particular, we derive a compartmental model that accounts for light and heavy prescription opioid users, heroin users, and the treatment-relapse cycle often observed in opioid addiction. We investigate the sensitivity of the models parameters to the heavy-prescription-opioid and heroin-using population. Finally, we derive and analyze the stability of the models fixed points, estimate several model parameters, and make predictions.

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PP1

A Computational Model for a Porous Viscoelastic Cytoskeleton with Applications to Cell Mechanics

Cell movement is crucial to physiological processes such as wound healing, cancer metastasis, and embryonic development. We present a computational framework to investigate cell movement involving either pressure-driven or polymer-rich protrusions. Our framework incorporates a porous viscoelastic cytoskeleton, a model of adhesion to the substrate, and a cell environment with changing material

properties. We quantify how cells mechanically sense their surroundings and react to changing environments by altering their shape and adhesion to the substrate to achieve optimal migration.

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PP1

Predicting Severity and Periodicity of Mountain Pine Beetle Outbreaks

We develop an age-structured forest demographic model that incorporates temperature dependent bark beetle infestation. The model is parametrized using data from a 1995-2005 outbreak in central Idaho. The stability of fixed points is analyzed as a function of (thermally controlled) growth rates, and indicates the existence of periodic outbreaks which increase with severity as growth rates increase. We devise an analytical method to predict outbreak severity and duration as well as expected time between outbreaks.

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PP1

Temperature Effects on REM/Non-REM Sleep Dynamics

Experimental work and prior models suggest changes in ambient temperature can affect sleep patterns in humans. We have designed a mathematical model describing numerous features of the human sleep/wake cycle and aspects of REM/non-REM dynamics. The model simulates temperature changes detected by neurons in the POAH that, in turn, affect the REM/non-REM cycles during sleep through a state-dependent homeostatic process. This model will help to better understand temperature and sleep relationships and support experimental findings.

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PP1

How Robust Is the Zero-Lag Synchrony When Two Neurons Interact Via a Third Relay Neuron

A remarkable zero time lag synchronization of two cerebral cortical areas with long distant, which results significant conduction delays, have revealed experimentally and numerically. It has been proposed that the synchronization of two delay-coupled oscillators can be achieved by relaying the dynamics via a third mediating element. Using phase oscillators, we have analytically investigated the dynamical relay problem for three oscillators.Our results show that the complete zero-lag synchrony can be achieved only in symmetric case, when the outer neurons are identical and the connections are symmetric. We have also shown that how phase lag of the outer neurons in the locked state depends on inhomogeneity in presence of small mismatch in the parameters of the neurons and the synapses. The results show very good agreement with numerical results of the conductance based models.

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PP1

Investigating the Effect of Atropine on Baroreceptor Heart Rate Regulation

Atropine and metropolol (betablockers) act as competitive antagonists of the neurotransmitters acetylcholine and noradrenaline within the autonomic nervous system. This study presents a non-linear baroreflex differential equations model, incorporating neurotransmitter concentrations. We investigate the impact of admission of atropine and metropolol on heart rate dynamics during head-up tilt. Global sensitivity analysis and optimization is used to validate and investigate the model using experimentally measured blood pressure and heart rate data for different doses of medication.

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PP1

Accelerated Uzawa Iteration for the Stokes Equations

The finite-element discretization of the Stokes equations leads to a saddle-point problem

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix} \quad (1)$$

where A is symmetric positive-definite and B is full-rank. The system (1) is explored using the Uzawa iteration

$$\begin{aligned} A\mathbf{u}_{k+1} &= \mathbf{f} - B^T p_k \\ p_{k+1} &= p_k + \omega B\mathbf{u}_{k+1}. \end{aligned}$$

Regarding this as a fixed-point iteration on $\mathbf{u}$ and p, we augment it with Anderson acceleration to improve the convergence. We show the results of a numerical study in which we compare the performance in several test cases of Uzawa iteration with and without acceleration as well as several alternative solution approaches.

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PP1

Determining An Optimal Mathematical Model for Tumor Growth

Cancer proves to be a major medical issue that is a leading cause of death and much research is devoted to finding effective treatments. Mathematical models play an important role in this effort by providing a framework to optimize proposed treatments. In order to make accurate predictions, models need to correctly predict tumor growth. We test previously proposed models of tumor growth by fitting them to data to determine an optimal model.

