Dynamics Days 2019: Poster Abstracts

Poster Session A

Friday, Jan. 4, 7:30 p.m.–9:30 p.m.

Flash talks correspond to posters with "*" appended.

A1. Dynamical Representations of Heterochrony and the Developmental Process

Bradly John Alicea, Open Worm Foundation, Orthogonal Research and Education Lab

The original theory of heterochrony provides us with a generalized quantitative perspective on the dynamics of developmental trajectories. While useful, these developmental trajectories merely characterize changes in the speed and extent of growth in developmental time. More recent work on sequence heterochrony reconsiders heterochrony as a series of developmental events such as tissue development or morphogenetic transformations positioned according to their relative occurrence. One open problem in the literature involves how to characterize developmental trajectories, particularly for rare modes of development. By applying better representations of development along with the appropriate mathematical constructs, we hope to reveal interesting features of changes in growth given the plasticity and complexity of developmental timing.

This talk will present a range of potential dynamical approaches to characterizing heterochrony in a way that goes beyond existing models. Our approach is unique in that we reconsider the developmental trajectory as a series of autonomous developmental programs that contribute to changes in growth and form. With a focus on developmental timing, we will use formal techniques to characterize delays and bifurcations in the developmental trajectory. We also consider the role of multiple developmental programs operating either in parallel or serially that are able to characterize some of the immense diversity observed in animal development. Along the way, we will employ concepts such as delay dynamical equations and bifurcation theory that can enrich our understanding of heterochrony and complex developmental processes more generally.

Digital notebook and other materials available at: https://github.com/Orthogonal-Research-Lab/ heterochrony-and-delays

A2. Quantum Correlations For a Simple Kicked System with Mixed Phase Space

Or Alus, Rockefeller University; Shmuel Fishman, Technion - Israel Institute of Technology; Mark Srednicki, University of California Santa Barbara

The classical and quantum dynamics for a simple kicked system (the standard map) that classically has mixed phase space were investigated. For initial conditions in a portion of the chaotic region that is close enough to the regular region, the phenomenon of sticking leads to a power-law decay with time of the classical correlation function of a simple observable. Quantum mechanically, we find a somewhat different behavior. Several possible explanations of this phenomenon were considered, from which a modification of the Meiss-Ott Markov tree model is the most probable. This modification takes into account quantum limitations on the flux through a turnstile between regions corresponding to states on the tree.

A3. Characterizing Atrial Fibrillation Dynamics Using Multiplex Visibility Graphs

Konstantinos N. Aronis, Anastasiya Salova, Ariadna Venegas-Li, Andrea Santoro, Johns Hopkins University

Atrial fibrillation is the most common arrhythmia world-wide. Despite technological advances, the current therapeutic options have only modest long-term success rates [1]. This partially reflects the incomplete understanding of the dynamics underlying atrial fibrillation. In this work we characterize healthy (normal sinus rhythm) and fibrillatory cardiac dynamics by using visibility graphs [2] on multivariate time series [3], derived from simulations and clinical data.

We performed simulations of normal rhythm and fibrillatory dynamics using the mono-domain formulation of the Rogers and McCulloch model. Clinical data were recorded from 4 patients with atrial fibrillation before and after successful catheter ablation procedure using a multi-electrode basket catheter. From multivariate times series of simulated and clinical data, we constructed multiplex visibility graphs. We then compared the structural properties of multiplex visibility graphs between time series from healthy and fibrillatory rhythms. For both simulations and clinical data, the giant component of the multiplex visibility graph was higher in time series of normal rhythm compared to time series of fibrillatory rhythms. The structural efficiency of the multiplex graphs was higher in normal rhythm compared to fibrillatory rhythms.

Multiplex visibility graphs provide novel insights in cardiac dynamics, paving the way for a more in-depth characterization of fibrillatory rhythms. In particular, normal sinus rhythm is associated with multiplex visibility graphs that have greater connectivity and structural efficiency compared to fibrillatory dynamics. Our long-term goal is to develop a network-based method that could be used to define procedural end-points and identify alternative therapeutic targets.

A4. Nonlinear Map Model of Functional Quantum Entanglement in Photosynthetic Bacteria*

Siegfried Bleher, Fairmont State University

Work of Graham Fleming, Birgitta Whaley and their colleagues indicates that green sulfur bacteria may utilize relatively long-lived quantum entanglement among chromophores in bacteriochlorophyll molecules to enhance the efficiency of photosynthesis. Quantum entanglement in this case persists despite thermal perturbation from the environment. In this talk we ask whether the quantized version of a classically nonlinear model system (Hénon-Siegel map) whose phase space contains a mixture of stochastic and regular regions can provide support for the idea that persistence of quantum entanglement in biological molecules comes from 'tuning' between thermal noise and quantum localization.

A5. Model-Free Control of Chaos with Deep Reservoir Computing*

Daniel M. Canaday, Aaron Griffith, Daniel Gauthier, Ohio State University

Control of dynamical systems is a ubiquitous problem in many areas of physics and engineering. Particularly difficult to control are chaotic systems, which are sensitive to the small perturbations introduced by controller efforts. Early methods, such as the Ott-Grebogi-Yorke method and time-delayed feedback, were shown to successfully stabilize unstable steady states and periodic orbits in a range of chaotic systems. However, these methods require the controller to be switched on in a small neighborhood of the desired orbit. The time required to wait for this condition may be large, resulting in long control times. Further, they are not capable of controlling more general motions, such as periodic orbits not embedded in the attractor.

In this work, we propose a control algorithm that overcomes these limitations and achieves robust control of an unknown dynamical system to an arbitrary trajectory. The algorithm is based on a type of recurrent neural network known as a reservoir computer. The network is trained to invert the dynamics of the chaotic system, thereby directly learning how to control it. The resulting controller is a fully nonlinear dynamical system that can be switched on at any time to quickly stabilize desired behavior. We demonstrate our technique by controlling the Lorenz system to unstable steady states, unstable periodic orbits, and periodic orbits not on the Lorenz attractor. Our results show that deep reservoir computers are a powerful new tool in control engineering and chaos control, capable of learning a wide range of control laws for completely unknown systems.

A6. Computation of Sensitivities of Statistics in Chaotic Systems

Nisha Chandramoorthy, Qiqi Wang, Massachusetts Institute of Technology

In a chaotic system, the derivatives of state functions with respect to system parameters such as design or control inputs, grow exponentially with time. However, the infinite-time average of a state function, equal to its average according to the steady-state distribution over state-space, has a bounded derivative to parameters. Computing this statistical response to infinitesimal changes in parameters without the unstable long-time evolution of instantaneous derivatives is the objective of the perturbation space-split sensitivity (S3) algorithm. An efficient computation of the statistical response would enable uncertainty quantification, mesh adaptation, parameter estimation and other gradient-based multidisciplinary design optimization techniques that are still nascent in chaotic systems.

Based on the fact that perturbations that lie in the stable subspace decay in time exponentially, the contribution to the overall sensitivity from them is computed similar to in non-chaotic systems. The unstable contribution is reduced by an integration-by-parts procedure to a variance-reduced Monte-Carlo sampling. Unlike Shadowing-based computation wherein the sensitivity is computed along a single trajectory that is not guaranteed to be typical, this method is provably convergent. The S3 algorithm will be demonstrated on low-dimensional uniformly hyperbolic systems.

A7. Long-range Interactions of Kinks*

<u>Ivan C. Christov</u>, Purdue University; Robert J. Decker, A. Demirkaya; <u>University of Hartford</u>; Vakhid A. Gani; National Research Nuclear University MEPhI (Moscow Engineering Physics Institute); P. G. Kevrekidis, University of Massachusetts, Amherst; R. V. Radomskiy, P. N. Lebedev Physical Institute of the Russian Academy of Sciences

Field-theoretic models with polynomial potentials are of great interest in theoretical physics: from cosmology to condensed matter. The scalar ϕ^4 model with two minima of the potential is widely used to model spontaneous symmetry breaking. Properties of kinks (topological solitary waves) of the ϕ^4 and ϕ^6 models are well understood. Recently, there has been interest in field theories with polynomial potentials of higher degrees, due to applications in material science. In these models, kink can have power-law asymptotics of either or both tails connecting two distinct equilibria. These slowly decaying tails lead to long-range interactions. We make the case that such asymptotics require particular care when setting up multi-soliton initial conditions for simulations of kink collisions and interactions. Through detailed numerical simulations we show that naive implementation of additive or multiplicative ansätze gives rise to highly pronounced radiation effects and eventually produces the illusion of a repulsive interaction between a kink and an antikink in such higher-order field theories. We propose and compare several methods of "distilling" the initial data into suitable ansätze, which can then lead to simulations that do capture the predicted attractive force. We combine our numerical approach with recent updates to Manton's method for analytically estimating the long-range force of interaction between topological defects. This force, now, decays as some algebraic power of their separation. Excellent agreement is obtained between theory and simulations for these challenging highly nonlinear interactions in some canonical examples of the ϕ^8 , ϕ^{10} and ϕ^{12} field theories.

A8. Mathematical Model of Gender Bias and Homophily in Professional Hierarchies*

Sara M. Clifton, University of Illinois at Urbana-Champaign; Kaitlin Hill, University of Minnesota; Avinash Karamchandani, Northwestern University; Eric Autry, Duke University; Patrick McMahon, Grace Sun, University of Illinois at Urbana-Champaign

Women have become better represented in business, academia, and government over time, yet a dearth of women at the highest levels of leadership remains. Sociologists have attributed the leaky progression of women through professional hierarchies to various cultural and psychological factors, such as self-segregation and bias. Here, we present a minimal mathematical model that reveals the relative role that bias and homophily (self-seeking) may play in the ascension of women through professional hierarchies. Unlike previous models, our novel model predicts that gender parity is not inevitable, and deliberate intervention may be required to achieve gender balance in several fields. To validate the model, we analyze a new database of gender fractionation over time for 16 professional hierarchies. We quantify the degree of homophily and bias in each professional hierarchy, and we propose specific interventions to achieve gender parity more quickly.

A9. Nonlinear-Linear Alchemy: Koopman Operators, Linear Chaos, and Tape Recorders*

Ned J. Corron, US Army AMRDEC

We naively apply Koopman operator theory to obtain a linear, infinitedimensional representation of a chaotic one-dimensional iterated map. At first glance, the result appears pathologically simple and of little interest; it is mathematically equivalent to a tape recorder that provides storage and playback of the chaotic time series. However, the result does not explicitly depend on the particular iterated map, and we find the same Koopman operator dynamics can model any iterated map, including higher dimensional systems and even random signals. We then make a connection to the mathematical oddity of linear chaos, with the surprising result that a tape recorder, when viewed as a dynamical system, is provably chaotic. That is, a storage-and-playback system formally satisfies the three conditions in Devaney's definition of chaos: a transitive orbit, dense periodic orbits, and sensitivity to initial conditions. We conclude by clarifying the meaning of chaos in a tape recorder, which is not simply a restatement of chaos in the original iterated map. Rather, the Koopman operator works in an immense function space comprising all possible waveform recordings, and its chaotic nature provides the flexibility to playback anything, including chaos.

A10. Nonequilibrium Statistical Mechanics of Sudden Stratospheric Warming

Justin M. Finkel, Dorian Abbot, Mary Silber, Jonathan Weare, University of Chicago

Climate models are often perturbed by stochastic forcing to capture uncertainty, unresolved processes, and possible regime shifts. Examples include sea ice instabilities, rapid intensification of hurricanes, and sudden stratospheric warming (SSW), all of which develop through complex pathways in highdimensional phase space. The causes and effects of SSW are being actively investigated through simulation experiments. We study SSW using transition path theory, a mathematical framework of nonequilibrium statistical mechanics to calculate reaction rates and most-probable paths. We compute these dynamical quantities both for the stochastically forced quasi-geostrophic potential vorticity model from Birner & Williams (2008), and observational data from the NOAA SSW Compendium. Transition path theory allows us to forecast SSW probabilistically given the initial state of the atmosphere, using a "reaction coordinate" for monitoring progress toward a transition. We also reconstruct a probability distribution of reaction paths, which reveals coherent structures (e.g. eddies) that typically accompany SSW events. In this way, transition path theory offers a data-driven perspective on physical onset mechanisms of SSW, and a useful comparison with previous studies on its relationship to the Madden-Julian Oscillation, blocking events, and planetary waves.

A11. Data-Driven Order Parameters For Coupled Oscillator Models

Oscar L. Goodloe, Joel Nishimura, Arizona State University

Coupled oscillator models are a useful testbed for studying temporal coordination in complex systems with many agents. Typically, an order parameter for such a model is based off of the centroid of oscillators traveling around the unit circle in the complex plane. While this centroid approach works well for oscillator models where oscillators are equally likely to be at any point on the circle, it is inappropriate for measuring coordination in many-agent models where the underlying dynamical structure is uneven. In this setting, the traditional order parameter method can artificially report coordination in regions of the cycle where oscillators spend a disproportionate amount of time. We propose the creation of a data-driven order parameter to address these issues, taking a model of the reproductive behavior of Fundulus heteroclitus, commonly known as mummichog, as a practical example. Additionally, we explore different implementations of data-driven order parameters and consider the possibility of different order parameters providing orthogonal information, thus yielding a more complete informational picture of coordination within a system. We anticipate that developing data driven order parameters will be an important advancement for the study of complex systems with agents whose individual behavior is nontrivial.

A12. Using Exact Coherent Structures to Tile the Infinite Spacetime Kuramoto-Sivashinsky Equation

Matthew N. Gudorf, Predrag Cvitanovic, Georgia Institute of Technology

Exact coherent structures have been the subject of many recent investigations in fluid dynamics. One of the many reasons that these solutions are important is because their stable and unstable manifolds shape the geometry of the solution space, thereby playing an important role in the dynamics.

