

10th Georgia Scientific Computing Symposium

Program and Abstracts

Georgia State University
February 24th, 2018

Introduction

The Georgia Scientific Computing Symposium (GSCS) is a forum for professors, postdocs, graduate students and other researchers in Georgia to meet in an informal setting, to exchange ideas, and to highlight local scientific computing research. The symposium has been held every year since 2009 and is open to the entire research community.

Organizing committee

- Vladimir Bondarenko (chair), Georgia State University
- Xiaojing Ye (co-chair), Georgia State University
- Tesfaye Negash Asfaw, Georgia State University
- Kevin Rozier, Georgia State University
- Benjamin Sirb, Georgia State University

Invited Presentation Speakers

- Gennady Cymbalyuk, Neuroscience Institute, Georgia State University
- Taufiqar Khan, Department of Mathematical Sciences, Clemson University
- Ming-Jun Lai, Department of Mathematics, University of Georgia
- Wenjing Liao, School of Mathematics, Georgia Institute of Technology
- Simona Perotto, Department of Mathematics, Emory University & Politecnico di Milano
- Michael Stewart, Department of Mathematics & Statistics, Georgia State University

Event Location

Helen M. Aderhold Learning Center, Room 24, 60 Luckie St NW, Atlanta, GA 30303

Event Time

8:30AM–5:00PM, Saturday, February 24th, 2018

Event Website

<https://math.gsu.edu/xye/public/gscs/gscs2018.html>

Acknowledgements

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Event Schedule

Time	Speaker	Title
8:30-9:45	Registration	Poster Setup and Breakfast
9:45-10:00	Sara Rosen	Welcome and Opening Remarks
10:00-10:45	Michael Stewart	Numerical rank computation in matrix quotient and product decompositions
10:45-11:30	Wenjing Liao	Multiscale methods for high-dimensional data with low-dimensional structures
11:30-12:00	Poster Blitz	
12:00-13:30	Break	Lunch and Poster Session
13:30-14:15	Ming-Jun Lai	On recent development of matrix completion
14:15-15:00	Simona Perotto	Anisotropic mesh adaptation in Finite Elements: from theory to practice
15:00-15:30	Break	Coffee Break and Poster Session
15:30-16:15	Gennady Cymbalyuk	Dynamics of neurons with multiple regimes of activity
16:15-17:00	Taufiqar Khan	Deterministic and statistical regularization approaches for ill-posed inverse problems in electrical impedance and diffuse optical tomography
18:00-21:00	Dinner	

Invited Presentations

Dynamics of Neurons with Multiple Regimes of Activity

Gennady Cymbalyuk
Georgia State University

Central pattern generating neuronal networks (CPGs) control and coordinate rhythmic tasks such as swimming, breathing, and walking. We investigate whether biophysical properties of ionic currents could support multiple functional bursting regimes in neuronal models and provide efficient mechanisms of operation of multifunctional CPGs. Here we investigated dynamics supporting multistability in single neurons and small networks ranging from invertebrates to mammalian neurons and circuits. More recently, we tested whether the idea of multistable CPGs could be applied to two rhythmic behaviors in the cat: walking and paw shake. Both behaviors can be elicited in a spinalized cat, and there have been conflicting evidence that the same circuitry could be used for rhythmic behaviors with two distinct frequencies. We have developed a parsimonious model of a half-center oscillator composed of two mutually inhibitory neurons. The model exhibits multistability of slow and fast bursting regimes: a fast, 7-10 Hz paw-shake rhythm and a slow, 1-2 Hz walking rhythm. It is possible to switch between paw shaking and walking regimes by pulses of conductance such as those that could come from sensory neurons in the paw or from higher centers of motor control. Our model explains new experimental data from Dr. Prilutsky Laboratory and suggests that a paw-shake response is a transient activity of the multifunctional locomotion CPG.

