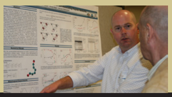
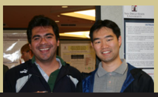
16th Annual ACSESS

Friday, April 12, 2019
12:00 pm - 5:00 pm
SDSU's Parma Payne Goodall
Alumni Center

For Applied Computational Sciences and Engineering Student Success

CSRC — gateway to the future — an interdisciplinary

San Diego State University

11:30am-12:00 pm	**Registration**	
12:00-1:00 pm	**Buffet Lunch**	
	Alfonso Limon Research & Development Oneirix Labs	Moderator
1:00-1:10 pm	**Stanley Maloy** Graduate & Research Affairs, SDSU	Welcome / Opening Remarks
	Jeffrey Roberts Dean, College of Sciences, SDSU	
1:10-1:30 pm	**Jose E. Castillo** Director Computational Science Research Center San Diego State University	Computational Science at SDSU & ACSESS Program
1:30-2:30 pm	**Melanie Hagerty** Vice President Engineering & Innovation Cubic Corporation	Keynote Speaker "Industry and University Innovation"
2:30-3:00 pm	**Blitz Oral Presentations**	
3:00-3:45 pm	**Poster Presentations / Reception**	
4:00-4:30 pm	**Guadalupe X. "Suchi" Ayala, Andrew Cooksy & Satchi Venkataraman** Associate Directors Computational Science Research Center San Diego State University	Poster Presentation Awards & Closing Remarks

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Welcome to the 16th Annual ACSESS Event

We cordially welcome our local tech and biotech industry executives, board members and CSRC faculty, and students to our Applied Computational Science and Engineering Student Success (ACSESS) Annual Event.

ACSESS was created sixteen years ago to provide graduate students an opportunity to work on real world problems. Also, with the vision to create stronger links between academic computational scientists, industry professionals and technology officers. This year's program is a reflection of that idea to continue the support and aspiration to foster CSRC educational and research missions; instilling graduate student's interest in industry problems and pursuing careers in technology and biotechnology sectors.

We appreciate the great interest of our administration, faculty and student participation in our event, and our special thanks go to our CSRC board members for their continuous advice, as well as our company sponsors for the financial commitment to our teaching and research missions.

Mission Statement

The mission of the Computational Science Research Center (CSRC), located at San Diego State University, is to promote development and advancement of the interdisciplinary subject of computational science. This is accomplished by fostering research, developing educational programs, and promoting industrial interaction, outreach, and partnership activities.

The Computational Science Research Center provides an excellent environment for scientific research at SDSU. The center facilitates the interaction between applied mathematics, computer science, and the sciences by providing the necessary infrastructure for productive research efforts.

Real world applications are the focus of the projects undertaken by the faculty and students of the center. Such projects provide a significant educational opportunity for our students to hone their industrially relevant computational skills.

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Coupling GCCOM and Swash for Analysis of Free Surface Conditions

By: Jared Brzenski
Advisor: Jose Castillo

No one ocean model can do everything in a computationally efficient way. Deep water models, optimized for large scale features, are not able to capture surface conditions or violent interactions accurately. Shallow water models, optimized for smaller distances, lack the sophistication to render global slow phenomenon impacted by temperature, pressure, and salinity. To overcome these drawbacks, coupling is used to combine the best features of different models to better resolve complex interactions between large and small scale phenomenon. Presented here is a coupling between GCCOM and SWASH using the Distributed Coupling Toolkit (DCT) to resolve free surface conditions for a lock release experiment. This coupled system is able to resolve free surface conditions from a non-hydrostatic experiment over a large vertical scale, something neither model can do efficiently alone.

This research is supported by the Computational Science Research Center at San Diego State University.

Improving Epileptic Seizure Detection from EEG Signals: A Patient-Specific Approach

By: Misha Kutzman
Advisor: Jerome Gilles

Epilepsy is one of the most common neurological disorders and is estimated by the World Health Organization to affect nearly 65 million people worldwide. Characterized by recurrent and unpredictable seizures, epilepsy can be associated with burdensome emotional, physical and social side effects. Various methodologies have been employed to detect and predict seizure events from electroencephalogram (EEG) recordings in order to assist with disease management. Our goal is to improve the seizure detection and prediction processes by enhancing the sensitivity and accuracy of information extracted from the epileptic EEG signal. To achieve this, we have implemented a novel application of a patient-specific wavelet transform, the Empirical Wavelet Transform, to extract spectral features from recordings of pediatric EEG seizure data. We then use these features to train a classification model to more accurately distinguish between seizure and non-seizure data, thereby improving the robustness of automated seizure detection and prediction.