While these exact coherent structures have proved to be important, finding them has proved to be a very difficult computational problem. The difficulty is significant enough that exact coherent structures have only been found for the smallest computational domains for three dimensional fluid flows. We attempt to circumvent this computational difficulty by developing a spatiotemporal theory which forgoes chaotic dynamics in favor of treating space and time on equal footing. We will formulate our theory in the context of the spatiotemporal Kuramoto-Sivashinsky equation; this equation serves as a simpler starting place than the (3 + 1) dimensional Navier-Stokes equation.

This investigative effort focuses on finding, studying, and utilizing doubly periodic spatiotemporal solutions of the Kuramoto-Sivashinsky equation. Our hypothesis is that the behavior on infinite spatiotemporal domains can be explained via the shadowing of invariant 2-tori solutions. This work will present current results of this formulation which include new methods for finding doubly periodic solutions on arbitrary domain sizes as well as constructing new solutions from combinations of old solutions.

A13. Enhancing the Dynamic Modeling of the Curing of Ethyl Linoleate: Reaction Pathways For Epoxidation

<u>Rebecca E.</u> <u>Harmon</u>, Lindsay H. Oakley, Linda J. Broadbelt, Northwestern University

The drying process of oils is a complex cascade of reactions. It can be difficult to experimentally capture all species involved. Modeling of the reaction dynamics can be used as a tool to develop a mechanistic understanding of what is going on at the atomic and molecular level. Reaction families are used to represent possible classes of chemistry in a kinetic model. In the drying of ethyl linoleate, a representative molecule of resins and drying oils, examples of reaction families include hydrogen abstraction for radical formation, beta-scission to form aldehydes, and crosslinking into the subsequent polymer network. Adding new reaction families to a kinetic model does increase the computational expense because of the additional pathways and new species, but it allows for a more accurate representation of the process.

This work expands the chemistry in the automated reaction network generation of unsaturated fatty acid autoxidation and curing. Epoxide ring formation and opening reactions were implemented to capture the dynamics of the experimentally observed concentrations of epoxy groups reported in literature. Further investigation into proposed ring-opening mechanisms and their respective kinetic parameters is necessary to offer a better chemical foundation of the optimized kinetic rates, but the foundation for developing a refined model that can be extended to higher molecular weight oils and polymer networks has been established.

A14. Scalable Learning of Time-varying Vector Autoregression By Low Rank Tensors*

Kameron Decker Harris, Aleksandr Aravkin, Rajesh Rao, Bingni Wen Brunton, University of Washington

Linear autoregressive models are a classical, statistically justified method for modeling stationary timeseries, but in many systems the true dynamics are nonlinear or vary over time. We present a windowed method to learn timevarying autoregressive models from multivariate timeseries. This is an unsupervised method for uncovering spatiotemporal dynamical structure in data. Specifically, we assume that the third order tensor formed by stacking each window's system matrix is a linear combination of a few rank-one tensors, i.e. the canonical polyadic decomposition. We find the components using alternating least squares. Because of its low rank structure, the model is scalable to high dimensional data and can easily incorporate priors such as smoothness over time. In a test case, our method can identify the true rank of a switching linear system in the presence of noise. We also illustrate its usefulness in a nonlinear model and present preliminary results on motion capture as well as electrocorticographic brain recording data.

A15. The Effects of Collisions on Observational Signatures of Nonlinear Charged Particle Dynamics in the Magnetotail

$\underline{\text{Daniel}} \ \underline{\text{Holland}}, \ \underline{\text{Phillip}} \ \underline{\text{Kovarik}}, \underline{\text{Jonathan}} \ \underline{\text{Sullivan-Wood}}, \ \underline{Illinois} \ \underline{State} \ \underline{University}$

A frequently used approximation for the quiet-time magnetotail magnetic field that maintains the basic structure of self-consistent numerical calculations, is the modified Harris model, $B = B_0[\tanh(z/L)e_x + b_z e_z]$ where B_0 is the magnetic field strength far from the sheet, L is the scale length of the current sheet thickness and b_z is the ratio of the magnitude of the field at the mid-plane to the asymptotic field. Simulations of nonlinear charged particle dynamics in the modified Harris field have predicted the existence of a series of peak in the ion distribution function who's separation scales as the fourth root of the normalized ion energy which in turn depends on the combination of parameters $S = z^2 L$. This signature is the result of an underlying partitioning of phase space into regions corresponding to three dynamically distinct classes of orbits: 1) transient, 2) chaotic, and 3) integrable. Measurements of the peaks in the ion distribution function or differential particle flux, when combined with measurements of the magnetic field produce, act as a remote sensing mechanism to determine the mesoscale structure of the magnetotail. In this poster, we show observational evidence of the distribution signature form several different satellites and demonstrate it application in data analysis. Furthermore, we examine the effects of stochastic collisions on the phase space structures and on the observational signatures. We show that both are robust to small to moderate levels of "noise".

A16. Interphase DNA As a Self-returning Random Walk

Kai Huang, Igal Szleifer Northwestern University

We introduce a self-returning random walk to describe the structure of interphase chromatin. Based on a simple folding algorithm, our de novo model unifies the high contact frequency discovered by genomic techniques, and the high structural heterogeneity revealed by imaging techniques, which two chromatin properties we theoretically prove to be irreconcilable within a fractal polymer framework. Our model provides a holistic view of chromatin folding, in which the topologically associated domains are liquid-tree-like structures, linked and isolated by stretched out, transcriptionally active DNA to form a secondary structure of chromatin that further folds into a "3D forest" under confinement. The model pivots a wide array of experimental observations and suggests the existence of a universal chromatin folding principle. Based on a global folding parameter, the model reveals a unique structure-function relation of chromatin, which is abnormal from a polymer point of view but explains some experimental observations of how chromatin responses to stress.

A17. The Unruly Effective Diffusion Coefficient of Phase-Locked Bursters

Avinash Jagdish Karamchandani, Hermann Riecke, Northwestern University

We investigate the noise response properties of phase-locked bursters, i.e. bursters in which the fast oscillations are phase-locked to the slower burst cycle. We find that the phase response of such bursters to noise is quite unruly: the effective "output" diffusion is non-monotonic in the input noise strength and greatly enhanced compared to a linear prediction.

The dynamics of the principal neurons of the mammalian olfactory bulb serves as a motivating example. The cells' membrane potentials exhibit mixedmode oscillations with both the large amplitude spikes typical of neurons and small amplitude, sub-threshold oscillations (STOs). Noisy input from upstream neurons can strongly perturb the patterns of spikes and STOs displayed, as is reflected in an unruly diffusion coefficient for spiking times. The noise-driven perturbations can greatly affect the spike-driven interactions between cells, and we note the implications of the diffusion on coherent, population-level behavior.

We show how the extreme sensitivity of the spiking to noisy inputs can be generalized. We capture the bursting mechanism of the specific 9-dimensional neuronal model in a 3-dimensional canonical burster model, which we reduce in turn to a simple stochastic circle map with a labeling of some states as "spikes" and some as "STO peaks". The dramatic qualitative features of the effective diffusion persist across this drastic simplification, and we make use of the simple model to elucidate them.

A18. Dynamical Stability of the Outer Solar System in the Presence of Hypothesized "Planet Nine"*

<u>Tali Khain</u>, University of Michigan; Konstantin Batygin, Michael E. Brown, California Institute of Technology

The outer Solar System is populated with a large number of small rocky bodies, called Kuiper Belt objects (KBOs), which orbit the Sun beyond Neptune. In the last few years, the orbital configuration of the most distant KBOs has been used as evidence for the existence of a new Neptune-sized planet ("Planet Nine") on a highly elliptical and distant orbit [1]. In this presentation, I will discuss the results of both numerical simulations and theoretical analysis that model the effect of Planet Nine on the KBO orbits. Not all objects remain stable in the presence of this external perturber; in fact, Planet Nine allows for the existence of two populations of KBOs, ones that are apsidally aligned with its orbit and ones that are apsidally anti-aligned. With the help of simple geometric arguments, we identify the mechanisms which enable the persistent stability of these objects and locate the regions of phase space in which they reside [2]. This analysis provides context for the observed orbital clustering of the known Kuiper Belt objects and offers insight to the ongoing search for Planet Nine.

 $\left[1\right]$ Konstantin Batygin and Michael E. Brown (2016), The Astronomical Journal, 151, 22

[2] Tali Khain, Konstantin Batygin, and Michael E. Brown (2018), The Astronomical Journal, 155, 250

A19. Levitating Granular Cluster: Typical Behavior and Noise-induced Rare Events*

Evgeniy Khain, Oakland University

Granular matter is ubiquitous in nature and exhibits a variety of nontrivial phenomena. In addition, granular medium is intrinsically far from equilibrium, as particles collide inelastically, and a continuous energy input is required to ensure a steady state. Within the same system, different regions of granular media can be at a solid or a gas phase. Here we focus on a granular Leidenfrost effect: a solid-like cluster is levitating above the "hot" granular gas [1]. This state was observed experimentally, when granular matter was vertically vibrated in a two-dimensional container [2]. The solid-gas coexistence can be described by using granular hydrodynamics with the properly measured transport coefficients [3]. We performed extensive molecular dynamics simulations of a simple model of inelastic hard spheres driven by a "thermal" bottom wall. Simulations showed that for low wall temperatures, the levitating cluster is stable, while for high wall temperatures, it breaks down, and the hot gas bursts out resembling a volcanic explosion [4]. We found a hysteresis: for a wide range of bottom wall temperatures, both the clustering state and the "volcanic" state are stable. However, even if the system is at the (stable) clustering state, a volcanic explosion is possible: it is a rare event driven by large fluctuations. We used techniques from the theory of rare events to compute the mean time for cluster breaking to occur: this required the introduction of a two-component reaction coordinate [4].

References:

[1] B. Meerson, T. Pöschel, and Y. Bromberg, Phys. Rev. Lett. 91, 024301 (2003).

[2] P. Eshuis, K. van der Weele, D. van der Meer, and D. Lohse, Phys. Rev. Lett. 95, 258001 (2005); N. Rivas, A.R. Thornton, S. Luding, and D. van der Meer, Phys. Rev. E 91, 042202 (2015).

[3] E. Khain, Phys. Rev. E 98, 012903 (2018).

[4] E. Khain and L. M. Sander, Phys. Rev. E 94, 032905 (2016).

A20. Dynamics of Multi-Agent Reinforcement Learning

Jimmy Kim, <u>Daniel Shams</u>, Northwestern University; David Schwab, ITS $_{CUNY}$

Reinforcement learning has been gaining popularity over past several years. Many of the algorithms require selection of hyperparameters, and it is unclear how these choices affect the learned policy. Often in practice, researchers choose hyperparameters for their simulations using brute force methods such as exhaustive grid search or heuristics without fully understanding how they may alter the effective reward structure and value function landscape. This approach is especially detrimental in the setting of multi-agent reinforcement learning where the learning dynamics of each agent depends on the complex interplay between all the parameters. Here, we investigate how different hyperparameters affect the learning dynamics in simple games and show that a dynamically informed choice of hyperparameters could lead to an exploitation of a naive agent.

A21. New Numerical Evidence That Nonlinearity and Local Depletion Reduce Variability in the Single Photon Response of Vertebrate Rod Photoreceptors

Colin Klaus, Mathematical Biosciences Institute; Giovanni Caruso, Italian National Research Council; Vsevolod Gurevich, Vanderbilt; Clint Makino, Boston University; Heidi Hamm, Emmanuele DiBenedetto, Vanderbilt

Rod photoreceptors are known to signal in dim-light even at the threshold of a single photon event. This single photon response (SPR) is detected in spite of inherent randomness in the transduction cascade. Sources of variability include the spatial site of photon detection, the random walk undertaken by activated GPCR, and its randomly distributed sojourn times before phosphorylation and arrestin shut-off. Using a novel and *homogenized* 3D spatiotemporal PDE model of rod photoreceptor cells, mechanisms that suppress the cascade's variability are numerically investigated. This model is a system for diffusing 2nd messengers cGMP and Ca²⁺ with nonlinear couple in their Neumann data. New numerical evidence demonstrates that nonlinear gating

of ion channels by cGMP, as well as local depletion of cGMP at the site of photon capture, play significant roles in reducing cascade variability. The effects of 3D geometry on variability are also explored through comparison with 1D and Well-Stirred models.

A22. Optimizing Simulations of Shaken Granular Media

<u>Anirrudh</u> Krishnan, Nicholas Corkill, Jonathan Bougie, Loyola University Chicago

We use modern computational techniques to numerically solve a set of granular hydrodynamics equations. A granular hydrodynamics approach models systems of grains as a continuous medium in order to apply methods originally developed for the study of fluids. As part of an ongoing series of investigations of patterns and shocks in vertically oscillated layers of granular media, we employ Forward-Time, Centered-Space (FTCS) differencing on a three-dimensional grid to simulate the evolution of continuous flow fields. We are optimizing our simulation to increase the efficiency of data collection in order to improve the accuracy of our analysis. Since our analysis requires large amounts of data, we employ distributed computing methods, using a hybrid openMP-MPI solution. MPI is used to distribute data throughout a network of computers, and openMP parallelizes the calculations on each node. Our open-MPSimulation shows significant speedup over a serialized version, and MPI will coordinate data streams between the cluster of nodes.