Deterministic and Statistical Regularization Approaches for Ill-Posed Inverse Problems in Electrical Impedance and Diffuse Optical Tomography

Taufiqar Khan
Clemson University

Techniques that combine ideas from both deterministic and statistical methods to solve inverse problems are getting a lot more attention in recent years. This type of blended expertise is relevant to solving ill-posed inverse problems such as Electrical Impedance Tomography (EIT) and Diffuse Optical Tomography (DOT). There is also tremendous growth in devising new techniques from regularization theory both deterministic and statistical such as sparsity regularization, Bayesian inversion using Markov Chain Monte Carlo (MCMC) methods etc. Statistical approaches are becoming more popular for solving inverse problems particularly ill-posed inverse problems due to the growth of computational power. In this talk, we will discuss several deterministic and statistical approaches for image reconstruction in EIT and DOT. The complete electrode model for the inverse problem in EIT for damage detection in concrete will also be presented. The appropriate function spaces and regularization required to solve this ill-posed inverse problem is also described. Both the deterministic and the statistical inversion approaches are compared with preliminary results using data.

On Recent Development of Matrix Completion

Ming-Jun Lai
University of Georgia

I shall first introduce the research on matrix completion based on Netflix problem. Then I will survey some classic methods based on various approaches. In particular, I will explain some recent approaches based on alternating minimization methods including least squares, steepest descent, Riemann gradient descent techniques. Finally, I shall explain our method of Alternating Projection Algorithm and present a convergence analysis under some conditions. Linear convergence will be shown under a sufficient condition. I will end my talk with numerical experimental results to demonstrate our method is excellent in completing a matrix of low rank.

Multiscale Methods for High-Dimensional Data with Low-Dimensional Structures

Wenjing Liao
Georgia Institute of Technology

Many data sets in image analysis and signal processing are in a high-dimensional space but exhibit a low-dimensional structure. We are interested in building efficient representations of these data for the purpose of compression and inference. In the setting where a data set in R^D consists of samples from a probability measure concentrated on or near an unknown d -dimensional manifold with d much smaller than D , we consider two sets of problems: low-dimensional geometric approximations to the manifold and regression of a function on the manifold. In the first case, we construct multiscale low-dimensional empirical approximations to the manifold and give finite-sample performance guarantees. In the second case, we exploit these empirical geometric approximations of the manifold and construct multiscale approximations to the function. We prove finite-sample guarantees showing that we attain the same learning rates as if the function was defined on a Euclidean domain of dimension d . In both cases our approximations can adapt to the regularity of the manifold or the function even when this varies at different scales or locations.

Anisotropic Mesh Adaptation in Finite Elements: From Theory To Practice

Simona Perotto
Emory University, Politecnico di Milano

Anisotropic phenomena are present in several contexts of Scientific Computing, e.g., when modeling shocks in compressible flows, steep boundary or internal layers in viscous flows around bodies, propagation of fronts of different nature. Anisotropic mesh adaptation has proved to be a powerful strategy in modeling these scenarios, ensuring high reliability to the approximation, despite the considerable computational saving. This justifies the progressive inclusion of mesh tools suited to manage anisotropic meshes in the softwares currently in use. In the first part of the presentation, we introduce possible mathematical tools driving an anisotropic adaptation of a computational mesh. The focus is on metric-based techniques, the metric being associated with the control of standard norms or physically-meaningful functional of the discretization error. The size, the shape and the orientation of the mesh elements will be automatically selected in order to follow the intrinsic directionalities of the solution at hand. The second part of the presentation will be devoted to possible applications of interest in engineering practice, such as propagation of cracks in brittle materials, image segmentation and topology optimization of structures.

Numerical Rank Computation in Matrix Quotient and Product Decompositions

Michael Stewart

Georgia State University

Generalizations of the SVD of a single matrix to an implicit decomposition of a product or quotient of two matrices can be used to reveal information about the relation between fundamental subspaces of two matrices, including row subspace intersections, common null spaces, and mutual orthogonality of row subspaces. Such implicit decompositions avoid numerical difficulties associated with the explicit computation of matrix products and inverses. Computing and partitioning implicit decompositions of two matrices typically involves multiple interdependent rank decisions in which small elements are truncated. This talk describes ways of making these rank decisions in an optimal way so that truncated elements are nearly as small as possible and the decomposition reliably reveals the distance of a pair of matrices from a pair with a prescribed quotient or product SVD structure.

