SMU-RTG Meeting, May 4, 2022

__Schedule__
Morning session: 9:30-12:10
Lunch (provided): 12:10-1:30
Afternoon session: 1:30-4-ish

126 Clements Hall

Date/time	***Presenter***	***Topic***
Wednesday, May 4	**Morning**	9:25 Opening AA
9:30am-9:55am	Sabrina Hetzel	*Pure Quartic Solitons in Novel Laser Designs*
10:00-10:25am	Ross Parker	*Existence and stability of coherent structures with applications to optical, mechanical, and neural models*
10:30-10:55am	Jimmie Adriazola	*A reduction-based strategy for optimal control of Bose-Einstein condensates*
11:00-11:25 am	Steven Walton	*Numerical Methods for Wave Kinetic Equations*
11:25- 11:45	Break	
11:45-12:10pm	Pake Melland	*Spiking neurons in extracellular recordings and numerical simulations*
12:10-1:30pm	LUNCH	

Date/time	***Presenter***	***Topic***
Wednesday, May 4	**Afternoon**	
1:30pm-1:55pm	Molly Robinson	*Adapting Weighted Gene Co-Expression Network Analysis for Next Generation Sequencing*
2-2:25pm	Elyssa Sliheet	*Predicting Protein Ligand Binding Affinity Using Machine Learning assisted by Electrostatics*
2:30-2:55pm	Tyler Evans	*Thin-film effects in the linear and nonlinear regimes of nanopatterning under ion-beam irradiation*
3:00-3:25pm	Ken Yamamoto	*Polarization of disc and ring electrodes in high-conductivity electrolyte solutions*
3:30-4:00 pm	AA	Final comments

Titles and abstracts

Jimmie Adriazola, New Jersey Institute of Technology
Title: *A reduction-based strategy for optimal control of Bose-Einstein condensates*
Abstract: Applications of Bose-Einstein Condensates (BEC) often require that the condensate be prepared in a specific complex state. Optimal control is a reliable framework to prepare such a state while avoiding undesirable excitations, and, when applied to the time-dependent Gross-Pitaevskii Equation (GPE) model of BEC in multiple space dimensions, results in a large computational problem. We propose a control method based on first reducing the problem, using a Galerkin expansion, from a PDE to a low-dimensional Hamiltonian ODE system. We then apply a two-stage hybrid control strategy. At the first stage, we approximate the control using a second Galerkin-like method known as CRAB to de- rive a finite-dimensional nonlinear programming problem, which we solve with a differential evolution (DE) algorithm. This search method then yields a candidate local minimum which we further refine using a variant of gradient descent. This hybrid strategy al- lows us to greatly reduce excitations both in the reduced model and the full GPE system.

Tyler Evans, RTG Graduate Fellow
Title: *Thin-film effects in the linear and nonlinear regimes of nanopatterning under ion-beam irradiation*
Abstract: Since around the 1960's, it has been observed that ion-beam irradiation of surfaces can result in a wide range of nanoscale pattern formation, from ripples, cones, hexagonal arrays of dots, to terraces and helical wire-like structures, and more. While it is well-understood that these phenomena depend on numerous system parameters, such as beam-angle, temperature, interfacial and bulk chemistry, and ion and target species, no single model has been able to correctly predict specific details of the nanopatterning process. In particular, for short time-under-irradiation (the "linear regime"), theories are currently lacking to explain the material-dependent selection ripple wavelength and the critical angle of transition from flat to patterned surfaces. Our linear-regime theoretical work has now established for the first time a tightly qualitative, nearly quantitative, agreement between theory and experimental observation at the nanometer scale. Secondly, for long exposure times (the "nonlinear regime"), we consider the effects of the inclusion of thin-film physics on the evolution of terraced nanostructures and nanopores, leading to the development of new modeling and numerical techniques.

Sabrina Hetzel, RTG Graduate Fellow
Title: *Pure Quartic Solitons in Novel Laser Designs*
Abstract: Pure quartic optical solitons are a special class of solitons that have properties of higher order dispersion (namely, fourth order dispersion) in novel laser designs. Investigation is done in the dynamics, bifurcation structure and stability of localized states under the pure fourth-order dispersion case and compared to the dispersion profile for conventional (quadratic dispersion) solitons. Numerical simulations are conducted to provide evidence of different kinds of pulse generation for a variety of initial conditions. Studies are also being done for the spatial eigenvalues which highlights a unique characteristic of pure quartic solitons, namely oscillatory tails on all localized states, and also reveals in which parts of the parameter space particular stationary solutions can potentially exist. A long-term goal is to generalize these studies to different dispersion profiles and look at optimal pulse generation in terms of physical characteristics (energy/pulse-width relation) and robustness (stability). These studies could find applications in communications, frequency combs, and ultrafast lasers.