A23. Computer Simulation of the Atomic Transfer Process in Slotted Systems with an Arbitrary Wall Inclination Angle

Alexander T. Kucher, L.V. Pletnev, G.M. Suslov, C. Zhang

The process of atoms transfer in systems is of interest, both from a theoretical and practical point of view. The motion of atoms in the intermediate and free-molecular flow regimes depends not only on the collisions of atoms in the gas phase, but also on the collisions of atoms with the walls of systems. The main problem is the gas-surface interaction. From a practical point of view, the movement of atoms evaporated from the surface of the condensed phase in slotted systems with different angles of inclination of the system walls allows controlling the flow of atoms emitted from the systems in the processes of molecular beam epitaxy. In all flow regimes atoms move in systems chaotically from the surface of the condensed phase from which they depart before colliding with the walls of the system. Of particular interest is the chaotic transfer of atoms with weak evaporation from the surface of the condensed phase, which leads to a free molecular flow regime in the gas phase, i.e. practically without collisions of atoms with each other. It turns out an interesting situation when a set of atoms makes a chaotic motion, but can accurately track the movement of each atom in the system. The analysis of such motion of atoms can be realized by the Monte Carlo method of direct modeling. In computer experiments, the distributions of collisions of atoms with the walls of systems, the angular distributions of departing atoms and the density of atoms distributions over

sprayed surfaces were determined depending on the relative heights of system's walls, the angles of inclination of the system's walls, the number of atoms collisions with the walls of systems and the dimensionless parameter r = U/kT. In this equation, U is the potential barrier on the surface of condensed phase, k is the Boltzmann constant and T is the temperature of the system.

A24. Frequency Shredding and Its Presence in Nonlinear Fluid Flows*

Michael Lee, Earl Dowell, Duke University

Computational simulations of a two-dimensional incompressible regularized lid-driven cavity flow were performed to characterize the flow's progression from periodic to chaotic flow. As the Reynolds number was increased, the flow was observed to progress from periodic to quasi-periodic flow without any observed period-doubling; the flow's toroidal attractor then became unstable and aperiodic flow resulted; single-periodic behavior, stable in long time, then suddenly appeared at a higher Reynolds number; the flow then quickly progressed back through quasi-periodicity to aperiodicity as the Reynolds number continued to increase. A power spectrum analysis, in which the novel concepts of frequency shredding and power capacity are introduced, was performed with the conclusion that although several qualitative changes in flow state were observed, only two bifurcations formally occurred: 1) the initial Hopf bifurcation and 2) when the flow first became quasi-periodic. All other changes in the flow's dynamics were explained by the known mechanism of frequency entrainment and the novel mechanism of frequency shredding. Frequency shredding, while currently founded in observation but not kinematics, therefore demonstrates potential as a mechanism by which known flow instabilities may interact. Such an analysis may serve as a new approach for characterizing multi-scale nonlinear dynamical systems.

A25. Comparing the Growth of Internet Access Worldwide

Jiachen Liu, Haley Yaple, Carthage College

In the past few decades, more and more people around the world started to have access to internet. The proportion of people who have access to internet has significantly increased about 10 times in the past 18 years. We evaluate and predict the trend of increasing internet usage in the future for different counties by using mathematical modeling methods. We use a differential equation to represent the rate of change of the proportion of internet users for any arbitrary population. In particular, we focus on 10 developed countries and 10 developing counties. Based on real data, we compare best-fit parameters for the two sets of counties. We use these fits to make predictions about the proportion of people who will have access to internet in the future.

A26. Puzzles and Piecewise Isometries - 1D, 2D, and 3D Possibilities *

Lachlan D. Smith, Paul B. Umbanhowar, Julio M. Ottino, <u>Richard M.</u> Lueptow, Northwestern University

An array of possibilities for cutting-and-shuffling mechanisms, also known as piecewise isometries (PWIs), are grounded in one-dimensional systems, evolving from there to two-dimensional planar, two-dimensional spherical, and three-dimensional geometries. Many of the higher dimensional cutting and shuffling motions are natural extensions of interval exchange transformations (IETs), which are defined as cutting-and-shuffling on a line interval and are the only way to cut-and-shuffle in one dimension. To guarantee that PWIs can be performed on solid bodies without solids overlapping or the domain needing to be deformed or extended, it is necessary to introduce the concept of PWIs that are time-continuous. PWIs with this property are easier to implement in experiments and applications, as we demonstrate through their connection to static mixers for fluids, mixing in spherical granular tumblers, and "twisty puzzles," such as the Cohan circle puzzle and the spherical version of the Rubik's cube. Partially supported by NSF grant CMMI-1435065.

A27. A Pharmacokinetic Model of Lead-Calcium Interactions

$\underline{\text{Tucker}} \ \underline{\text{Lundgren}}, \ \text{Anca Radulescu}, \ State \ University \ of \ New \ York \ at \ New \\ Paltz$

Lead is a naturally-occurring element. It has been known to man for a long time, and it is one of the longest established poisons. The current consensus is that no level of lead exposure should be deemed "safe." New evidence regarding the blood levels at which morbidities occur has prompted the CDC to reduce the screening guideline of 0.01 mg/dl to 0.002 mg/dl. Measurable cognitive decline (reduced IQ, academic deficits) have been found to occur at levels below 0.01 mg/dl.

Knowledge of lead pharmacology allows us to better understand its absorption and metabolization mechanisms that produce its medical consequences. Based upon an original and simplistic compartmental model of Rabinowitz (1973) with only three major compartments (blood, bone and soft tissue), extensive biophysical models sprouted over the following two decades. However, none of these models have been specifically designed to use new knowledge of lead molecular dynamics towards understanding its deleterious effects on the brain. We will present and analyze a compartmental model of lead pharmacokinetics, focused specifically on neurotoxicity. Our model captures mathematically the complex nonlinear interaction between lead and calcium along their dynamic trajectory through the body. We will focus on showing how an imbalance in this interaction may readily lead to the neuro-behavioral effects.

A28. Connected Tiling Structures Within a Fractal Sea

<u>Thomas F. Lynn</u>, Northwestern University; Lachlan D. Smith, University of Sydney; Julio M. Ottino, Paul B. Umbanhowar, Richard M. Lueptow, Northwestern University

Mixing due to cutting-and-shuffling has been studied using the mathematical framework of piecewise isometries (PWIs). Specifically, the mixing of a hemispherical shell rotated about two orthogonal axes has become a canonical example. A new computational method for efficiently executing the cuttingand-shuffling using parallel processing allows for extensive parameter sweeps. This permits a relaxing of the restrictions of orthogonal rotation axes allowing for the exploration of a new degree of freedom that can break the symmetries inherent in the orthogonal axes PWI, leading to better mixing. Expanding the parameter space to include non-orthogonal axes arrangements reveals underlying Arnold tongues when rational rotations appear in the PWI. Outside of these tongues, mixing happens within a fractal set of accumulated discontinuities, but Arnold tongues inside a fundamental plane of symmetry correspond to a connected class of PWIs that tile the hemisphere in polygons.

A29. Modes of Information Flow

Blanca Daniella Masante Ayala, Ryan G. James, James P. Crutchfield, University of California Davis; Bahti Zakirov, College of Staten Island

Information flow between components of a system takes many forms and is key to understanding the organization and functioning of large-scale, complex systems. We demonstrate three modalities of information flow from time series X to time series Y. Intrinsic information flow exists when the past of X is individually predictive of the present of Y, independent of Y's past; this is most commonly considered information flow. Shared information flow exists when X's past is predictive of Y's present in the same manner as Y's past; this occurs due to synchronization or common driving, for example. Finally, synergistic information flow occurs when neither X's nor Y's pasts are predictive of Y's present on their own, but taken together they are. The two most broadly-employed information-theoretic methods of quantifying information flow—time-delayed mutual information and transfer entropy—are both sensitive to a pair of these modalities: time-delayed mutual information to both intrinsic and shared flow, and transfer entropy to both intrinsic and synergistic flow.

To quantify each mode individually we introduce our cryptographic flow ansatz, positing that intrinsic flow is synonymous with secret key agreement between X and Y. Based on this, we employ an easily-computed secret-keyagreement bound—intrinsic mutual information—to quantify the three flow modalities in a variety of systems including asymmetric flows and financial markets.

A30. Hebbian Model of the Structural Plasticity in the Olfactory System

John Hongyu Meng, Hermann Riecke, Northwestern University

How animals can discriminate between different sensory stimuli, e.g. similar odors, is an intriguing question. In the olfactory system the olfactory bulb is the first brain area to receive sensory input from the nose. It exhibits persistent structural plasticity: i) synaptic connections between excitatory principal neurons and inhibitory interneurons are formed and eliminated, ii) interneurons are added and removed from the network. This structural plasticity is crucial for the learning of certain odor tasks. Here we present a Hebbian-type model to understand how synaptic structural plasticity can contribute to this learning.

Based on experiments, we assume that synaptic structural plasticity follows Hebbian-type rules: co-activation of a principal cell and an interneuron leads to the formation of a synapse connecting them; if the principal cell is active, but not the interneuron, the connecting synapse is removed; if the principal neuron is not active the synapse is unchanged. In addition, the total number of synapses of each interneuron is limited.

Experiments show that during learning the responses of the principal cells and the discriminability of odors change qualitatively in a different way depending on the difficulty of the task. Our model captures key aspects of these results if we allow the network to be exposed to other stimuli before the learning of the relevant tasks. This suggests that previous memory influences the behavior during learning

A31. Detecting Dynamically Generated Communities in Complex Networks

Alex Mercanti, Adilson E. Motter, Northwestern University

Statistical network models have often been proposed as tools for inferring latent community structure in observed networks. It is commonly believed that such communities inferred by these models roughly correspond to groups of nodes in the network that behave similarly in some sense. While this can often be verified empirically for networks with known annotations, these models typically offer little insight into what types of communities they are capable of detecting and additionally fail to propose a plausible mechanism for their generation. In contrast, recent research in the field of network dynamical systems has related equitable or balanced partitions of networks to cluster synchronized states for a broad range of systems. Such partitions truly group together nodes with identical behavior or dynamics, but are prohibitively restrictive in practice as the required partitions tend to have few non-trivial clusters. Here, we bridge the gap between these two lines of research and present a novel generative network model based on a statistical relaxation of the notation of an equitable network partition. We further demonstrate the efficacy of our model for the tasks of network metadata inference, link prediction for recommendation systems, and dynamical system model reduction.

A32. Dimer Chain with Single Impurity

Abhik Mukherjee, Igor Barashenkov, University of Cape Town, South Africa

Not long ago, Bender and Boettcher [Phys.Rev.Lett 80, 5243,1998] suggested that parity (P) and time (T) symmetries can be responsible for purely real spectra of non-Hermitian operators. These developments suggested further extension of the theory to include nonlinearity, which is inherent in many fields of physics and is responsible for a wide variety of new phenomena. More analysis on the PT symmetric discrete lattice has been done in the last decade[Rev.Modern.Phys, Vol88,July-Sept 2016]. Our problem is to study the properties of a long chain of PT-symmetric dimers of equal gain and loss in presence of a single impurity. We have first considered linear system, which can easily be decomposed in to an eigenvalue problem. If the number of dimers be N where each waveguide interacts with each other with a nearest neighbor interaction, the corresponding matrix of the eigenvalue problem would be of the order (2N X 2N). It can be shown that for the homogeneous system, when the gain/loss coefficient is > 1, PT symmetry breaking occurs. For a threshold value of the gain/loss coefficients instability in the system sets in and PT symmetry breaking occurs. This is a very important phenomena to observe scientifically. Our main objective and aim is to study this symmetry broken phase of the system. Such theoretical problem may have useful applications in Nonlinear Optics, Photonics, Communications etc. In order to look at the problem with more details, we will first consider an infinitely long array of dimers with the impurity at the center(origin). The PT-symmetry breaking threshold is found out with depends on the coupling constant. Next, the problem is extended to consider finite chain of dimers with periodic and vanishing boundary conditions. The results are shown to differ from the infinite case. More intricate situation arises when we consider the nonlinear terms, which is our future problem.

A33. Multifaceted Dynamics of Janus Oscillator Networks*

Zachary G. Nicolaou, Deniz Eroglu, Adilson E. Motter, Northwestern University

Recent research has led to the discovery of fundamental new phenomena in network synchronization, including chimera states, explosive synchronization, and asymmetry-induced synchronization. Each of these phenomena has thus far been observed only in systems designed to exhibit that one phenomenon, which raises the questions of whether they are mutually compatible and of what the required conditions really are. Here, we introduce a class of remarkably simple oscillator networks that concurrently exhibit all of these phenomena, thus ruling out previously assumed conditions. The dynamical units consist of pairs of non-identical phase oscillators, which we refer to as Janus oscillators by analogy with Janus particles and the mythological figure from which their name is derived. In contrast to previous studies, these networks exhibit: i) explosive synchronization in the absence of any correlation between the network structure and the oscillator's frequencies; ii) extreme multi-stability of chimera states, including traveling, intermittent, and bouncing chimeras;

and iii) asymmetry-induced synchronization in which synchronization is promoted by random oscillator heterogeneity. These networks also exhibit the previously unobserved possibility of inverted synchronization transitions, in which transition to a more synchronous state is induced by a reduction rather than increase in coupling strength. These various phenomena are shown to emerge under rather parsimonious conditions, and even in locally connected ring topologies, which has the potential to facilitate their use to control and manipulate synchronization in experiments.

A34. Motif Dynamics on Signed Directed Complex Networks

Youngjai Park^(1,2), Young Jin Kim^(1,3), Seung-Woo Son^(1,2). ¹Hanyang University, Korea; ²University of Calgary, Canada; ³Korea Institute of Science and Technology, Korea

Complex systems such as ecosystems, financial markets, brains, and our society can be expressed as evolving complex networks, where a node presents each species or component and a connecting link presents interactions or effect between them. We are considering signed directed networks which are evolving as time goes, where each connection contains a positive or negative sign and a in- or out-direction. In these networks, one can find more various kinds of network motifs, which are patterns that appear in a network much more than one would expect in degree conserved randomized networks, than before when only considering the directionality. We investigate the motif dynamics by counting the number of each motif as a function of time. The motif dynamics, i.e., changes in motif patterns are essential for understanding the stability of the corresponding networks.