Poster Presentations

Markov Models of The Human Cardiac Sodium Channel

Tesfaye Negash Asfaw and Vladimir E. Bondarenko
Georgia State University

Voltage-gated sodium channels play an important role in the function of excitable cells. Upon activation, they initiate action potentials in cardiac muscle cells. Experiments show complex dependency of sodium channels on voltage. Therefore, it is important to understand their behavior under different physiological conditions. We developed and investigated six Markov models of the human cardiac sodium channel. The models were tested with major voltage-clamp protocols for activation, deactivation, inactivation, and recovery from inactivation. In addition current-voltage relationships, steady-state inactivation, and voltage dependence of normalized channel conductance were analyzed. Good agreement with the experimental data provides us with the mechanisms of the fast and slow inactivation of the human sodium channel and the coupling of its inactivation states to the closed and open states in the activation pathway.

Computer Simulation of the Bursting Dynamics in the Normal and Failing Mouse Hearts

Vladimir E. Bondarenko and Andrey L. Shilnikov
Georgia State University

Heart failure is a cardiac disease, which manifests in impaired cardiac function. On the cellular level, cardiomyocytes possess impaired Ca^{2+} transients, upregulation of $\text{Na}^+/\text{Ca}^{2+}$ exchanger function, reduction of Ca^{2+} uptake to sarcoplasmic reticulum, and reduced K^+ currents. Significant effort are applied to investigate this disease experimentally and by computer simulations. We used a comprehensive mathematical model of mouse ventricular myocytes to investigate mechanisms underlying the transition towards a state of heart failure and found that such a transition can be described as a sequence of bifurcations that the healthy myocytes undergo while transforming into failing myocytes. The sequence of bifurcation include periodic action potentials and $[\text{Ca}^{2+}]_i$ transients, action potential and $[\text{Ca}^{2+}]_i$ alternans, and bursting behaviors. Such bifurcations are observed in the experimental studies of heart failure. We also found that the slow component of the fast Na^+ current is a key factor for the bursting activity in mouse ventricular myocytes.

Multistable Clusters and Chimeras in Networks of Phase Oscillators

Barrett Brister
Georgia State University

Patterns of synchronized clusters are observed in many networks, including neuronal populations and other biological systems. Despite significant interest, the emergence and hysteretic transitions between stable clusters in a network of phase oscillators have still not been fully understood. In particular, the celebrated Kuramoto model of identical phase oscillators is known to exhibit multiple spatiotemporal patterns, including co-existing clusters of synchrony and chimera states in

which some oscillators form a synchronous cluster, while the others oscillate asynchronously. In this paper, we contribute toward an improved understanding of the emergence of stable clusters in networks of Kuramoto phase oscillators with inertia. We derive the conditions under which patterns of synchrony stably co-exist and demonstrate how inertia affects the hysteretic transitions between the patterns. Our stability results also shed light on the emergence of transient and stable chimeras.

Augmented Graph Synchronization Method for Directed Networks

Kevin Daley

Georgia State University

What is the stability criterion for synchronization in networks of identical (or nearly identical) oscillators stable, especially in regard to network topology? This general question has been widely discussed, and powerful stability methods for studying network synchronization have been developed. The most popular approaches include the Master Stability function and the Connection Graph method. Both methods, originally developed for undirected networks, have been generalized to handle networks with directed connections. In this paper, we present a modification of the Generalized Connection Graph method that gives tighter bounds on the coupling strength required for the onset of globally stable synchronization in a wide class of directed networks (typically, the sparse ones). We demonstrate how the directed network can be turned into an augmented undirected network with weighted connections. As a result, the stability conditions for synchronization in this augmented directed network also ensure stable synchronization in the original directed network. The obtained graph-based quantities also serve as estimates for the real part of algebraic connectivity for the underlying asymmetric Laplacian matrix.