Pake Melland, RTG postdoctoral fellow
Title: *Spiking neurons in extracellular recordings and numerical simulations*
Abstract: In this talk, I will discuss two projects connected through spiking neurons. The first portion is an applied project using neural data obtained by researchers at UT Southwestern. The second portion focuses on theoretical work that I began during my PhD at the University of Iowa. Both are described below.
Researchers use electrophysiological data to study the behavior and dynamics of neurons. When sampled at a high enough frequency, action potentials can be detected in the neural data. Spike-sorting is the process of identifying the detected action potentials (spikes) with unique neural units. When recording over multiple hours or days, writing the full signal to a storage device may be unrealistic, and in some instances, only brief time periods near the spikes are saved. This yields a sparse data set, but many spike-sorting algorithms require input sampled at a fixed frequency. What are appropriate ways to prepare sparsely-sampled data as input into these algorithms? In this talk, we will discuss two approaches we have taken to preparing sparse data sets and how to assess the effectiveness of each.
The FitzHugh-Nagumo (FH-N) oscillator model is an autonomous system of two equations that can produce biologically relevant dynamics observed in a spiking neuron. When smooth periodic input is added, broader classes of spiking activity (including mixed-mode oscillations and bursts) are observed. In this talk, we will highlight numerically observed spiking regimes, and discuss the current theoretical approaches we are taking to analyze the non-autonomous forced system.

Ross Parker, RTG postdoctoral fellow
Title: *Existence and stability of coherent structures with applications to optical, mechanical, and neural models*
Abstract: This is a summary of research performed over the past year on the existence and stability of coherent structures, with applications to optics and neuroscience. First, I have studied the existence and stability of multi-kink and multi-breather solutions in the discrete Klein-Gordon equation, which is.a Hamiltonian system describing the dynamics of chain of particles with nearest-neighbor coupling and a nonlinear, on-site potential. I have also explored coherent structures in networks of optical fibers. One example is a twisted, circular, multi-core optical fiber, where we showed that the twist can produce complete suppression of one of the fibers in the ring. Another system is an optical lattice in which the coupling between waveguides varies periodically in the propagation distance z. We showed that such systems admit localized breather solutions in which the bulk of the optical intensity moves around a single group of four sites in the lattice. Future work includes exploring phase transitions between stationary and mobile solutions in these periodically modulated lattices. Finally, I have explored bifurcations in a large neural network model in the presence of permutation symmetries in the network.

Molly Robinson, RTG Graduate Fellow
Title: *Adapting Weighted Gene Co-Expression Network Analysis for Next Generation Sequencing*
Abstract: New technologies such as single-cell RNA-sequencing (scRNA-seq) have become vital to the understanding of cell type heterogeneity. One limitation of this technique is that the resulting datasets are sparse. That is, genes often have read counts of zero in a given cell. Computational challenges arise when sparse data sets are analyzed with Weighted Gene Co-Expression Network Analysis (WGCNA), a technique that has been used to study the underlying genetic network of bulk data sets.
This project aims to study how sparsity degrades the performance of WGCNA. This is done by modifying datasets where the method has been successfully applied. Gene clusters, or modules, of the generated network can then be tracked from the original dataset across varying levels of sparsity. This gives insight into how the network construction is altered when a sparse dataset is used. We will then study

imputation and smoothing techniques to recover performance. Finally, we will seek to determine significant statistical features of the data that predict model performance.

Elyssa Sliheet, RTG Graduate Fellow
Title: *Predicting Protein Ligand Binding Affinity Using Machine Learning assisted by Electrostatics*
Abstract: Electrostatics plays a significant role in bimolecular structure, interaction, and dynamics. However, due to its long range and pairwise natures, consideration of electrostatics is often challenging in accuracy and computational cost. In this talk, we present a novel efficient and accurate approach to include electrostatic features for predicting protein binding affinities using machine learning.

Steven Walton, RTG Graduate Fellow
Title: *Numerical Methods for Wave Kinetic Equations*
Abstract: Wave Kinetic Equations (WKEs) have remained principle objects of study in the theory of weak wave turbulence since the pioneering work of Nordheim, Peierls and Hasselmann. However, relatively little is known about the long-time behavior of solutions to these equations. We describe some numerical methods which are able to capture the long-time behavior of the energy of solutions to isotropic 3-WKEs. The results are compared with known theory for the decay rate of the total energy and are found to be in good agreement.

Ken Yamamoto, RTG Postdoctoral Fellow
Title: *Polarization of disc and ring electrodes in high-conductivity electrolyte solutions*
Abstract: Studies of electrical double layers near charged surfaces in electrolyte solutions are important for a wide range of applications including biophysics, colloidal science, and micro/nanofluidics. We investigate the polarization of disc and ring electrodes immersed in an electrolyte solution and subjected to a small external AC voltage governed by the Debye−Falkenhagen equation (a linearization of the Nernst−Planck equations) and the Poisson equation. Based on integral transforms, analytical techniques are developed for predicting the space charge density and complex impedance of the system. The effect of electrode dimension on the impedance is examined and compared with experiments. These mathematical models enable uncovering detailed knowledge of the surface charge densities on the electrodes from experimental impedance spectroscopy measurements.