In this work, we evaluate the motif dynamics in order to interpret the role of each motif affecting the stability of complex networks. We define 22 kinds of 3-node-motifs and measure their Z-scores, which evaluate how much an occurrence deviates from the mean of null models conserving the degree information. We analyze the motif dynamics by measuring these Z-scores as a function of time to quantify how much significant the observed motifs are in terms of dynamic stability. Other network properties such as clustering coefficient and the burstiness of network size are also investigated as well as motif dynamics while the size evolves as a function of time in order to compare their effects to network stability. We find that particular motifs relate to conserving the network stability and their meaning on the corresponding complex networks. We expect analysis with the motif dynamics helps us for better understand about our surrounding complex systems. Furthermore, this approach provides new insight into complex systems management by measuring a sign of network stability.

A35. The High Forecasting Complexity of Noisy Periodic Orbits Limits the Ability to Distinguish Them From Chaos*

Navendu S. Patil, Joseph P. Cusumano, Pennsylvania State University

A long-standing question in applications of dynamical systems theory is how to distinguish noisy signals from chaotic steady states. Information-theoretic complexity measures hold promise to resolve this problem. For example, while stochastically perturbed limit cycles become increasingly unpredictable with noise, they are nevertheless less complex than chaotic states. Thus, one might hope that quantification of dynamical complexity, taken together with a measure of stochasticity, could help classify a system's qualitatively distinct steady states. Here, we explore two information measures applied to numericallycomputed phase-space trajectories of continuous-state nonlinear oscillators: forecasting or statistical complexity (Grassberger, 1986; Crutchfield & Young, 1989), which quantifies the minimum memory required for the optimal prediction of discrete observables; and the entropy rate, which quantifies their intrinsic unpredictability. We estimate empirical generating partitions (Patil & Cusumano, 2018) to obtain discrete observables which faithfully represent continuous-state time series. We find that a stable, high-period (p = 15) orbit of a stochastically perturbed, periodically driven Duffing oscillator admits high values of both information measures, making it difficult to distinguish it from chaotic states at adjacent parameters, even with small noise. However, for a low period (p=3) orbit, such a distinction becomes easier, as both measures admit considerably lower values compared to a chaotic attractor at a nearby parameter. Furthermore, we find that the complexity of periodic orbits increases with noise ("noise-induced chaos"), while that of chaotic attractors decays. We discuss how the possibility of chaos-noise distinction is severely impacted by the ambiguity of model order selection when estimating forecasting complexity, and how the exact choice of discrete observables used to encode phase-space trajectories affects the information measures.

A36. Asymptotic Sets in Networks of Coupled Quadratic Nodes

Anca Radulescu, Simone Evans, SUNY New Paltz

We study asymptotic behavior in networks of n nodes with discrete quadratic dynamics. While single map complex quadratic iterations have been discussed over the past century, considering ensembles of such functions, organized as coupled nodes in an oriented network, generates new questions with potentially interesting applications to the life sciences.

We discuss extensions of traditional results from single map iterations, such as the existence of an escape radius; we then investigate whether crucial information about the network is encoded in the behavior of the critical orbit. We consider the network Mandelbrot set (i.e., the set of quadratic parameters in n complex dimensions for which the network is postcritically bounded). Using a combination of analytical techniques and numerical simulations, we study topological properties of the diagonal slice of the Mandelbrot set, which we call the equi-M set. We find that, while equi-M sets no longer have a hyperbolic bulb structure, some of their geometric landmarks (e.g., the cusp) are preserved for any network configuration, and other properties (such as connectedness) depend on the network structure. We finally explore potential implications to dynamic networks in the life sciences.

A37. Improved Newton Linearization for L^1 -Norm-Type Minimization with Application to Viscoplastic Fluid Solvers

Johann Rudi, Argonne National Laboratory; Georg Stadler, New York University: Omar Ghattas, University of Texas at Austin

We target highly nonlinear applications in CS&E that are modelled by optimization problems with Hessians exhibiting a problematic (near) null space upon linearization with Newton's method.

The null space is caused by a projector-type coefficient in the Hessian, which is created by terms in the objective functional that resemble the L^1 -norm. This occurs, e.g., in nonlinear incompressible Stokes flow in Earth's mantle with plastic yielding rheology, which effectively limits stresses in the mantle by weakening the viscosity depending on the strain rate. Another example is total variation regularization for inverse problems. Using a standard Newton linearization for such applications is known to produce severe Newton step length reductions due to backtracking line search and stagnating nonlinear convergence. Additionally, these effects become increasingly prevalent as the mesh is refined.

We analyze issues with the standard Newton linearization in an abstract setting and propose an improved linearization, which can be applied straightforwardly to Stokes flow with yielding and total variation regularization. Finally, numerical experiments compare the standard and improved Newton linearizations in practice. When we employ our improved linearization within our inexact Newton-Krylov method, a fast and highly robust nonlinear solver is attained that exhibits mesh-independent convergence and scales to large numbers of cores with high parallel efficiency.

A38. Wavenumber Selection in Pattern Forming Systems

Saloni Saxena, J. Michael Kosterlitz, Brown University

Pattern forming systems are characterized by the emergence of a band of stable spatially periodic states as a control parameter is varied. Wavenumber selection refers to the evolution of such systems to one of these states at long times, irrespective of initial conditions. Numerical studies of pattern forming phenomena indicate that the presence of noise is a mechanism for wavenumber selection at long times [1]. We investigate this for the Stabilized Kuramoto Sivashinsky (SKS) equation. Computational difficulties restricted earlier numerical simulations of this equation to small system sizes and a narrow range of control parameters. Our aim now is two-fold: to determine whether state selection occurs for larger and larger system sizes and to do so for a broader range of control parameter values. By simulating large system sizes, we hope to identify the noise selected wavenumber in the thermodynamic limit. With the use of spectral methods of integration, we have been able to simulate larger system sizes and obtain a crude probability distribution of final states. We present our results for various system sizes and demonstrate a possible connection to large deviation theory [2]. The drawbacks of our approach and possible improvements are also discussed.

[1] D. Obeid, J. M. Kosterlitz, and B. Sandstede, Phys. Rev. E 81, 066205 A41. Effects of Shear-rate Dependent Viscosity on the Flow of a (2010).

[2] H. Touchette, Physics Reports 478, 1, (2009).

A39. Examining Human Unipedal Quiet Stance By Characterizing Smoothness

Matthew R. Semak, Jeremiah Schwartz, Gary Heise, University of Northern Colorado

We investigate the quality of smoothness for human unipedal balance. In particular, we are interested in its temporal scaling character. Although force measurements were carefully examined, the study will focus on the jerk concerning the center-of-pressure (COP) for each foot. Data were collected via a force plate for individuals attempting to maintain upright posture using their dominant and non-dominant legs (with eyes open). Positive tests for stochasticity allowed us to treat the time series as a stochastic process. Then, the jerk is seen as proportional to the increment of the force realizations. Detrended fluctuation analysis is the primary tool used to explore scaling behavior. Results suggest that both the medial-lateral and anterior-posterior components of the jerk display persistent and antipersistent correlations which can be modeled by fractional Gaussian noise over different temporal scaling regions. Moreover, in one region of temporal scaling, it is suggested that behavior for the jerk's anterior-posterior component could be modeled by pink noise. Finally, the possibility of a jerk-based control over the force on the foot's COP is discussed.

A40. Data-driven Model Selection For a Coarse-Grained **Description of Coupled Oscillators**

Jordan Snyder, UC Davis; Andrey Lokhov, Anatoly Zlotnik, Los Alamos National Laboratory

Quantitative science has produced successful models of the world at scales spanning dozens of orders of magnitude in space, time, and energy. While in principle, the most finely detailed models are sufficient to reproduce the predictions of any less-detailed model, there is clearly scientific value in deriving and studying models that do not resolve details that are not directly relevant to the question at hand. The procedure of systematically reducing the degrees of freedom of a model goes by many names depending on context (renormalization group in statistical physics) but can be generally be referred to as "model reduction". In this talk I will discuss progress towards general principles of model reduction obtained by studying synchronization of phase oscillators on a modular network. This system is an ideal test-bed because it exhibits a controllable transition from high- to low-dimensional behavior: moreover, the resulting low-dimensional behavior is well-described by coarsegrained equations of a known form.

Cement Slurry

Chengcheng Tao, Barbara Kutchko, Eilis Rosenbaum, Mehrdad Massoudi, U.S. DOE National Energy Technology Laboratory

Rheological behavior of cement slurries is important in well cementing operation in petroleum industries. In this talk, we study the fully developed flow of a cement slurry inside a wellbore. We assume cement behaves as a nonlinear fluid. We use a constitutive relation for the viscous stress tensor which is based on a modified form of the second grade (Rivlin-Ericksen) fluid; we also present a diffusion flux vector for the concentration of particles. The onedimensional forms of the governing equations and the boundary conditions are made dimensionless and solved numerically with ODE solver in MATLAB. A parametric study is performed to present the effect of shear-rate-dependent viscosity by varying the dimensionless numbers.

A42. Forecasting U.S. Elections with Compartmental Models of Infection

Alexandria Volkening, OSU Mathematical Biosciences Institute; Daniel F. Linder, Augusta University: Mason A. Porter, University of California Los Angeles: Grzegorz A. Rempala, Ohio State University

U.S. election forecasting involves polling likely voters, making assumptions about voter turnout, and accounting for various features such as state demographics and voting history. While elections in the United States are decided at the state level, errors in forecasting are correlated between states. With the goal of better understanding the forecasting process and exploring how states influence each other, we develop a data-driven framework for forecasting U.S. elections from the perspective of dynamical systems. We combine a compartmental model with public polling data from HuffPost and RealClearPolitics to forecast gubernatorial, senatorial, and presidential elections at the state level. Our results for the 2012, 2016, and 2018 U.S. races are largely in agreement with those of more complex popular pollsters, and we use our model to discuss how subjective choices about uncertainty impact forecast interpretations and suggest future research questions.

A43. Variational and Phase Response Analysis For Limit Cycles with Hard Boundaries, with Applications to Neuromechanical Control Problem

Yangyang Wang, Mathematical Biosciences Institute, Ohio State University; Peter Thomas, Hillel Chiel, Jeff Gill, Case Western Reserve University

Central pattern generators (CPGs) are neural networks that are intrinsically capable of producing rhythmic patterns of neural activity without receiving sensory inputs and are adaptable to sensory feedback to produce robust motor behaviors such as breathing, walking, and swallowing. The mechanism underlying robust motor control mediated by the sensory feedback would be to

adjust both the timing and the path of neuromechanical trajectories that can have hard boundary conditions. Motivated by this, we generalize variational and phase response analysis developed for stable limit cycle systems to the piecewise smooth neuromechanical system to uncover the mechanism underlying robust sensory feedback control, in comparison with experimental data from the food-swallowing behavior in the sea slug *Aplysia*.

A44. Frequency Entrainment of Coupled Oscillators with Dynamic Interaction

<u>Seong-Gyu</u> <u>Yang (양성규)</u>, Sungkyunkwan University (성균관대학교); Hyunsuk Hong (홍현숙), Chonbuk National University (전북대학교); Beom Jun Kim (김범준), Sungkyunkwan University (성균관대학교)

Music play and applause for the performance show opposite synchronization phenomena. For music play, without a director, it has been reported that the paired synchronous rhythmic in finger tapping shows a faster rhythm than that of solo play. On the other hand, for applause, it has been reported that a sound of many hands clapping gets tuned into a slower one. With curiosity on such real-world phenomena, we here suggest a simple model that can mimic the faster and slower synchronous rhythm. We revise the Kuramoto model in such a way that interaction ranges dynamically depend on the phase of oscillators. In more detail, each oscillator interacts with others only when the phase difference $\Delta \phi$ satisfies $\Delta \phi \in [-\beta \pi, \alpha \pi]$. The conventional Kuramoto model corresponds to the full range of interaction, i.e., $\alpha = \beta = 1$ and $\alpha \neq \beta$ introduces asymmetry. We numerically investigate the shift of synchronized frequency with respect to the original distribution of the oscillator frequency and find that the parameter β plays an important role.

A45. Pattern Formation in a Fully-3D Segregating Flow

<u>Mengqi</u> Yu, Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow, Northwestern University

Segregation patterns related to elliptic non-mixing regions for size-bidisperse particle mixtures have been previously observed only in quasi-two-dimensional systems. Here we identify such segregation patterns for the first time in a fully three-dimensional flow, specifically that generated by alternately rotating a half-filled spherical tumbler containing a mixture of mm-size particles of two sizes about two perpendicular axes. We consider this flow both experimentally and from a dynamical systems perspective with a continuum model of the flow. Pattern formation, observed both directly at the tumbler wall and from x-ray imaging, results from the interaction of size segregation with chaotic regions and non-mixing islands of the flow identified from Poincare maps based on continuum modeling. Specifically, large particles in the flowing surface layer preferentially accumulate in non-mixing islands despite the effects of collisional diffusion and chaotic transport. The protocol-dependent structure of the unstable manifolds of the flow surrounding the non-mixing islands provides further insight into why certain segregation patterns are more robust than others. Partially funded by NSF Grant #CMMI-1435065.

A46. Random Beats Design in Network Synchronization*

Yuanzhao Zhang, Adilson E. Motter, Northwestern University

A fundamental and widely held assumption on network dynamics is that similar agents are more likely to exhibit similar behavior than dissimilar ones, and that generic differences among them are necessarily detrimental to synchronization. Here, we show that this assumption does not hold in networks of coupled oscillators. We demonstrate, in particular, that random oscillator heterogeneity can consistently induce synchronization in otherwise unsynchronizable networks. Remarkably, at intermediate levels of heterogeneity, random differences among oscillators are far more effective in promoting synchronization than differences specially designed to facilitate identical synchronization. Our results suggest that, rather than being eliminated or ignored, existing mismatches can be harnessed to help maintain coherent network dynamics in experiments and real systems.