The Effects of Moderate Stimulation of the β_1 -adrenergic Signaling System in Mouse Ventricular Myocytes

Mark Grinshpon and Vladimir E. Bondarenko

Georgia State University

The β_1 -adrenergic signaling system plays an important role in cardiac cells. It regulates action potential, calcium transients, and contraction force. We explored a comprehensive mathematical model of the β_1 -adrenergic signaling system for mouse ventricular myocytes to simulate the effects of moderate stimulations of β_1 -adrenergic receptors on the electrical activity, Ca^{2+} and Na^+ dynamics, as well as the effects of inhibition of protein kinase A and phosphodiesterase of type 4. Simulation results show that the action potential prolongations reach saturating values at relatively small concentrations of isoproterenol ($\sim 0.01 \mu\text{M}$), while the $[\text{Ca}^{2+}]_i$ transient amplitude saturates at significantly larger concentrations ($\sim 0.1 - 1.0 \mu\text{M}$). We also observed the differences in the response of Ca^{2+} and Na^+ fluxes to moderate stimulation of β_1 -adrenergic receptors. Sensitivity analysis of the mathematical model is performed and the model limitations are discussed.

The Shapes of Cell Migration

Xiuxiu He and Yi Jiang

Georgia State University

Cell migration is a highly integrated, multi-step process involving different morphologies and mechanisms of molecular and mechanical origins. Cell migration changes cell shape; cell shape also affects cell migration. Directed cell migration requires highly coordinated processes of cell shape deformation. For efficient movement, these processes must be spatiotemporally coordinated. The major remaining challenge is to identify mechanisms that couple these processes in space and time. How cell shape and migration influence each other through the intracellular molecular and mechanical mechanisms is not well understood. We analyzed images of cell migration to determine if and how the spatial-temporal dynamics of membrane contraction and protrusion can describe and predict cell migration features.

LAP Method for Coupled Problems in Imaging

James Herring

Emory University

Many inverse problems involve two or more sets of variables that represent different physical quantities but are tightly coupled with each other. For example, image super-resolution requires joint estimation of image and motion parameters from noisy measurements. Exploiting this structure is key for efficiently solving large-scale problems to avoid, e.g., ill-conditioned optimization problems. We present a new method called Linearize And Project (LAP) that offers a flexible framework for solving inverse problems with coupled variables. LAP is most promising for cases when the subproblem corresponding to one of the variables is considerably easier to solve than the other. LAP is based on a Gauss-Newton method, and thus after linearizing the residual, it eliminates one block of variables through projection. Due to the linearization, the block can be chosen freely and can represent quadratic as well as nonlinear variables. Further, LAP supports direct, iterative, and hybrid regularization as well as constraints. Therefore LAP is attractive, e.g., for ill-posed imaging problems. These traits differentiate LAP from common alternatives for this type of problem such as variable projection (VarPro) and block coordinate descent (BCD). Our numerical experiments examine LAP's performance for three coupled imaging problems: 3D super resolution, MRI motion correction, and image registration with local rigidity constraints.

Inferring Stage of HCV Infection Via Next Generation Sequencing and Multi-Parameter Analysis

Pelin Burcak Icer

Georgia State University

The research consist of evaluating the stage of HCV infection by applying machine learning methods on a multi-parameter analysis of strains sequenced from patients.

Path Optimization for Surface Surveillance

Benjamin Ide

Georgia Institute of Technology

Consider a cluttered environment in which there are surfaces that need to be surveyed. We propose an algorithm to find the shortest path to follow to achieve full surveillance. We propose a finite dimensional space of paths in which to search. In this space, we use a global optimization strategy given by intermittent diffusion.

In addition to the application of real life surveillance, this is also of mathematical interest. We provide evidence in favor of Zalgaller's conjecture for the Asteroid Surveillance Problem, and we use related solved problems to provide evidence that our algorithm does approximate global optima.

Effects of Temperature on Rhythmic Activity in Interstitial Cells of Cajal of the Small Intestine

Sarah Johnson, Nataliya Maksymchuk, Gennady S. Cymbalyuk

Georgia State University

The cause of many intestinal motility disorders lies in the dysfunctional dynamics of Interstitial Cells of Cajal (ICC) located in the myenteric region of the small intestine. They are electrically coupled to circular and longitudinal smooth muscle cells and generate spontaneous rhythmic electrical activity which is the origin of smooth muscle contractions. Factors such as temperature influence oscillatory activity, which changes the waveform of the slow waves. The goal of our study is to understand the mechanisms of slow-wave activity of the ICC in the small intestine under different temperature conditions. Here, we have systematically changed the temperature as a parameter of a biophysically based model of ICC to investigate the effects of temperature sensitivity. Temperature was increased in steps of 2°C from 25 to 45°C and the slow oscillations were analyzed at each parameter value. Changes in each of the currents were evaluated to determine whether they are critical for the observed changes in the waveform. We also investigated the role of the intracellular geometry of the cell with focus on the Mitochondria, Endoplasmic Reticulum and Submembrane Space. This study will help us understand functional and pathological dynamics of intestinal motility. This research was supported by GSU Brains & Behavior grant for G.C., GSU University Assistantship Program to S.J., and GSU Honors College to S.J.