This research is supported by a STEM scholarship award funded by the National Science Foundation (DUE- 1259951) and the Computational Science Research Center at San Diego State University.

Adaptive Pre-Shaping of Ultrashort Pulses in AZO/ZnO at the Epsilon-Near-Zero Spectral Point

By: Priscilla Kelly
Advisor: Lyuba Kuznetsova

Metamaterials that can operate at the epsilon-near-zero (ENZ), where the material's optical permittivity is << 1, have demonstrated unique opportunities for light-matter interactions. Applications such as all-optical switching, radiation phase tailoring, and deformation-free propagation at the ENZ have shown potential for real-world optical devices. We are interested in ENZ devices made from aluminum-doped zinc oxide (AZO) as its Kerr coefficient has a 6-fold increase and the dynamics of its inter- and intra-band transitions can be controlled at the ENZ wavelength. Here, we numerically investigated how ultrashort pulse preshaping affects propagation in AZO and zinc oxide (AZO/ZnO) multilayered materials. This study uses the finite-difference time-domain (FDTD) method and aims to minimize sideband development using an evolutionary optimization algorithm.

This research is supported by the Graduate Research Fellowship Program (1321850) and the Computational Science Research Center at San Diego State University.

Machine Learning of Load-Balancing for a Large Parallel Code

By: Jordan Fox
Advisor: Calvin Johnson

Load-balancing is a ubiquitous problem in high-performance computing (HPC), and it is often constrained by physics in scientific codes. This work uses state of the art machine learning (ML) techniques to assist load-balancing in highly parallelized runs of BIGSTICK, a configuration-interaction nuclear shell-model code. BIGSTICK breaks up work into bundles of operations which are in turn distributed over MPI processes. Our challenge is to accurately predict the time each bundle will take to compute, so that the total work can be distributed efficiently. We turn to sophisticated ML techniques to predict compute-time of bundles by their physical features. By training random forest and gradient boosted trees classification models on bundles from many BIGSTICK runs, we can predict bundle cost more accurately and in turn execute more efficient runs on world-class supercomputers.

This research is supported by U.S. Department of Energy funds (DE-FG02-03ER41272), a STEM scholarship award funded by the National Science Foundation (DUE- 1259951), and the Computational Science Research Center at San Diego State University.

PHANOTATE: A Novel Approach to Gene Identification in Phage Genomes

By: Katelyn McNair
Advisor: Robert Edwards

Background: Currently there are no tools specifically designed for annotating genes in phages. Several tools are available that have been adapted to run on phage genomes, but due to their underlying design they are unable to capture the full complexity of phage genomes. For example, prokaryotic genomes typically have long genes separated by non-coding regions that are distinct and non-overlapping, but phage genomes are composed of shorter, overlapping, genes that are predominantly all on the same DNA strand. Phage genomes also contain very few non-coding nucleotides, as the size of their genome is limited by packaging into rigid capsid structures. Phages have therefore adapted their genomes to be extremely compact, having adjacent genes that overlap, and genes completely inside of other longer genes. This non-delineated genome structure makes it difficult for gene prediction using the currently available gene annotators.

Methods: To fill this need for an accurate phage genome annotation program, we implemented a novel method for gene caller specifically designed for annotating phage genomes: THEA (The Algorithm). While the compact nature of genes in phages is a problem for current gene annotators, we exploit this property by treating a phage genome as a network of paths: where open reading frames are favorable, and overlaps and gaps are less favorable, but still possible. We represent this network of connections as a weighted graph, and use graph theory to find the optimal path.

Results: We compared THEA to other gene callers by downloading a set of 2,133 complete phage genomes from GenBank. We then predicted the open reading frames using THEA and the three most popular gene callers: GeneMarkS, Glimmer, and Prodigal. We found that the four programs find a consensus of 82% of the total predicted genes, with THEA predicting significantly more genes than the other three. We found these extra genes in both GenBank's non-redundant protein database, as well as in GenBank's sequence read archive, at levels that suggest that these are functional protein coding genes.