References:

(1) Y. Zhang and A. E. Motter, "Random beats design in network synchronization", to be published

(2) Y. Zhang and A. E. Motter, "Identical synchronization of nonidentical oscillators: when only birds of different feathers flock together", Nonlinearity 31 R1-R23 (2018)

(3) Y. Zhang, T. Nishikawa and A. E. Motter, "Asymmetry-induced synchronization in oscillator networks", Phys. Rev. E 95 062215 (2017)

Poster Session B

Saturday, Jan. 5, 7:30 p.m.–9:30 p.m.

Flash talks correspond to posters with "*" appended.

B1. Forecasting Events in the Complex Dynamics of a Semiconductor Laser with Optical Feedback

Andres Aragoneses, Meritxell Colet, Eastern Washington University

We study, under an ordinal patterns analysis, the output intensity of a semiconductor laser with feedback in a regime where it develops a complex spiking behavior.

We demonstrates the presence of a nontrivial dual dynamics underlying the complex dynamics of a stochastic high-dimensional optical system, that can be used to forecast events in the dynamics of the system.

We consider the output intensity of a commercial semiconductor laser with optical feedback. The laser intensity displays an apparently random sequence of spikes. This irregular spiking dynamics has received a great deal of attention in the past three decades, as it can be used to understand the general features of complex systems, but also because of the connection between the optical spikes and biological neurons spikes.

We use an ordinal patterns analysis, where we transform the time series of the output intensity of the laser into a series of patterns. By analyzing the probabilities of these patterns we can detect if temporal correlations are present in the time series of events.

The patterns show temporal and intensity correlations among consecutive spikes, that allow us to distinguish that two different behaviors coexist in the transition regimes of the laser. These correlations can be used to separate the different types of behaviors, one that triggers shallow events and another that triggers deep events. We use the correlation patterns to anticipate when the systems changes from triggering one type of events to the other type of events.

We show that the method developed in this work can be used to forecast transition events in complex systems that present a dual dynamics. Particularly, because the complex dynamics of this optical system has similarities with neuronal networks, our results are relevant to understand how neurons compute and process information, and open new avenues for ultra-fast computing through optical spikes.

B2. A Step Towards Personalized Cardiac Electrophysiology: Calibrating Virtual Heart Models Using Disease-Specific Action Potential Restitution Curves.

Konstantinos N. Aronis, Patrick M Boyle, Suyeon Ju, Jonathan Chrispin, Joseph Marine, Sunil Sinha, Hari Tandri, Ronald Berger, Hiroshi Ashikaga, Natalia A Trayanova, Johns Hopkins University Introduction: Virtual heart modeling is an emerging approach used for arrhythmia risk-stratification and ablation planning. Current models do not account for disease-specific electrophysiology of the remote-from-scar myocardium. Our aims are: (a) to assess for differences in action potential duration restitution (APDR) properties of remote-from-scar myocardium between patients with ischemic cardiomyopathy (ICMP) and structurally normal left ventricles (SNLV), and (b) to calibrate a phenomenological action potential model using these APDR curves using a stochastic optimization approach.

Methods: We enrolled 22 patients that underwent ablation for VT, PVCs or AF (10 ICMP; 12 SNLV). We performed programmed electrical stimulation to construct APDR from remote-from-scar LV myocardium. We compared APDR slopes between patients with ICMP and SNLV. We calibrated an action potential model to the derived restitution curves using a genetic algorithm that iteratively assesses the "fitness" of a population of model parameters and uses the principles of natural selection to derive the optimal parameter set. We compared the dynamics of the uncalibrated and calibrated models in singlecell, and monolayer simulations.

Results: Mean age is 63.5 ± 13 years (41.3% women). ICMP patients have a significantly steeper APDR compared to those with SNLV (higher by 30.8 ± 10 , p < 0.01). The SNLV model has more pro-arrhythmic dynamics compared to uncalibrated model and the ICMP model has the most pro-arrhythmic dynamics. On single-cell simulations the ICMP model developed electrical alternans earlier compared to the SNLV and uncalibrated model (380, 350 and 325 msec). In monolayer simulations, sustained functional reentry was induced with the ICMP model but not with the SNLV or uncalibrated model.

Conclusions: The remote-from-scar myocardium of patients with ICMP has a steeper APDR compared to that of SNLV, reflecting myocardial remodeling. Optimization of action potential models is feasible using patient-derived APDR. Ionic models calibrated to the myocardium of patients with ICMP exhibit the greatest pro-arrhythmic propensity.

B3. On Host-genetic Parasite Models

Faina Berezovskaya, Howard University; Georgy Karev; NCBI, NIH

Genetic parasites are ubiquitous satellites of cellular life forms most of which host a variety of mobile genetic elements. Theoretical considerations and computer simulations suggest that emergence of genetic parasites is intrinsic to evolving replicator systems (Koonin et al., Biol. Direct, 2017,12(1);31).

Using methods of bifurcation analysis, we created and investigated the characteristics of simple models of replicator (R)-parasite (P) co-evolution in a well-mixed environment. The one of the simplest considering model that describes the stable co-evolution of the system is of the form

$$dR/dt = 1/((1+\alpha e))R^{2}(1-(R+P/q)/K)e_{R}R - \beta RP, dP/dt = q/((1+e))RP - e_{P}P$$

where $\alpha, \beta, e_R, q_e, e$ are non-negative parameters of the model.

We show that for reasonable fixed α, β, e_R, e_P the parameter plane (e, q) is divided into four domains of qualitatively different behaviors of the model,

and two of them correspond to the stable coexistence of host and parasites (latter in equilibrium or oscillation modes).

B4. Snakes and Lattices: Understanding the Bifurcation Structure of Localized Solutions to Lattice Dynamical Systems*

Jason Bramburger, Bjorn Sandstede, Brown University

A wide variety of spatially localized steady-state solutions to partial differential equations (PDEs) are known to exhibit a bifurcation phenomenon termed snaking. That is, these solutions bounce between two different values of the bifurcation parameter while expanding the region of localization and hence ascending in norm. The mechanism that drives snaking in PDEs has been understood by analyzing the evolution of the ordinary differential equation in the spatial variable governing steady-state solutions to the PDE. In this talk we extend this theory to lattice dynamical systems by showing that the associated steady-state equations in this context can be written as a discrete dynamical system. We can then interpret localized solutions to the lattice system as homoclinic orbits of the associated discrete dynamical system, and show that the bifurcation structure is determined by bifurcations of nearby heteroclinic orbits. We supplement these results with examples from a well-studied bistable lattice differential equation which has been the focus of many works to date.

B5. Rheology of Transient Polymer Networks and Polymer-Nanoparticle Composites: A Molecular Dynamics Study

$\underline{\text{Xue-Zheng}} \underline{\text{Cao}}, \text{ M. Gregory Forest, } University of North Carolina at Chapel Hill$

The remarkable functionalities of transiently crosslinked, biopolymer networks are increasingly becoming translated into synthetic materials for biomedical and materials science applications. Various computational and theoretical models, representing different transient crosslinking mechanisms, have been proposed to mimic biological and synthetic polymer networks, and to interpret experimental measurements of rheological, transport, and self-repair properties. Our computational model leverages the LAMMPS open source software as a platform to input stochastic non-equilibrium binding /unbinding kinetics of transient crosslinking, parametrized by probabilities both to form and break crosslinks. The emergent crosslink mean density and fluctuations, and the induced rheology, are determined across the 2-parameter space of binding and unbinding affinities for a moderately long chain, entangled polymer melt. Moreover, we reveal that nanoparticle loading of unentangled polymers induces entanglement-like relaxation modes and a broad sol-gel transition, in the presence of strong nanoparticle-polymer attraction, i.e. nanoparticles are effectively long-lived crosslinks. The computational results are placed in context with the experimental and theoretical literature on transient polymer networks and polymer-nanoparticle composites.

B6. When Is One Variable Enough to Reconstruct a Dynamical System?*

Tom Carroll, US Naval Research Lab

We typically attempt to reconstruct a dynamical system from a single variable using the method of delays. Recently, Letellier, Aguirre and others have applied the theory of nonlinear observability to show that such reconstructions are not always possible. I supplement their method with estimations of the likelihood of a continuous function between two signals, and I also find how accurately I can train a reservoir computer to reproduce a dynamical system. These three measures sometimes give conflicting answers on whether it is possible to reconstruct a dynamical system from a particular signal.

B7. Non-linear Time Series Analysis of Density-Stratified Gravity Current

<u>Saurabh</u> Chawdhary, Anshu Dubey, Argonne National laboratory; Fotis Sotiropoulos, Stony Brook University

Non-linear dynamics have been observed in a variety of turbulent flows. We consider the case of dense underflow, called density or gravity current, forming as a result of saline water jet introduced at the top of a sloping bed placed in a fresh-water tank. Different set of parameters, such as, jet-velocity, salinity, bed-slope angle, give rise to different flow characteristics and dynamics. The large-eddy simulation of gravity current flow developing over bed slopes of 5 degrees revealed existence of large-scale structures in the flow, shedding at discrete intervals. We analyzed the time-series velocity data near the bed using the method of delays to construct the phase space. The phase space indicates the presence of an attractor near a fixed velocity in space. A positive value of maximal Lyapunov exponent was found, thus, confirming the presence of a chaotic attractor. However, a similar analysis for the gravity current over bed-slope of 15 degrees and lower salinity results in different dynamics.

B8. Shock Instability and Pattern Formation in Vertically Oscillated Granular Media

<u>Nicholas</u> Corkill, Anirrudh Krishnan, Jonathan Bougie, Loyola University Chicago

We study shocks and patterns in vertically oscillated layers of grains using methods of granular hydrodynamics. Granular layers are thrown off an oscillating plate when the downward acceleration of the plate exceeds that of gravity. When the layer contacts the plate later in the cycle, a shock forms that travels through the layer. Simultaneously, standing wave patterns form, similar to Faraday waves in fluids. We analyze these patterns as a result of an instability in an initially flat shock front. To do so, we numerically solve a set of three-dimensional, time-dependent granular hydrodynamics equations, treating the layers of grains as a continuous medium. We analyze results from this simulation to characterize the base state of the shock in order to perform a linear stability analysis of this base state. We find a frequency dependence of this base state which indicate multiple flow regimes. A transition between regimes appears to correlate with the transition between stripe and square patterns that are observed experimentally.

B9. Relation Between Sensitive Systems, Topological Entropy and Baire Set in MDS

Mauricio Díaz, Universidad Nacional Andrés Bello

In this article we going to use a Measurable dynamical system of the form (X,B,μ,T,S) for do some analysis about the connection between the dynamics that are present in C(X) and the strong relation between ω -scrambled set and topological entropy for homeomorphics maps with horse-shoe property.

B10. Geometrical Methods For Stochastic Dynamics

Jinqiao Duan, Illinois Institute of Technology

Dynamical systems arising in engineering and science are often subject to random fluctuations. The noisy fluctuations may be Gaussian or non-Gaussian, which are modeled by Brownian motion or α -stable Levy motion, respectively. Non-Gaussianity of the noise manifests as nonlocality at a "macroscopic" level. Stochastic dynamical systems with non-Gaussian noise (modeled by α -stable Levy motion) have attracted a lot of attention recently. The non-Gaussianity index α is a significant indicator for various dynamical behaviors.

The speaker will overview recent advances in geometrical methods for stochastic dynamical systems, including random invariant sets, random invariant manifolds, stochastic bifurcation, mean exit time, escape probability, tipping time, most probable orbits, and transition pathways between metastable states.

B11. Encoding of Multimodal Sensory Information in a Sensorimotor System*

<u>Rosangela</u> <u>Follmann</u>, Christopher J. Goldsmith, Wolfgang Stein, *Illinois* State University

Nervous systems constantly receive and process input from various sensory modalities. Incoming information converges at many neural centers, including those that directly control motor output and behavioral plasticity. How these sensory inputs are encoded and separated so that organisms can carry out appropriate behavioral responses is poorly understood. To address this question, we use network analysis to investigate responses to distinct sensory inputs of a population of neurons involved in processing of sensory information. Our analysis is applied to the commissural ganglion in the crab nervous system where

fewer than 220 neurons process mechanosensory and chemosensory information to control aspects of feeding (Follmann et al., J Comp Neurology, 2017). Stimulation of these two sensory modalities is known to produce distinct motor outputs. In this study, we use voltage-sensitive dye imaging to record the neuronal population activity at individual neuron resolution under different sensory conditions. We provide evidence that differences between modalities are encoded in the combination of activated neurons (whether neurons were excited or inhibited). Moreover, we found a new combination of excitation and inhibition when both pathways were activated simultaneously (Follmann et al., PLoS biology, 2018). Our results are consistent with the idea that this small sensorimotor network encodes different sensory modalities in a combinatorial code of neurons. Each perceived modality results in a different combination of activated and inhibited neurons, providing the downstream motor networks with the ability to differentially respond to distinct categories of sensory conditions.

B12. Electrochemical Signaling and Oscillatory Growth in Bacillus Subtilis

Noah Ford, David Chopp, Arthur Prindle, Northwestern University

Biofilms are communities of bacteria that grow on surfaces. Bacteria in biofilms have developed complicated modes of interdependence. Recent studies suggest that bacteria at the center of a biofilm, far from the nutrient source, can communicate starvation to their neighbors. Bacteria near the exterior receive this signal and will halt growth periodically to allow nutrients to penetrate deeper into the biofilm. It is unclear how bacteria signal starvation to their neighbors, however, it is known that when bacteria stop growing, they also hyperpolarize by releasing potassium. We have developed a model that shows it is possible for bacteria to use potassium as the signal. In this model bacteria actively propagate a potassium wave from the interior to the exterior of the biofilm, which causes the entire biofilm to temporarily and synchronously halt growth.