Modeling Patterns of Slow Wave Oscillations in Interstitial Cells of Cajal

Taylor Kahl, Parker Ellingson, and Gennady S. Cymbalyuk

Georgia State University

Proper digestive functioning requires a variety of coordinated activities in the gastrointestinal tract. Within the small intestine, three types of motility patterns regularly occur: silence, peristaltic propulsion, and mixing motions. The activity of muscles depends on input from interstitial cells of Cajal (ICC), known as pacemaker cells in the gut. ICCs generate spontaneous rhythmic depolarizations called slow waves that spread through a network of ICCs and smooth muscle cells to cause synchronous depolarizations and muscle contractions. We investigated whether all three patterns of small intestinal motility can be produced by altering the ICC slow wave. The frequency of muscle contractions matches the frequency of the slow wave in the ICC. The intrinsic

frequency of the slow wave is thought to be controlled by the dynamics of intracellular calcium release and reuptake through the endoplasmic reticulum (ER). However, the dynamics of calcium current through T-type calcium channels are also sufficient to generate oscillating depolarizations. We hypothesized that calcium oscillations through both the ER and T-type calcium channels interact to create multiple patterns of activity in the ICC. Specifically, if calcium oscillations through the ER occur at a slightly different frequency than calcium oscillations through T-type channels, then this interaction will produce a beating pattern in ICC that corresponds to mixing motions. Using a mathematical model of cellular dynamics, produced in MATLAB, we show that ICCs are capable of producing patterns corresponding to silence, propulsion, and mixing patterns recorded in the small intestines. Acknowledgements: This project was supported by the GSU Brains and Behavior program.

Asymmetrically Modeling Locomotor and Paw-Shaking Rhythms in a Multifunctional Central Pattern Generator

Rashid Khwaja, Jessica Parker, and Gennady S. Cymbalyk
Georgia State University

Central pattern generators (CPGs) are neuronal circuits controlling rhythmic motor functions such as walking and breathing. We developed a model of a multifunctional CPG which generates a paw-shaking regime and a locomotory regime in cats. Our CPG consists of two neurons organized in a half-center oscillator motif (HCO). An HCO consists of two neurons which mutually inhibit each other. A single interneuron represents the muscular activity of a hindlimb flexor while the other neuron represents a hindlimb extensor. We investigated how changes in the biophysical parameters associated with intrinsic cellular currents on a single interneuron in the HCO control these rhythms. We constructed our model such that the slow calcium current (ICaS) drives the locomotory regime while the slow sodium current (INaS) current drives the paw-shaking regime. We investigated how asymmetries in the strength of these currents between hindlimb flexors and extensors controls active phases of these motor regimes. By investigating bursting dynamics within the two regimes we discovered that controlling the conductance of the slow calcium current (gCaS) in a single neuron asymmetrically controls the locomotory regime, but it does not control the paw-shaking regime. From a locomotory regime, controlling gCaS in one neuron, we observed burst characteristics in each of the two interneurons such as burst duration, duty cycle, interburst interval, and spike frequency. By using linear and non-linear regressions in MATLAB, we determined that the burst duration changes in both and linearly and a square root-like when controlling the strength of ICaS in a locomotory rhythm. By asymmetrically controlling the gCaS and gNaS, we observed asymmetries in in the burst durations within both the locomotory and paw-shaking regimes. When gCaS is asymmetrically controlled from 12.3 nS within a locomotory regime, the burst duration changes linearly in the neuron with the with the lower burst duration. The burst duration in the other neuron changes proportionally to the square root function. This mechanism can explain the control of locomotory and paw-shaking regimes at different cycle periods.