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PP1

Synchrony in Metapopulations with on-off Stochastic Dispersal

We consider ecological networks in which migration between patches and other intrinsic system parameters are stochastic in nature. We study the role of this stochasticity and how it relates to synchronization, especially in cases when the time scale of the stochastic process is slow with regard the inherent time scale of the system. We find that such a system can favor synchrony, despite the network being disconnected for large time intervals.

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PP1

Two-Theta Neuron: Phase Models for Bursting Networks

We propose a reduction approach to study bursting outcomes of central pattern generators using coupled two-theta phase models. We examine several configurations of 3-cell CPGs with inhibitory, excitatory and electrical synapses, and compare our findings with corresponding exemplary networks comprised of plausible Hodgkin-Huxley models. Occurrence, robustness and transformations of CPG outcomes are studied using 2D return maps, whose stable fixed points and invariant circles correspond to bursting patterns with fixed and varying phase lags.

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PP1

A Linear Analysis of a Straight Rod under Tension Both With and Without Drag

Starting with a straight rod under tension, we are studying the perturbations in twist and bend using the Kirchhoff Rod Model. Additionally, we can include the effects of drag approximated by resisted force theory. Finally, this model can inform us about the response of internal forces compared to external ones. This work has applications to the study of worm locomotion, bacterial flagella, and DNA.

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PP1

Conserved NPZ Models with Time Delay

Nutrient-Phytoplankton-Zooplankton (NPZ) models are used to describe the bottom two trophic levels of an underwater ecosystem. Time delays arise naturally in these models, such as the time it takes for juvenile plankton to reach maturity. Our focus is on models in which the total biomass in the system is conserved. We then explore how the quantity of biomass and the delay properties have on behaviour such as persistence and stability.

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PP1

Prediction of Biphasic Mitogenic Activity by Hgf, a Cancer-Associated Stroma-Derived Growth Factor, Using a Multi-Species Continuum Model.

A large number of growth factors and drugs are known to act in a biphasic manner: at lower concentrations they cause increased division of target cells, whereas at higher concentrations the mitogenic effect is inhibited. Often, the molecular details of the mitogenic effect of the growth factor are known, whereas the inhibitory effect is not. Hepatoctyte Growth Factor, HGF, has recently been recognized as a strong mitogen that is present in the microenvironment of solid tumors. Recent evidence suggests that HGF acts in a biphasic manner on tumor growth. We build a multi-species model of HGF action on tumor cells using different hypotheses for high dose-HGF activation of a growth inhibitor and show that the shape of the dose-response curve is directly related to the mechanism of inhibitor activation. We thus hypothesize that the shape of a dose-response curve is informative of the molecular action of the growth factor on the growth inhibitor.

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PP1

The Role of CD200-CD200R in Cancer Suppression and Promotion

CD200-CD200R is an inhibitive signal that tumor cells use it to silence macrophages in tumor microenvironment. It has been shown that CD200-CD200R has apparently two contradictory experimental results in tumor growth: inhibition and promotion. We develop a mathematical model to qualitative fits with experimental results and explain why these two opposite experimental results can both take place depending on the "affinity" of M1 and M2 macrophages to form the complex CD200-CD200R with tumor.

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PP1

Patient-Specific Modeling of Average Cerebral Blood Flow During Orthostatic Stress

Cerebral autoregulation is a combination of local mechanisms responsible for maintaining a stable cerebral blood flow during changes in arterial blood pressure. This talk presents a simple patient-specific autoregulatory model that predicts the average cerebral blood flow velocity amidst dramatic changes in arterial blood pressure during the sit-to-stand procedure. The model will be validated against experimental data and results will be compared to explore physiological differences between healthy young, healthy elderly, and hypertensive elderly individuals.

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PP1

Periodic Accumulation of Genetic Variation in the Genome of the Plant *Sorghum bicolor*

An organism's genome is a key determinant of its phenotype. Genetic variation produces much of the phenotypic variation on which evolutionary forces act, and we aim to identify signatures of factors influencing the accumulation of genetic variation. We show that periodic accumulation of genetic variation exists in the genome of the plant *Sorghum bicolor* and suggest that this periodicity is the result of biological phenomena, such as chromatin structure and selection.