B13. Connecting Gene Expression to Cellular Movement: a New Transport Model For Cell Migration

<u>Alexis</u> <u>Grau Ribes</u>, Yannick De Decker, Laurence Rongy, Université libre de Bruxelles (ULB), Belgium

The epithelial-to-mesenchymal transition (EMT) is a key step in metastasis. Understanding the connection between the gene regulation network orchestrating this transition and cell migration and invasion abilities could help identify targets to prevent malignant spreading. E-cadherin, the protein mediating cellcell adhesion in epithelial tissues, is a key marker of EMT. Wound-healing cell migration assays have indeed been used to demonstrate that E-cadherin loss results in tumor progression. However, existing reaction-diffusion models for cell migration are mostly phenomenological and cannot consider the feedback of cellular composition on migration properties. In particular, to the best of our knowledge, no model is available in which the cell mobility depends on E-cadherin level.

In this work, we present a multiscale reaction-diffusion model that successfully reproduces wound-healing cell migration experiments showing the influence of E-cadherin on cell mobility. To do so, we connect the mobility of cells and gene expression dynamics inside the cells. The model also includes the regulation of E-cadherin by an extracellular factor. We thereby highlight the role of extracellular secretion in conferring local heterogeneity in the system by modifying locally E-cadherin expression and, consequently, cell mobility. Since extracellular vesicles have been found to play a key role in pathological conditions, our approach can help understand this cell-cell communication mechanism. Furthermore, our approach brings a new look at cell proliferation by considering the spatial impact of this phenomenon which is, by essence, nonlocal but treated locally in previous models.

The model we propose establishes an elegant connection between E-cadherin and cell mobility. This is the first time that the spatial density profiles for different experimental conditions can be modeled with a unique set of parameter values instead of resorting to ad hoc sets of parameters.

B14. Understanding and Designing Emergent Behavior Via Stability Analysis of Mean Field Games

<u>Piyush</u> <u>Grover</u>, <u>Mitsubishi Electric Research Labs</u>; Kaivalya Bakshi, Evangelos A. Theodorou, <u>Georgia Tech</u>

Mean Field Games (MFG) have emerged as a promising tool in the analysis of large-scale self-organizing networked systems. The MFG framework provides a non-cooperative game theoretic optimal control description of emergent behavior of large population of rational dynamic agents in a distributed setting. In this description, each agent's state is driven by optimally controlled dynamics that result in a Nash equilibrium between itself and the population. The agent's optimal control is computed by minimizing the sum of its control effort, and a mean-field interaction term that depends on its own state and statistical information about the population. The agent distribution in phase space evolves under the optimal feedback control policy. Mathematically, a MFG system is described by a coupled forward-backward system of nonlinear Fokker-Planck and Hamilton-Jacobi-Bellman PDEs.

In this talk, we discuss a class of MFGs whose qualitative behavior mimics certain well known empirical flocking models. Using a combination of numerical and analytical methods, we provide a closed-loop stability analysis of the non-local forward-backward PDE system demonstrating that these MFGs exhibit bifurcations similar to those found in the empirical model. The present work is a step towards developing a set of tools for systematic analysis, and eventually design, of collective behavior of non-cooperative dynamic agents via an inverse modeling approach. We also briefly discuss ongoing efforts to develop low-order models of MFGs that possess rich phase space structure and undergo global bifurcations.

References:

1). A mean-field game model for homogeneous flocking; Chaos: An interdisciplinary journal of nonlinear science, 2018 DOI:10.1063/1.5036663; Grover,

Bakshi and Theodorou

2). On mean field games for agents with Langevin dynamics; IEEE Transactions on Control of Network Systems (Conditionally accepted), 2019; Bakshi, Grover and Theodorou

B15. Data-driven Spatiotemporal Modal Decomposition For Time Frequency Analysis

Seth Michael Hirsh, Bing Brunton, Nathan Kutz, University of Washington

We propose a new solution to the blind source separation problem that factors mixed time-series signals into a sum of spatiotemporal modes, with the constraint that the temporal components are intrinsic mode functions (IMF's).

The key motivation is that IMF's allow the computation of meaningful Hilbert transforms of non-stationary data, from which instantaneous timefrequency representations may be derived. Our spatiotemporal intrinsic mode decomposition (STIMD) method leverages spatial correlations to generalize the extraction of IMF's from one-dimensional signals, commonly performed using the empirical mode decomposition (EMD), to multi-dimensional signals.

Further, this data-driven method enables future-state prediction. We demonstrate STIMD on several synthetic examples, comparing it to common matrix factorization techniques, namely singular value decomposition (SVD), independent component analysis (ICA), and dynamic mode decomposition (DMD). We show that STIMD outperforms these methods at reconstruction and extracting interpretable modes. Next, we apply STIMD to analyze two real-world datasets, gravitational wave data and neural recordings from the rodent hippocampus.

B16. A Minimal Mathematical Model For Free Market Competition Through Advertising*

Joseph D. Johnson, Daniel M. Abrams, Northwestern University

Firms in the U.S. spend over 150 billion dollars a year in advertising their products to consumers. Given the clear importance promotion has in market competition, it is of great interest to understand how that budget could be optimally distributed, and how market prices should be affected. Constructing a system of differential equations to model dynamics of competition, we explore firm behavior under idealized conditions and find a surprising prediction: firms should split into two groups, one with significantly less advertising (a "generic" group) and one with significantly more advertising (a "name-brand" group). We use consumer data to compare predictions from the model with real world pricing and find qualitative agreement.

B17. Growing Network Model For Knowledge Space: Micro to Macro Views

Hyunuk Kim, Pohang University of Science and Technology, Korea; Daniel Kim, Natural Science Research Institute, Korea; Young-Ho Eom, University of Strathclyde, UK; Hawoong Jeong, Korea Advanced Institute of Science and Technology, Korea; Woo-Sung Jung Pohang University of Science and Technology, Korea; Hyejin Youn, Northwestern University

Human knowledge expands through the combination of exploration and exploitation. Individuals exploit existing ideas and explore knowledge space to forage novelties of high impact. Their microscopic behaviors are accumulated, thereby shaping knowledge structure over time. We introduce a network model replicating the microscopic behavior with a sublinear growth of synthetic space that corresponds to Heaps' law. This growing network model reproduces hetering coefficient that are observed in an empirical technology space extracted from US patent data. More importantly, it generates knowledge modules which have strong intra- and weak inter-connections. Emergence of knowledge modules happens without prior information on node characteristics, inferring collective human behaviors create domain knowledge in some extent. Our findings explain why humans consistently face a new domain of knowledge and experience gradual changes in knowledge structure.

B18. Delay Differential Analysis of Sensory Processing Dysfunction in Schizophrenia

<u>Robert Kim</u> (1,2), Aaron L. Sampson (1, 2), Claudia Lainscsek (1, 2),
Michael L. Thomas (2, 3), Karen Man (1), Xenia Lainscsek (4), The COGS Investigators, Neal R. Swerdlow (2), David L. Braff (2, 5), Terrence J.
Sejnowski (1, 2), Gregory A. Light (2, 5); Affiliations: (1) Salk Institute for Biological Studies; (2) University of California San Diego; (3) Colorado State University; (4) Technische Universitat Graz, Austria; (5) VISN-22 Mental Illness, Research, Education and Clinical Center (MIRECC), VA San Diego Healthcare System

Neural data, like data from other natural systems, often appears chaotic since it is generated by complex nonlinear dynamics. Disruption of the coordination of brain regions may underlie the impairments to information processing in neuropsychiatric disorders. Schizophrenia is among the most debilitating of mental illnesses and is thought to be caused by network dysfunction leading to impaired auditory information processing along with cognitive and psychosocial deficits. Since current techniques for the analysis of neurophysiologic biomarkers are based principally on linear methods, they do not take into account the full breadth of information available in the electroencephalogram (EEG). Here, Delay Differential Analysis (DDA), a novel nonlinear classification tool based on embedding theory, was applied to EEG recordings from 877 schizophrenia (SZ) patients and 753 nonpsychiatric comparison subjects (NCS) who underwent mismatch negativity (MMN) testing via their participation in the Consortium on the Genetics of Schizophrenia (COGS-2) study. Changes

in DDA features were associated with auditory information processing in both groups, and these changes preceded those observed with traditional, linear methods. Marked abnormalities in the SZ patients can be observed using both linear and nonlinear features. In addition, a novel clustering algorithm was developed to utilize the DDA features in order to identify subgroups with similar dynamical signatures. The subgroups identified from the COGS-2 cohort were correlated with previously established neurophysiological biomarkers and cognitive functioning assessed by numerous neuropsychological test scores.

These results highlight the benefits of applying the tool of nonlinear dynamics to the analysis of brain signals in general, as well as the particular need for further studies to explore the relationship between DDA features and neural information processing.

B19. Sliding on Moving Strings: From Regular Motions to Nonlinear Resonances and Chaos*

Steven R. Knudsen, Leonardo Golubovic, West Virginia University

We consider the dynamics of objects sliding on moving strings. We introduce a powerful computational algorithm that can be used to investigate the dynamics of objects sliding along non-relativistic strings. We use the algorithm to numerically explore fundamental physics of sliding climbers on a unique class of dynamical systems, Rotating Space Elevators (RSE) [L. Golubovic and S. Knudsen, Europhys. Lett. 86, 34001 (2009); S. Knudsen and L. Golubovic, Eur. Phys. J. Plus 129, 242 (2014), ibid., 130, 243 (2015), ibid., 131, 400 (2016)]. Objects sliding along RSE strings do not require internal engines or propulsion to be transported from the Earth's surface into outer space. By extensive numerical simulations, we find that sliding climbers may display interesting non-linear dynamics exhibiting both quasi-periodic motion, nonlinear resonances, and chaotic states of motion. While our main interest in this study is in the climber dynamics on RSEs, our results for the dynamics of sliding object are of more general interest. In particular, we designed tools capable of dealing with strongly nonlinear phenomena involving moving strings of any kind, such as the chaotic dynamics of sliding climbers observed in our simulations.

B20. Noise-indused Frequency Increase in Synchronization of Human Rhythmic Activities

<u>Wataru</u> <u>Kurebayashi</u>, Masahiro Okano, Masahiro Shinya, Kazutoshi Kudo, Shiga University

In the field of experimental psychology, Okano *et al.* (Sci. Rep., 2017) reported that a nontrivial frequency increase is ubiquitously observed in synchronized finger tapping of two persons. This experimental result shed a light on an unclear dynamical aspect of human rhythmic responses. In this study, we describe this phenomenon by a simple mathematical model without loss of generality by using the phase reduction theory, and show that the frequency increase is ubiquitously observed under a certain general condition through mathematical analysis.

B21. A New Frame For Phase Plane Analysis: Using Differential Geometry to Reveal Local Dynamics

Benjamin G. Letson, Jonathan Rubin, University of Pittsburgh

In this talk, we introduce a new change of coordinates, which we term local orthogonal rectification or LOR, that can be applied at any selected manifold in the phase space of a dynamical system. LOR yields a coordinate system, the LOR frame, which allows us to rigorously study dynamics near the selected manifold. We have used the LOR approach to derive a novel definition for rivers, long recognized but poorly understood trajectories that locally attract other orbits yet need not be related to invariant manifolds or other familiar phase space structures, and to identify rivers within several example systems. We also use the LOR frame to identify periodic orbits in higher-dimensional flows and construct novel invariant manifolds attendant to periodic orbits.

B22. Variable Cutting-and-Shuffling to Enhance Mixing*

Lachlan Smith, <u>Paul B.</u> <u>Umbanhowar</u>, Julio M. Ottino, Richard M. Lueptow, <u>Northwestern University</u>

Mixing by cutting-and-shuffling can be understood and predicted using dynamical systems based tools and techniques. Typically, mixing is generated by maps that repeat the same cut-and-shuffle process at every iteration thereby producing weak mixing. However, mixing can be greatly improved by varying the cut-and-shuffle parameters at each step. To demonstrate this, we show how mixing can be significantly improved for an interval exchange transformation (IET), which is cutting-and-shuffling on a one-dimensional line interval. While the optimal IET operations can be found analytically for an arbitrary number of iterations, for more complex cutting-and-shuffling systems, computationally expensive numerical optimization methods are required. Furthermore, the number of control parameters grows linearly with the number of iterations, making optimization over a large number of iterations computationally prohibitive. Nevertheless, an ad hoc approach to cutting-and-shuffling that is computationally inexpensive guarantees that the mixing is within a constant factor of the optimum. This ad hoc approach yields significantly better mixing than normal IETs, because cut pieces never reconnect. The general principles of this method can be applied to more general cutting-and-shuffling systems. Partially supported by NSF grant CMMI-1435065.

B23. Automatic Recognition of Multiple Sclerosis Through Gait Data Using Machine Learning Algorithms

Sanjana Menon, <u>Richard</u> <u>Sowers</u>, <u>Manuel</u> <u>Hernandez</u>, <u>University</u> of Illinois at <u>Urbana-Champaign</u>

This paper proposes a system that automatically recognizes individuals with Multiple sclerosis, which is a disorder that is clinically manifested by gait dysfunction. The objective of the system is to identify the onset of a relapse in the disease and automatically notify a physician and provide an explanation of the automatic diagnosis. The gait patterns of 40 subjects that included 20 with multiple sclerosis and 20 healthy age-matched and gender-matched individuals were captured using an instrumented 1m x 3m treadmill. Each stride was categorized into three events, namely - Toe Off, Mid-foot stance and Heel strike of the left and right leg. The center of pressure position coordinates and time of occurrence of each of these events were recorded for the entire duration that the individual was walking at a comfortable pace. The resulting time series of these coordinates were analyzed using machine-learning algorithms. Time series of the detected positions of the body parts from the motion-capture system was transformed into a form suitable for supervised machine-learning methods using novel semantic features for the recognition of Multiple sclerosis. The extraction and normalization of gait features such as center of pressure and ground reaction force were used to distinguish between persons with and without Multiple sclerosis. The results show that the proposed approach achieves high classification accuracy through k-means clustering, covariance matrices, and can be used as a guide for further studies of diagnosing different levels of disability in persons with Multiple sclerosis.