Community Detection in Graphs Using Compressive Sensing

Daniel Mckenzie
University of Georgia

In many areas of Applied Mathematics it is of interest to partition the vertex set V of a graph G into disjoint sets C_1, \dots, C_k , called clusters, such that the clusters are densely connected with few edges between them. For example, one could be trying to find communities in a social network, sets of related neurons in the human brain or collections of similar webpages on the World Wide Web. More generally, any data set X equipped with some notion of distance can be turned into a graph by inserting an edge between data points which are appropriately close. In this poster we present recent work of the author, in collaboration with Professor Ming-Jun Lai, on a new algorithmic approach to finding clusters that utilizes ideas from the signal processing field of Compressive Sensing. In particular, we show that our algorithm is able to ‘extract’ a single cluster of size n_0 in $\mathcal{O}(n \ln(n)n_0)$ operations, where n is the total number of vertices in the graph.

Simulations of the β_1 -Adrenergic Regulation of Mouse Ventricular Myocyte Contraction

Paula Mullins¹, J. Jeremy Rice², and Vladimir E. Bondarenko³

¹University of North Georgia, ²IBM T.J. Watson Research Center, and ³Georgia State University

The β_1 -adrenergic regulation plays an important role in regulating heart function. Activation of this system leads to the changes in the cardiac action potential and Ca^{2+} dynamics resulting in an increased heart rate and stronger myocyte contraction. On the other hand, prolonged stimulation of the β_1 -adrenergic signaling system can lead to cardiac hypertrophy and heart failure. To understand the cardiac myocyte behavior upon stimulation of the β_1 -adrenoceptors, a mathematical model of cardiac myocyte contraction was developed. The model was verified by the simulation of the major experimental protocols, such as the steady-state force-calcium relationship, time course of force redevelopment, cell shortening, force-velocity relationships, etc. Simulation data revealed the mechanisms of increased contraction force and myocyte shortening upon stimulation of the β_1 -adrenergic signaling system.

A Bayesian Framework for Strain Identification From Mixed Diagnostic Samples

Lauri Mustonen
Emory University

We present a mathematical framework and computational methods for disambiguation of pathogen strains in mixed DNA samples. Mathematically, strain identification aims at simultaneously estimating a binary matrix and a real-valued vector such that their product is approximately equal to the measured data vector. The problem has similarities with blind deconvolution, but binary constraints are present. The specific problem structure allows us to efficiently decouple the problem into smaller subproblems, for example when considering maximum a posteriori estimation or uncertainty quantification. Relevant applications in public health include identification of pathogens and monitoring disease outbreaks.

Modeling a Multifunctional Central Pattern Generator That Generates a Locomotor-Like Rhythm and Transient Paw-Shake Responses

Jessica Parker¹, Alex Klishko², Boris Prilutsky², and Gennady S. Cymbalyuk¹

¹Georgia State University and ²Georgia Institute of Technology

We investigate whether mammalian central pattern generators (CPGs) could be multifunctional, controlling more than one functional rhythmic behavior. We constructed a model of a single CPG that controls both locomotion (1 Hz) and paw-shaking (10 Hz) in cats to propose general biophysical mechanisms, supporting vastly different rhythms of a multifunctional CPG. This model consists of four neurons: two inhibitory neurons carry reciprocal inhibition between two excitatory neurons. Each of these neurons represents a neuronal population in the cat CPG. The excitatory neurotransmission is conducted by NMDA and AMPA glutamatergic synaptic currents and the inhibitory neurotransmission is GABAergic and glycinergic. This model exhibits coexistence of the locomotion rhythm and the paw-shaking rhythm. Transient paw-shake-like activity can be elicited by applying an excitatory pulse of current in either the multistable model or a monostable model. The described mechanism of multistability provides various testable predictions about bursting dynamics throughout a paw-shake response. These predictions were also tested in a corresponding population model, consisting of two inhibitory populations of 10 neurons each that carry reciprocal inhibition between two excitatory populations of 10 neurons each. The population model also exhibits coexistence of locomotion and paw-shaking and provides predictions consistent with the four neuron model. We also tested these predictions experimentally. The paw-shake responses were elicited in cats by attaching an adhesive tape on the hind paw and letting the cat walk on a walkway. The cats performed paw-shake responses intermittently while walking. We recorded EMG activity of multiple hindlimb muscles and hindlimb kinematics, and we found that these experimental results agreed with model predictions.