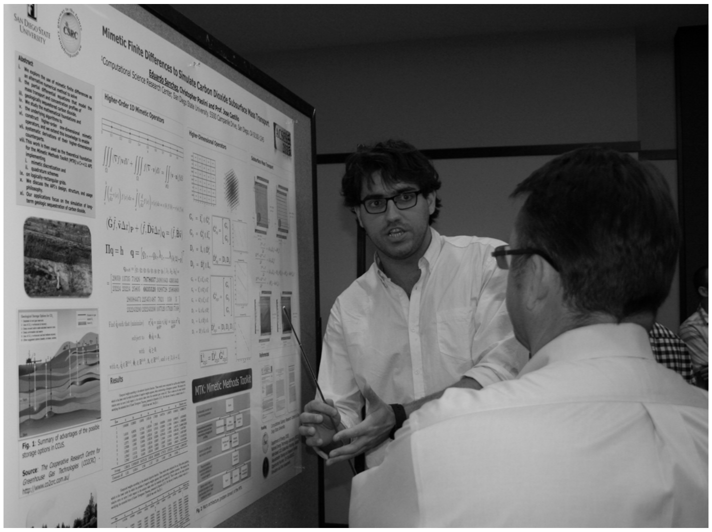
This research is supported by Department of Defense funds (IAA: DTRA10027-20149), the Graduate Research Fellowship Program (1321850), and the Computational Science Research Center at San Diego State University.

Random Forest Based Matching Algorithm for Observational Data with Missing Values, Applied to Student Success Studies

By: Tristan Hillis, Maureen Guarcello, Richard Levine, and Juanjuan Fan
Advisor: Juanjuan Fan

Observational studies require matching across groups over multiple confounding variables putting more emphasis on each observation and increasing the issue of missing data. Across the literature, matching algorithms fail to handle this issue. In this way, missing values are regularly imputed to be considered in the matching process. However, imputing is not always practical forcing us to drop the observation due to the deficiency of the chosen algorithm decreasing the power of the study, and possibly failing to capture crucial latent information. We present a study of missingness on a large data set involving student success in an introductory business statistics course. We have two groups of students: those who attend multiple supplemental instruction sessions and those who do not. To perform the matching, we leverage our own developed R package iterOptMatchWM. This package finds a one to one matched subsample of data that incorporates missing values in an iterative fashion. The underlying framework utilizes random forest as a natural tool in constructing a distance matrix where there might be missing values; then feeding into an optimal matching algorithm as proposed by Hansen et al., 2006. We evaluate the robustness of the matching results by injecting varying amounts of missingness into the data. Additionally, we present results utilizing surrogate splits as an enhancement to handling missing data within the random forest construction.

This research is supported by National Science Foundation funds (1633130) and the Computational Science Research Center at San Diego State University.



Wide Angle Beam Steering Cylindrical Parabolic Reflector with Phased Array as a Feed Source for Ku-Band Applications

By: Ghanshyam Mishra
Advisor: Satish K. Sharma

A 3D metal printed cylindrical parabolic reflector is investigated at Ku-band for wide angle beam steering using phased array antenna as a feed source. The parabolic cylindrical reflector provides wide beam scanning at low f/D compared to a conventional parabolic reflector antenna. In addition to wide beam scanning, the sidelobe level can also be reduced by distinct control of the excitation weights. Also, the cost of the beamforming components is reduced significantly due to less RF components. The wide angle beam scanning is achieved in a single plane along the cylindrical axis. The stacked patch antenna array is used to illuminate the reflector and is arranged along the focal line of the cylindrical axis of the reflector.

The cylindrical parabolic reflector surface is generated in MATLAB and analyzed using Ticra GRASP. The maximum dimension of the reflector is 50 cm and is placed in an offset arrangement with f/D = 0.4. The stacked patch antenna is analyzed in Ansys HFSS to provide wide impedance matching bandwidth, low cross polarization and stable radiation pattern from 12 GHz to 15 GHz. The phased array of size 8 × 4 is used to illuminate the cylindrical parabolic reflector. The peak directivity of the secondary pattern is around 27 dBi and an overall beam scanning of ±35° is achieved along the cylindrical axis of the reflector. The simulated reflector will be 3D metal printed and the effect of finite conductivity, surface roughness and strut effects will also be analyzed.