B24. Machine-learning Inference of Variables of a Chaotic Fluid Flow From Data Using Reservoir Computing*

Kengo Nakai, Yoshitaka Saiki, University of Tokyo

We infer macroscopic behaviors of a three-dimensional fluid flow with chaotic behaviors using reservoir computing. A reservoir is a recurrent neural network whose internal parameters are not adjusted to fit the data in the training process. What is done is to train the reservoir by feeding it an input timeseries and fitting a linear function of the reservoir state variables to a desired output time-series. Due to this approach of reservoir computing we can save a great amount of computational costs, which enables us to deal with a complex deterministic behavior.

Recently it is reported that the reservoir computing is effective in the inference of time-series and some characteristics using the Lorenz system, Rossler system and Kuramoto-Sivashinsky system (J. Pathak, Z. Lu, B. Hunt, M. Girvan, and E. Ott, Chaos 27, 121102 (2017).). We apply the same method to a chaotic fluid flow.

In our procedure of the inference, we assume no prior knowledge of a physical process of a fluid flow except that its behavior is complex but deterministic. We present an inference of the complex behavior, which requires only past time-series data as training data.

We show that the reservoir dynamics constructed from only past data of energy functions can infer the future behavior of energy functions and reproduce the energy spectrum. It is also shown that we can infer a time-series data from only one measurement by using the delay coordinates. These imply that the obtained two reservoir systems constructed without the knowledge of microscopic data are equivalent to the dynamical systems describing macroscopic behavior of energy functions. It should be remarked that such dynamical systems describing macroscopic behaviors cannot be derived from the Navier-Stokes equation.

The choice of appropriate delay coordinates and some other technical issues will also be discussed. Partial results in this work are published (K. Nakai and Y. Saiki, Physical Review E, 98, 023111 (2018)).

B25. Quasi-Periodicity to Period-Doubling of Parallel-Input/Parallel-Output Buck-Boost DC-DC Converter

<u>Ammar Nimer</u> Natsheh, Higher Colleges of Technology; Dubai Women's College

This work describes the bifurcation behavior of a modular peak current-mode controlled DC-DC buck-boost converter from quasi-periodicity to perioddoubling. A nonlinear mapping in closed form is derived and bifurcation diagrams are generated using MATLAB. In this paper, another bifurcation parameter is defined arising from variation of a suitably chosen parameter, which referred to as secondary bifurcation parameter, and based on which observed a "super"-bifurcation that leads quasi-periodicity to period-doubling. Routes to chaos via quasi-periodic orbits and period-doubling are possible. However, there has been no attempt to find out the condition that determines the type of the route to chaos for a given set of parameters. So a secondary bifurcation parameter Gamma is introduced. As Gamma increases, the route to chaos initially goes through quasi-3T-periodic orbits, then goes through quasi-6T-periodic orbits, and continues to go through quasi-periodic orbits of 12T, etc. It eventually becomes period-doubling for large values of Gamma. The transition of the bifurcation path for the proposed system from one that goes through quasi-3T-periodic orbits via progressively longer quasi-periodic orbits to one that goes through period-doubling is summarized using the mapping derived.

Observation 1

Stable 1T orbits, stable 2T orbits, quasi-3T orbits, and eventually exhibits chaos.

Observation 2

After the stable 1T and 2T regions, enters a region of stable 3T orbits (instead of quasi-3T), and then quasi-6T, and eventually chaos.

Observation 3

The bifurcation path goes through a region of quasi-12 orbits before it enters the chaotic region.

Observation 4

Typical period-doubling route to chaos.

A panoramic view is reported in this paper. For small values of the secondary parameter, the route to chaos is via quasi-3T-periodic orbits. As we increase

the secondary parameter, the quasi-3T-periodic orbits become stable 3T subharmonic orbits, and the route to chaos is via quasi-6T.

B26. Strain Rate Effects on Quasi-two-dimensional Advection-reaction-diffusion Experiments

Thomas D. Nevins, Douglas Kelley, University of Rochester

The growth of a reactive scalar in a flowing medium is controlled by the combined influence of advection, reaction, and diffusion (ARD). Phytoplankton in the ocean, growing flame fronts, and reactions in industrial mixers all match this description. Due to the complexity of these systems it is often convenient to consider just the motion of a reaction front. The front is advected by flow—just like any material surface—but a constant outward chemical velocity is then added, which gives an ordinary differential equation known as the Eikonal equation. The Eikonal equation is much faster to simulate than the full ARD equations and provides good intuition. However, it is not clear how accurate this approximation is in unsteady, physical situations, and even in simple laminar flows. In fact, in previous work we found the chemical speed to be apparently increasing with flow speed, with no critical flow speed below which the Eikonal equation held. In this prior work we constructed a system for measuring chemical front speed separately from total front speed in a reactive, flowing, quasi two-dimensional experiment. In this system we measure both fluid flow and reaction state simultaneously, allowing us to study unsteady, physical flows, and to separate the flow displacement from the portion due to chemical growth (chemical speed). In this talk I will detail analytic models, simulations, and finally experiments using our front speed measurement system which show that the apparent front speed increase is entirely consistent with the Eikonal equation, if strain-rate throughout the experimental depth is taken into consideration. We will also show that this effect is present in most current quasi-two-dimensional flow experiments and suggest methods for experiments that more closely match two-dimensional dynamics.

B27. Multistability in Chemical Networks: Interplay of Coupling Strength and Delay

Simbarashe Nkomo, Emory University

Multistability has mostly been reported in theoretical studies of coupled network. We present here results of experimental demonstrations of multistability in populations of globally coupled chemical oscillators. Using photosensitive Belousov-Zhabotinsky chemical oscillators, we explore the switching behavior between the fully synchronized state, n-cluster state and incoherent behavior for different specific coupling strength and delay parameter values. The ZBKE model is used for the numerical investigation of dynamic states in populations of homogeneous and heterogeneous oscillators. Results show the existence of regions in the parameter space where the effect of delay significantly influences the exhibited behavior and vice versa. The presentation includes a discussion of possible connections between regions of multistability and the likelihood of finding chimera behavior in networks of chemical oscillators.

B28. Magnetic Resonance Imaging of Porous Media Flow

Blake Gigout, Jeffrey S. Olafsen, Baylor University

Magnetic Resonance Imaging can be used to probe 3D fluid flow in otherwise opaque porous media. In this study, coconut oil is the fluid used to extract three dimensional fluid flow within porous media comprised of porcelain spheres. Coconut oil was chosen due to the thermophysical properties of this phase change material (PCM) near the fluid solid phase transition. As the melting temperature of coconut oil is around room temperature, the transition point and temperatures near it allow for a manner in which to increase the viscosity of the fluid, slowing its flow through the porous media, permitting data to be obtained from MRI scans each of which take several minutes. Calibration is necessary to correct for the magnetic field gradient, effects of temperature on MRI images as well as the temperature dependence of the fluid parameters. Three dimensional image analysis of the MRI scans is accomplished using software programs written in-house in the Interactive Data Language (IDL). Volumetric flux through the entire imaging volume as well as fluid flux through a single MRI slice are both used to characterize the gravity driven fluid flow in the vertically oriented porous media. Bulk measurements of coconut oil in the absence of the porous media are used for MRI calibration as well as to characterize the phase transition, first using a 1-D model of Newton's Law of Cooling and eventually a complete 3D application of the heat equation.

B29. Complex Contagion Leads to Complex Dynamics in Models Coupling Behavior and Disease*

<u>Matthew T. Osborne</u>, Ohio State University; Xueying Wang, Washington State University; Joseph H. Tien, Ohio State University

Models coupling behavior and disease as two unique but interacting contagions have existed since the mid 2000s. In these coupled contagion models behavior is typically treated as a 'simple contagion'. However, empirical evidence suggests the means of behavior spread may be more complex.

In this talk I will present a simple compartmental model coupled contagion framework that highlights the dynamical differences that can occur when behavior is treated as a 'simple contagion' vs a 'complex contagion'. We find that behavioral contagion type can have a significant impact on overall disease behavior dynamics.

I will also present preliminary results from numerical simulations of behavior spread on networks aimed at providing a better understanding of the force of infection curve for both simple and complex contagions.

B30. Stability of Multi-pulse Solutions to Nonlinear Wave Equations*

Ross Hamilton Parker, Björn Sandstede, Brown University

Higher order nonlinear wave equations, such as the fifth-order Korteweg-de Vries equation (KdV5) and the Chen-McKenna suspension bridge equation, are used to model phenomena such as capillary-gravity water waves and traveling waves on a suspended beam. For certain parameter regimes, these equations exhibit multi-pulse traveling wave solutions. Linear stability of these multipulse solutions is determined by eigenvalues near the origin representing the interaction between the individual pulses. We locate these small eigenvalues using spatial dynamics techniques such as Lin's method and the Krein matrix. We are able to give analytical criteria for the stability of these multi-pulse solutions. We also present numerical results to support our analysis.

B31. Empirical Determination of the Optimum Attack For Fragmentation of Modular Networks

Carolina A. Pereira, Sebastián Gonçalves, Federal University of Rio Grande do Sul (UFRGS); Bruno Requião da Cunha, Federal Police

All possible removals of n = 5 nodes from networks of size N = 100 are performed in order to find the optimal set of nodes which fragments the original network into the smallest giant connected component. The resulting attacks are ordered according to the size of the largest connected component and compared with the state of the art methods of network attacks. We chose attacks of size 5 on relative small networks of size 100 because the number of all possible attacks, $\binom{100}{5} \approx 10^8$, is at the verge of the possible to compute with the available standard computers. We applied the procedure in a series of networks with controlled and varied modularity, comparing the resulting statistics with the effect of removing the same amount of vertices according to disruption strategies known to be efficient, *i.e.*, High Betweenness Adaptive attack (HBA), Collective Index attack (CI), and Modular Based Attack (MBA). Results show that modularity has an inverse relation with robustness, with $Q_c \approx 0.7$ being the critical value. For modularities lower than Q_c , all heuristic methods give in general the same result as random attacks, while for bigger Q, networks are less robust and highly vulnerable to malicious attacks.

B32. Drainage Through Holes Drives Arctic Sea Ice Melt Ponds to the Critical Percolation Threshold*

Predrag Popovic, Mary C. Silber, Dorian S. Abbot, University of Chicago

During the summer, vast regions of the Arctic sea ice are covered by meltwater ponds that significantly lower the ice reflectivity and accelerate melting. Despite their importance, melt ponds are still not well-understood. Ponds develop over the summer melt season through an initial stage of rapid growth followed by drainage through macroscopic holes. Recently, we showed that ponds after drainage resemble percolation clusters near a critical percolation threshold. Understanding the physical mechanism behind this previously-unrecognized constraint on pond evolution provides an unprecedented opportunity to improve representation of ponds in large-scale climate models. Here, we show that organization towards the percolation threshold is a consequence of pond drainage through macroscopic holes. The threshold, a tractable statistical property of ice topography, sets the upper limit and scales the pond coverage throughout its evolution after the beginning of drainage. Furthermore, we show that, after rescaling, pond coverage fraction as a function of number of open holes follows a universal curve. This curve governs pond evolution during and after pond drainage, which allows us to formulate an equation for pond coverage evolution that captures the dependence on physical properties of the ice. Our work reveals some of the fundamental properties of melt pond physics. As such, it can be used in large-scale models to create a reliable albedo parameterization and improve predictions of Arctic sea ice's response to warming.

B33. Standard Map-like Models For Single and Multiple Walkers in an Annular Cavity

Aminur Rahman, Texas Tech University

Recent experiments on walking droplets in an annular cavity showed the existence of complex dynamics including chaotically changing velocity. This talk presents models, influenced by the kicked rotator/standard map, for both single and multiple droplets. The models are shown to achieve both qualitative and quantitative agreement with the experiments, and makes predictions about heretofore unobserved behavior. Using dynamical systems techniques and bifurcation theory, the single droplet model is rigorously analyzed to prove dynamics suggested by the numerical simulations.

B34. Active Suspension of Self Rotating Particles

Cody <u>Reeves</u>, Northwestern University; Igor Aronson, Penn State; Petia Vlahovska, Northwestern University

Suspensions of self-propelled particles, such as bacteria, have received considerable attention. Recently there has been increased interest in suspensions of self-rotating particles, such as Quincke rotors in electric fields and ferromagnetic colloids in alternating magnetic fields. While the individual particles are governed by relatively simple dynamics, the interaction of the particles can result in incredibly complex and interesting phenomena. Experiments show phase separation, macroscopic directed motion, and structure formation (e.g. vortices and asters). Modeling these systems as discrete particles at the micro-scale (Yeo et al, Physical Review Letters (2015)) is computational expensive and limits the study of the rotors collective dynamics. We develop a continuum model for such rotor systems based on derivation for dielectric fluids with internal rotation (Rosensweig, The Journal of Chemical Physics (2004)). This model allows us to study properties of the fluid and the existance of active turbulence caused by the rotors. We can also study the interaction between the rotors and the interface for both a fixed and deformable interface.

B35. Chaos Mediated Synchronous Neuronal Transitions

Epaminondas Rosa, Annabelle Shaffer, Zach Mobille, George Rutherford, Rosangela Follmann, *Illinois State University*

No two neurons are the same. However diverse neurons should be, many times they are capable of working together in synchrony, actively performing specific functions that can be crucial for the survival of the animal. Importantly, neurons in synchrony may undergo transitions that allow them to perform tasks associated with changes in the rate as well as in the pattern of their firing. For example, transitions between tonic (fixed rate spiking) and bursting (trains of fast spiking alternated with periods of quiescence) are known to be present in thalamocortical neurons at sleep-wake transition states (Sherman, Trends Neurosci 2001). These transitions may also play a role in sensory-motor nuclei that generate tremors in Parkinson's disease (Llinas et al. J Neurophysiol 2006). Even though of fundamental relevance, little is known about the underlying mechanisms operating this type of neuronal transition. In this study we use a physiologically relevant computational model to investigate neuronal tonic-to-bursting transitions, exploring aspects found in the dynamical evolution of the firing rate. Usually, the transition from tonic to bursting starts with a period doubling cascade going to chaos with the well-known windows of periodicity, eventually reaching a regular bursting regime. The transition is therefore mediated by chaos, where a critical firing rate is present. This critical firing rate found initially as a signature of the individual neuron actually is passed on to the collective of distinct networked synchronous neurons (Shaffer et al. PRE 2016: Shaffer et al. EPJST 2017: Follmann et al. Chaos 2018). We further discuss additional features including how temperature may play a role in the setting off of the transition.