Modeling Phenotypic Differentiation in *B. Subtilis* Through an Environmentally Regulated Nested Feed-forward Loop Network

Andira Putri

Georgia State University

Biofilms are colonies of microbial organisms held together by a polymeric extracellular matrix (ECM) on surfaces. Biofilms are prevalent in natural, industrial, and health settings. Much of the molecular mechanisms for biofilm formation are still unclear, in particular how cells switch their phenotypic behavior. To gain an understanding of this phenotypic switch, we focus on sporulation in *Bacillus subtilis* (*B. subtilis*). Empirical evidence shows that Spo0A is the master protein determining cell phenotype: High concentrations of phosphorylated-Spo0A (Spo0A~P) trigger sporulation while low levels lead to ECM production. We constructed a nested incoherent feed-forward genetic network that integrates both nutrient and quorum-sensing pathways. We used a system of coupled differential equations to study this biological circuit in response to nutrient availability and surrounding cell density. Dynamical systems analysis of these equations reveal that both starvation and overcrowding can raise Spo0A~P levels and trigger sporulation. This simple model of the *B. subtilis* genetic network is the first step in understanding the growth mechanisms of biofilms under varying environmental conditions.

ACHILES: An Asynchronous Iterative Sparse Linear Solver

Paritosh Ramanan

Georgia Institute of Technology

Asynchronous methods are becoming more popular for solving linear systems offering faster performance in many cases. In such methods, local updates are performed using the latest available information from other sub problems eliminating the need for synchronization. In this poster, we present ACHILES, an asynchronous iterative linear solver that uses MPI Remote Memory Access (RMA) to asynchronously communicate data. We further show the performance of ACHILES for asynchronous Jacobi Schwarz.

Uncovering the Physiological Role of β_2 -Adrenoceptors in Mouse Ventricular Myocytes Via Computational Simulations

Kelvin Rozier and Vladimir E. Bondarenko

Georgia State University

Advances in technology have led to an increase in the use of computational tools as a means of exploring and understanding complex systems in an array of disciplines, including the biological sciences. In this study, we developed a molecular based, compartmentalized model of the combined β_1 - and β_2 -adrenergic signaling systems in mouse ventricular myocytes. Simulations of the experimentally verified model were then used to assess the role of β_2 -adrenergic receptors. Stimulation of the signaling system in normal/healthy mouse ventricular myocytes suggests that β_2 -adrenoceptors render insignificant or no contribution to calcium transients and the action potential. Simulations show that the physiological effects of β_2 -adrenoceptors can be revealed with the inhibition of phosphodiesterase 3 and 4 by cilostamide plus rolipram or with the inhibition of inhibitory G protein, G_i , by the application of pertussis toxin.

Optimal Control Methods for Deep Learning

Lars Ruthotto

Emory University

This poster presents a new framework for deep learning that exploits the relationship between the training of deep networks to optimally controlling a system of nonlinear partial differential equations (PDEs). This new interpretation leads to a variational model for deep learning, which provides new theoretical insight into CNNs, new approaches for designing learning algorithms, and a myriad of opportunities for research and teaching.

Fast Estimation of Genetic Relatedness Between Members of Heterogeneous Populations of Closely Related Genomic Variants

Viachaslau Tsyvina

Georgia State University

Many biological analysis tasks require extraction of families of genetically similar sequences from large datasets produced by Next-generation Sequencing (NGS). Such tasks include detection of viral transmissions by analysis of all genetically close pairs of sequences from viral datasets

sampled from infected individuals or studying of evolution of viruses or immune repertoires by analysis of network of intra-host viral variants or antibody clonotypes formed by genetically close sequences. The most obvious naïve algorithms to extract such sequence families are impractical in light of the massive size of modern NGS datasets. In this paper, we present fast and scalable k-mer-based framework to perform such sequence similarity queries efficiently, which specifically targets data produced by deep sequencing of heterogeneous populations such as viruses