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PP1

Gene Regulatory Network Based on a Novel Evolvable Partially Connected Artificial Neural Network

DNA microarray technology provides the expression levels of thousands genes and make it possible to investigate the complex biological processes. Finding relationships between genes and construct a Gene regulatory Network (GRN) is subject of interest. To this aim, we proposed a novel Partially connected Artificial Neural Network with Evolvable Topology (PANNET) in inferring the GRN from time series gene expression data. This approach can illustrate the underlying biological behaviors without prior knowledge of the system

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PP1

Accumulation Behavior

We introduce a Markov Chain variant to model the accumulation behavior of a population and provide a forecasted confidence set of items to be accumulated in a future period which may differ in length from the derived period. In non-sequential accumulation it will be established that the eigenvalues of this model are always real.

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PP1

Distribution of Correlated Spiking Events in Integrate-and-Fire Networks

Randomly connected populations of spiking neurons display a rich variety of dynamics. We address the conceptual issue of how to mathematically characterize the partially synchronous multiple firing events (MFEs) which manifest in between homogeneous and total synchronous dynamics. Using a geometric method for obtaining the distribution of magnitudes of these MFEs, we recast the cascading firing event process as a first-passage time problem, establishing a link between the voltage distribution of excitatory and inhibitory neurons and the number of neurons firing in an MFE.

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PP1

Modeling Dynamics of Mosquito Populations and Assessing Abatement Strategies for West Nile Virus

We designed a mathematical model and compared it with surveillance data for mosquitoes that are primary vectors of West Nile Virus (WNV). Based on the best fit of the model to the data, we estimated key parameters such as the effectiveness of insecticide treatments. We used these estimates for modeling the spread of WNV to obtain more reliable disease outbreak predictions and performed numerical simulations to test various mosquito abatement strategies.

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PP1

Activity Patterns of Neuronal Network with Voltage-Sensitive Piecewise Smooth Coupling

We present an analysis of activity patterns in a neuronal network of three mutually inhibitory cells with voltage-sensitive piecewise smooth coupling. While standard fast-slow analysis fails to describe the dynamics during fast jumps due to the voltage-sensitive nature of coupling, piecewise smoothness of coupling enables us to consider a sequence of fast subsystems in piecewise way. Our analysis shows that slow dynamics as well as fast dynamics incorporate to determine where fast jumps actually go.

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PP1

Modeling the Effects of Craniosynostosis on Intracranial Pressure

Craniosynostosis is a condition where the plates in a newborns skull fuse prematurely. In some cases cognitive development is impaired. Impairment is caused by increased intracranial pressure that arises in untreated craniosynostosis. Our research attempts to quantify the effect of craniosynostosis by mathematically modeling the growing skull/brain system and investigating how the fusion of various plates affects pressures in this system. We use the finite element method to solve the model equations, and conclude that in certain cases intracranial pressures rise above the critical value of 15 mmHg.

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PP1

Investigation of Dual Virus Infection of Human Respiratory Tract

Recent studies have revealed that about 40 percent of influenza like illness are caused by simultaneous infections by more than one virus. The effect of multiple virus infections on the severity of illness is not clear. We investigate a mathematical model of dual virus infections to determine conditions that make these infections more or less severe than single virus infections.

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PP1

Synchronization of Bursting Neurons: a Synergetic Effect of Excitation and Inhibition

We study synchronization of bursting neurons with excitatory and inhibitory connections. Fast inhibition is known to promote pairwise asynchrony in inhibitory bursting networks. We show that the addition of such repulsive inhibition to excitatory networks induces bursting synchrony,

in contrast to one's expectations. Through stability and geometrical analysis, we reveal the mechanism underlying this purely synergetic phenomenon and show that it originates from the transition between bursting of different types caused by excitatory-inhibitory synaptic coupling.

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PP1

Determining Mechanism of Action and Efficacy of Novel Influenza Antivirals

Influenza is a serious viral infection common in humans that can cause deadly pandemics. Drug treatment is a first line of defense against pandemics and many compounds are tested as influenza antivirals. We use mathematical models to identify experiments that can determine the mechanism of action of an influenza antiviral.

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PP1

Within-Host Models of Influenza Virus Infection: The Role of Macrophages

Influenza strains can be categorized as either with low (LP) or high pathogenicity (HP). We developed a mathematical model which includes the pathogenic role of the immune system cells to study the within-host dynamics influenza infections caused by the HP viruses. By comparing modeling predictions with both macrophage and viral kinetic data, we examined their contribution to the overall pathogenesis of HP viruses and quantified the difference between seasonal and HP viruses.