B36. Parametrically Excited Birhythmic Generalised Van Der Pol Model

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Birhythmic oscillator is a variant of van der Pol oscillator as proposed by Kaiser to model enzyme reaction in bio-system which can provide complex response dynamics. Our goal is to characterize birhythmic oscillator in terms of the subharmonic resonance behaviour. From their stability and bifurcation scenario, one can identify excitation induced oscillation between two stable limit cycles. Unlike the resonance and antiresonance features here we find nonlinear resonances which are obtained analytically from Krylov-Bogoliubov(K-B) analysis.

B37. Koopman Operator and Its Approximations For Dynamical Systems with Symmetries*

<u>Anastasiya</u> <u>Salova</u>, Jeffrey Emenheiser, Adam Rupe, James Crutchfield, Raissa D'Souza, *University of California, Davis*

Dynamical systems often exhibit symmetries. Understanding these symmetries can help simplify analysis of these systems and gain insights into their behavior, such as their attractor basin structure, bifurcations, and synchronization patterns. Yet a particular challenge is that modern systems are increasingly high-dimensional and nonlinear, making them inaccessible to approaches based on traditional dynamics of states. Thus, operator based approaches to dynamical systems, which consider the evolution of functions which operate on the states of the system, have gained popularity in recent years. Moreover, the approximations of these operators provide ways to apply these methods directly to data. We employ an operator based approach to systems with point symmetries (for instance, networks with dynamics equivariant with respect to node permutations). In particular, we focus on the Koopman operator, an infinite dimensional linear operator which is an adjoint of the Perron-Frobenius operator. Using tools from representation theory we study the structure of the eigendecomposition of this operator, which we show is especially revealing of the symmetries through an appropriate isotypic component basis. The Koopman operator can be well approximated via the recently proposed extended dynamic mode decomposition method that requires a dictionary of observables. We apply the knowledge of the structure of the eigenspace gained via our symmetry considerations to produce dictionaries of observables that ensure that the matrix corresponding to the Koopman operator approximation is block diagonal. That can offer computational advantages, can illuminate the attractor stricture of the underlying system, and can potentially lead to new methods of detecting symmetries in high dimensional nonlinear dynamical systems.

B38. A Mechanistic Framework For Transcriptional Regulation Through Intranuclear Crowding Kinetics

Anne R. Shim, Rikkert J. Nap, Luay Almassalha, Hiroaki Matusda, Vadim Backman, Igal Szleifer, Northwestern University

The nuclear environment is highly crowded by biological macromolecules, including proteins and non-coding chromatin, which affects gene expression by altering the kinetics and efficiency of transcriptional machinery. However, previous studies of the crowded nuclear environment have not considered time as a variable; therefore, little is known about how crowding kinetics integrate with gene expression. Moreover, macromolecular crowders are highly mobile, owing to processes such as chromatin translocation, protein diffusion, and DNA loop extrusion. Therefore, we investigate how transcription kinetics are altered by the time-evolving, crowded nanoenvironment of the nucleus. We constructed a computational model of transcription, dependent upon temporal changes in crowding density ("dynamic crowding"), which alter the steric and thermodynamic landscape of transcriptional chemical reactions. We show that while transcription is governed by the local average crowding density as shown in previous studies, it also depends critically on the temporal properties of dynamic crowding. Furthermore, while dynamic crowding constitutively influences all reactions of the transcription pathway, the mechanisms which determine transcription levels switch from altering pre-mRNA processing kinetics to altering transcriptional protein search and binding kinetics at later time points. Therefore, this work demonstrates that macromolecular crowding may play an even greater role in regulating transcription kinetics than previously understood, as it presents crowding kinetics within the bulk nuclear nanoenvironment as a novel regulatory framework for gene expression.

B39. Bayesian Parameter Estimation in the Spatial Organization of Metabolism *

Sasha Shirman, Svetlana P. Ikonomova, Taylor Nichols, Keith E.J. Tyo, Danielle Tullman-Ereck, Niall Mangan, Northwestern University

Enteric bacteria live in the intestines of other animals. Some enteric bacteria utilize spatial organization of the metabolic pathway, allowing them to survive in the hostile environment. This spatial organization can be useful in generating local regions of high concentration within the cell thus improving metabolic flux through the associated portions of the metabolic pathway. One type of spatial organization is microcompartments (MCPs): protein bound structures which encapsulate a subset of the metabolic pathway and segregate it from the rest of the cytosol. The localization capabilities of MCPs may be used to engineer metabolic pathways to maximize flux into a desired chemical product. Unfortunately, characteristic properties of the MCPs, such as their permeability to reactants, and the internal dynamics of the MCP are not directly measurable. Additionally bacterial metabolic pathways are often assumed to exist predominantly in steady state. This steady state is determined by a combination of environmental conditions, thermodynamic constraints, and intrinsic chemical properties of the system. We develop computational methods through which time series data of the transient behavior of externally measured metabolites may be used to infer unknown parameters and model dynamics. The dynamics of reactant and product concentrations within the cell and MCPs can be described with different levels of fidelity by a set of coupled partial or ordinary differential equations. We use Bayesian methods to analyze simulated time series data to determine the regions of parameter space in which unknown parameters are recoverable. We demonstrate the estimation of previously inaccessible model parameters and the internal dynamics of the MCP through constraints determined by the structure of the model equations. Results of these analyses are used to guide experimental design and the development of engineered metabolic pathways. This research is supported by DOE grant DE-SC0019337.

B40. The Lotka Model: One Century Later

Gessner Antonio Soto, University of Colorado

One century later, the prevalence of computational machinery allows a substantial sub-set of our species to have access to hardware that is able to adequately handle the numerous sequential steps required to analyze the solution structure of related differential-equation relationships. An arrangement related by Dr. Ilya Prigogine in the third edition of "An Introduction to Thermodynamics of Irreversible Processes"—one whose structure is simply an ornamentative modification to the arrangement Dr. Alfred Lotka formally related in his 1.920 contribution "Undamped Oscillations Derived from the Law of Mass Action"—was un-packed more fully with the aid of contemporary machinery. Two interests currently seem to both have had been nourished and continue to be nourished with this project: 1) exposure to and development of numerical algorithms related to the deconstruction of the solution sets associated with collections of differential-equation relationships (a two dimensional differentialequation collection with three parameters was partially deconstructed) and 2) an explicit grounding in the terms and logic utilized in the non-equilibrium thermodynamics lineage (one of the aspects Dr. Prigogine emphasized in the analysis he relates are the associated thermodynamically grounded conjectures and their place within the context of the associated kinetic differential-equation system. The generality potential associated with these thermodynamic constructs merits the investment.

B41. Controlling a Belousov-Zhabotinsky Droplet Using a Light Intensity Gradient

<u>Syed Jazli Syed Jamaluddin</u>, West Virginia University; Kritsana Khaothong, Kasetsart University, Thailand; Mark Tinsley, Kenneth Showalter, West Virginia University

A Belousov-Zhabotinsky (BZ) droplet that is immersed in an oil-phase can self-propel due to a surface tension gradient that exists on the droplet surface. The surface tension gradient is created as a result of the reactions that occur within and on the surface of the BZ droplet. By influencing the rates of these reactions, the directionality of the BZ droplet motion can be controlled. In our experiment, we tune the reactions that occur within and on the BZ droplet surface by imposing a light intensity gradient on the droplet. We have analyzed the BZ droplet motion and demonstrated that we can control the droplet directionality via the light intensity gradient. We also demonstrated that the shape of the light intensity gradient imposed on the BZ droplet can help us fine-tune our ability to control the directionality of the BZ droplet motion.

B42. New Amplitude Equations For Ocean Waves*

<u>Jim</u> <u>Thomas</u>, Dalhousie University and Woods Hole Oceanographic Institution

This talk will discuss the application of a new set of amplitude equations to model various ocean waves interacting with oceanic vortices and topography. Three types of waves will be examined: internal gravity waves, surface gravity waves, and acoustic waves. The amplitude equations faithfully capture complex and intricate features of the wavefield, while being much faster to numerically integrate. Numerical simulations will be presented to demonstrate that in suitable parameter regimes, the amplitude equations can replace the full set of nonlinear governing partial differential equations.

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B43. Measurement Induced Complexity in Quantum Dynamics

<u>Ariadna E.</u> <u>Venegas-Li</u>, Fabio Anza, James P. Crutchfield, *University of California Davis*

Time series of qubits are a key part of important quantum computation protocols, such as quantum key distribution. This has driven the experimental development of single photon sources, such as color centers, which output time series in which the experimenter has no control over the state of the outgoing photons. If a classical observer performs measurements on the output qubits. the outcomes of such measurements generate a time series—a classical stochastic process. The aim of our work is to understand the apparent randomness and complexity of the output qubit process when observed through measurement. For this purpose we use simple hidden Markov models to generate qubit time series and study the properties of those processes when measured by an observer. We show that, in general, the observed classical processes are highly complex. Specifically, they have positive Shannon entropy rate and require an infinite number of predictive features for optimal prediction. We identify the specific mechanisms for the resulting complexity and examine the influence that the choice of measurement has on the randomness and structural complexity of the observed classical process.

B44. The Effect of Diffusion on Mixing By Cutting and Shuffling

<u>Mengying</u> <u>Wang</u>, Northwestern University; Ivan C. Christov, Purdue University

Dynamical systems are commonly used to model mixing of fluid or granular materials under flow. We consider a one-dimensional discontinuous dynamical system model (termed "cutting and shuffling" of a line segment), and we present a comprehensive computational study of its finite-time mixing properties. To improve the mixing efficiency and avoid pathological cases, we incorporate diffusion into this dynamical system. We show that diffusion can be quite effective at homogenizing a line segment of initially differing "colors." If the decay of the normalized mixing norm is plotted against the number of cutting and shuffling map iterations rescaled by the characteristic e-folding time. then universality emerges. Specifically, the mixing norm decay curves across all cutting and shuffling protocols collapse onto a single stretched-exponential profile. Next, we propose a way to predict the characteristic e-folding time (i.e., this critical number of iterations) a priori using the average length of unmixed subsegments of continuous color during cutting and shuffling, as compared to a minimal length scale set by diffusion. This prediction, called a "stopping time" for finite Markov chains, compares well with the e-folding time of the stretched-exponential fit. Finally, we analyze the effect of diffusion on cutting and shuffling through a Péclet number (a dimensionless inverse diffusivity). We show that the system transitions more sharply from an unmixed initial state to a mixed final state as the Péclet number becomes large. Our numerical investigation of cutting and shuffling of a line segment in the presence of diffusion thus present some evidence for the phenomenon known as a "cut-off" in finite Markov chains, but now in an interval exchange map.

B45. Enhancing the Synchronization of Coupled Rhythms Through Intrinsic Network Heterogeneity

Xize Xu, Hermann Riecke, Northwestern University

The study of collective oscillations or rhythms is an intriguing subject. In the brain the interaction of rhythms is thought to play a functional role. Here we focus on the interaction between the rhythms of two heterogeneous populations of mutually inhibiting oscillators. To gain insight into that interaction we first utilize the previously developed framework of the macroscopic phase-resetting curve (mPRC) for spiking networks [1]. Surprisingly, although the PRC of each individual oscillator is strictly positive, we find that the mPRC of the population is biphasic: external inhibition can both delay and advance the network depending on the time when it is applied. This biphasic mechanism results from the competition between the external inhibition and a decrease in the self-inhibition within the network caused by a reduction in the number of neurons spiking in a given cycle. The advancing component of the mPRC allows coupled networks to synchronize if the frequencies of the oscillators in each network are sufficiently heterogeneous. This heterogeneity plays a role similar to that of uncorrelated noise, which has been found to enhance the synchronization of ING rhythms [2].

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B46. Emotions Predict Presidential Voting Choices

Vicky Chuqiao Yang, Santa Fe Institute

Using a US national election survey dataset from 1980 to 2016, we find that pre-election self-reported emotional responses towards presidential candidates predict the individual's voting choice to over 90% accuracy. Emotions are more predictive than party identification, liberal-conservative identification, and stance on a combination of policy issues (abortion, defense spending, etc). Among the emotions reported in the dataset, the positive emotions (hope and pride) are more predictive than the negative ones (anger and fear). The predictive power of emotions also increased over time. These results suggest that besides studying "opinion dynamics", "emotional dynamics" can be worth considerable attention.

B47. Decoys and Dilution: the Impact of Incompetent Hosts on Prevalence of Chagas Disease

<u>Mondal Hasan</u> Zahid, Christopher M. Kribs, University of Texas at Arlington;

Biodiversity is commonly believed to reduce risk of vector-borne zoonoses. This study focuses on the effect of biodiversity, specifically on the effect of the decoy process (additional hosts distracting vectors from their focal host), on reducing infections of vector-borne diseases in humans. Here, we consider the specific case of Chagas disease and try to observe the impact of the proximity of chickens, which are incompetent hosts for the parasite but serve as a preferred food source for vectors. We consider three cases as the distance between the two host populations varies: short (when farmers bring chickens inside the home to protect them from predators), intermediate (close enough for vectors with one host to detect the presence of the other host type), and far (separate enclosed buildings such as a home and hen-house). Our analysis shows that the presence of chickens reduces parasite prevalence in humans only at an intermediate distance and under the condition that the vector birth rate associated with chickens falls below a threshold value, which is relative to the vector birth rate associated with humans and inversely proportional to the infection rate among humans.