Influence of the Na^+/K^+ Pump on Pathological Bursting Dynamics in Pre-Bötzinger Complex

Alex Vargas and Gennady S. Cymbalyuk
Georgia State University

The medulla of the brain stem contains regions necessary for maintenance of normal breathing patterns dedicated for each phase of breathing. These neuronal populations, if responsible for generating respiratory rhythm, do so for either the inspiratory or expiratory phases of breathing (Feldman & Del Negro 2006). The Pre-Bötzinger Complex (PBC) is one of those regions that generates rhythm governing the inspiration phase of breathing (Smith et al. 1991, Ramirez & Richter 1996). This region consists of neurons when isolated, that exhibit bursting, tonic spiking, or silence and when connected in a network produce bursting through excitation (Ramirez et al. 2004). Some of these neurons burst through maintaining a ratio of persistent sodium conductance to leak current conductance (Del Negro et al. 2002). Leak current can be divided into Na^+ and K^+ dominated components that we believe have the potential to modify burst characteristics alongside the Na^+/K^+ pump. The Na^+/K^+ pump plays an important role within the PBC such as post-burst hyperpolarization, maintaining external potassium concentration and increasing the reversal potential of the potassium component of leak current (Krey et al. 2010, Bacak et al. 2016). Differential equations implemented in a Hodgkin Huxley formalism (Hodgkin & Huxley 1952) in MATLAB were used to simulate the PBC at the neuronal level in a biophysically accurate manner. Experimental data from previous studies of the characterization of persistent sodium was used in the model to make the model more experimentally accurate. Differential equations were integrated using the ode15s solver and Gear's method. Varying the strength of the Na^+/K^+ pump shifted the neuron into and out of rhythmic behavior and silence. At higher pump strengths the burst frequency increased whereas lower pump strength values, the interburst period increased. The pump's effect on modulation of bursting properties in the full model and dynamics in the oscillatory model add evidence to the implication of Na^+/K^+ pump in physiological disorders stemming from arrhythmia in respiratory rhythm generating regions of the brain like the PBC.

Cardiovascular Mathematics: From Theory to Practice

Alexander Viguerie
Emory University

This poster summarizes the many different activities of our research group regarding the application of computational fluid dynamics and finite element methods to problems in cardiology.

A Characterization of the Domain of Beta-Divergence and Its Connection to Bregman Variational Model

Hyenkyun Woo
Korea Tech

In machine learning and signal processing, the beta-divergence is well known as a similarity measure between two positive objects. However, it is unclear whether or not the distance-like structure of beta-divergence is preserved, if we extend the domain of the beta-divergence to the negative region. In this poster, we introduce the domain of the beta-divergence and its connection to the Bregman-divergence associated with the convex function of Legendre type. In fact, we show that the domain of beta-divergence (and the corresponding Bregman-divergence) include negative region under the mild condition on the beta value. Additionally, through the relation between the beta-divergence and the Bregman-divergence, we can reformulate various variational models appearing in image processing problems into a unified framework, namely the Bregman variational model. This model has a strong advantage compared to the beta-divergence-based model due to the dual structure of the Bregman-divergence. As an example, we demonstrate how we can build up a convex reformulated variational model with a negative domain for the classic nonconvex problem, which usually appears in synthetic aperture radar image processing problems.

An Uncertainty-Weighted Asynchronous ADMM Method for Large-Scale PDE Parameter Estimation

Samy Wu Fung
Emory University

We consider a global variable consensus ADMM algorithm for computing the maximum a posteriori (MAP) estimate of large-scale PDE parameter estimation problems. We obtain an efficient optimization scheme by partitioning the data and solving the resulting subproblems in parallel. The parallelization can be implemented asynchronously, and each subproblem can be associated with different forward models and/or right-hand-sides, leading to ample options for tailoring the method to different applications.

A drawback of consensus ADMM is its slow convergence, especially when there are a large number of subproblems. This is particularly challenging in PDE parameter estimation due to the immense costs per iteration. To accelerate the convergence in the first few iterations, we introduce a novel weighting scheme in the algorithm that accounts for the uncertainty associated with the solutions of each subproblem. We exemplarily show that the weighting scheme reduces the time-to-solution of a multiphysics parameter estimation problem.