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PP1

Bursting in the Pituitary Corticotroph: The Role of Bk Ion Channels

Pituitary corticotrophs from male rats exhibit a variety of electrical activity patterns, including spiking and several forms of bursting. Stimulation with corticotrophin releasing hormone and arginine vasopressin convert the spiking to bursting. Surprisingly, the bursting occurs even though the SK type of calcium-activated potassium ion channels are not expressed. We use mathematical modeling to understand how calcium- and voltage-dependent BK channels can produce the bursting produced by stimulated corticotrophs.

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PP1

Identifiability of Linear Dynamical Systems from a Single Trajectory

In parameter estimation, before implementing numerical methods, it is important to determine whether the parameter estimation problem will have a unique solution in the presence of unlimited and error free data. This is the question of structural identifiability. For linear systems of ODEs , I will present a straightforward criterion for identifiability from one trajectory, solely based on geometric properties of the trajectory. Several illustrative examples will be discussed.

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PP1

From Chaos to Periodicity: Revisiting the Logistic Map with an Ecologically Realistic Spatial Structure and Dispersal Mechanism

We improve on traditional applications of the logistic map to spatially extended systems by explicitly introducing spatial length scale, dispersal shape, and absorbing boundary conditions. In this way we greatly improve ability to apply model outputs to real-world ecological systems. For a large range of parameters we find spatiotemporally chaotic population distributions abruptly give way to periodicity. As growth rate and dispersal distance increase, we witness an evolving metapopulation structure with three phases.

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PP1

Identifying Physiological Origins of Baroreceptor Firing Characteristics Through a Conductance Based Neural Model

In this study we investigate aortic baroreceptors, stretch

sensitive neurons with endings embedded in the arterial walls. The firing rate of these neurons is a key physiological signal in cardiovascular regulation. We investigate the physiological basis of key characteristics of this firing pattern through an ion channel based model of the membrane voltage. Comparisons of models with differing ensembles of ion channels provide insight into the origins of certain firing characteristics.

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PP1

Leaf Inclination Angle Regulates the Distribution of Light in the Sorghum Canopy

Light interception is the first step in photosynthesis. Mathematical modeling of the light environment of sorghum, an agriculturally important crop, predicts that changes in the angle that a leaf emerges on a plant will confer changes in its light interception. This led to the identification of loci associated with the genetic regulation of leaf inclination angle and continues to guide field experimentation toward optimizing light interception in sorghum.

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PP1

Modeling the Effect of Antiarrhythmic Agents on the Action Potential of Human Ventricular Cells

Sudden cardiac death from ventricular fibrillation is a major cause of death worldwide. Several different classes of antiarrhymia drugs are currently available each of which alters a different membrane ion conductance. A human cardiac cell model is used to study the effect of the different antiarrhythmia drugs on the physical characteristics of cardiac action potentials.

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PP1

Understanding and Distinguishing Three Time Scale Oscillations

Our goal is to understand bursting dynamics in three time scale systems. Such systems arise in biological settings such as the interaction of intrinsic calcium oscillations with a calcium-dependent, voltage-gated membrane potential oscillation mechanism. With this motivation, we construct a model having three time scales with two copies of Morris-Lecar equations. Using techniques from geometric singular perturbation theory, we explain the mechanisms underlying the dynamics and elucidate which characteristics truly represent three time scale features.

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PP1

Coupling-Induced Synchronization of Mexican Jumping Beans

Mexican jumping beans jump to move from higher to lower temperatures for optimal survival. By characterizing their jumping pattern containing two characteristic frequencies of jumping and rest, and by inducing a physical nearest neighbor coupling through the attachment of string, we seek to synchronize their motions experimentally. We compare this to computational results relating the behavior of the beans to an adaptation of Kuramoto model with frequency modulated oscillators accounting for the atypical jumping behavior.

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PP1

Phenotypic Modulation of Virulence Facilitates Pathogen Invasion of the Gut

The interior lining of the human intestine is inhabited by populations of commensal microbiota, which provide defense against invasive bacteria. Surprisingly, *Salmonella Typhimurium* gains an environmental advantage over the commensals by provoking the hosts inflammatory defenses. We develop and analyze a model of the competition between the commensals and Salmonella, which incorporates a simple model of the inflammatory response, to explore possible mechanisms by which Salmonella exploits the immune response to outcompete the commensals.

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