The phased array feed source is steered using the integrated analog beamforming network (BFN). Beam steering is achieved using Ku-band Anokiwave AWMF-0117 integrated silicon core chips. The chip features half duplex operations with +20 dB transmit channel gain, +28 dB receive channel gain with 3 dB noise figure. 6-bit amplitude and 6-bit phase controls are included with low RMS amplitude and phase errors. The fabricated BFN board will be assembled with the 3D metal printed cylindrical parabolic reflector and the scan performance will be experimentally verified.

This research is supported by Department of Defense funds, the Graduate Research Fellowship Program (1321850), and the Computational Science Research Center at San Diego State University.

All Metal Heat Sink Dual Linear Polarized Phased Array Antenna for Ku-Band Applications

By: Rudraishwarya Banerjee
Advisor: Satish K.Sharma

In this abstract, a new 8×8 dual linear polarized phased array antennas, with 128 innovatively designed metallic radiators, each working as heat sink as well, is proposed for Ku band applications. Each single radiator is half wavelength in height, and fed by a stripline through a intuitively shaped balun. Two shaped radiators are placed at right angles within a metal cavity of square cross section and overall dimension of nearly $\lambda/2 \times \lambda/2$. This constitutes the unit dual linear polarized radiating cell. A multi-layered substrate is used to accommodate stripline feed for two radiators of an unit cell and surface waves generated due to thick substrate is supressed by using a number of vias, placed underneath each metal cavity, with a period of nearly $\lambda/6$ and diameter 12 mils. The single radiating element is designed to provide wideband performance with respect to S11 of 10dB between 12-15 GHz and acceptable radiation pattern is observed over the entire bandwidth. A 8×8 array will be designed with 64 radiating unit cells, each unit cell having two feed points. Spacing between unit cells depends on expected beam scan range of ±45 degree. Active S-parameter will be calculated for this array structure for the desired scan range over the matching bandwidth. Peak gain versus frequency will be evaluated as beam scans. The beamforming network will be directly integrated with the phased array antenna aperture. 3D metal printing technology will be employed to build the phased array antenna aperture. The full fabricated phased array antenna and the beamforming network will be tested for its impedance matching and radiation pattern in Antenna and Microwave lab at San Diego State University.

This research is supported by SPAWAR and the Computational Science Research Center at San Diego State University.

Spatio-Temporal Graph Inference for Multi-Variate Time Series

By: Siddhi Tavildar
Advisor: Ashkan Ashrafi

In this research we propose spatio-temporal model for graph inference using multi-variate time series as graph signals. The purpose of spatio-temporal graph inference is to infer and analyze instantaneous (static) and dynamic connections in graphs. Additionally, the underlying directed graph can be represented as the augmented spatio-temporal graph structure and the directions can be inferred from the temporally delayed graph connections. We establish the temporal relationship equation (TRE) to infer the inter-relationship of the signals in causal multivariate time series data. The theoretical and mathematical framework for spatio-temporal graph inference is developed using TRE with existing symmetric graph inference methods. With the proposed model, we aim to provide a generic model leveraging the existing undirected graph inference methods that can be used to infer spatial and temporal connections which later can be translated into directed graph inference.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

What Bacteriophage Proteins Know

By: Diana Lee
Advisor: Antoni Luque

Bacteriophages (or phages) are viruses that prey on bacteria, and are the most abundant lifeform on earth. At an estimated 10^31 particles, they are in fact more abundant than all other lifeforms combined, are prevalent in nearly all environments on the earth, from the human body to the deep ocean, and play a major role in the health of ecosystems and organisms. Metagenomic investigation leaves 70% of phage proteins unidentified, many of which cannot be cultured in the lab. We must then return to the investigation of the genomic information and find novel approaches to uncover those functions. In this project, we look specifically the proteins that form phage capsids and find that we can use them to successfully predict T-number, and in turn make determinations about phage structure lifestyles.

This research is supported by a STEM scholarship award funded by the National Science Foundation (DUE- 1259951), the Viral Information Institute Interdisciplinary Fellowship, the SDSU University Grant Program, and the Computational Science Research Center at San Diego State University.

Post-Treatment Control of HIV Infection Under Conditioning of Drugs of Abuse

By: Peter Uhl
Advisor: Naveen K. Vaidya

Despite tremendous successes of antiretroviral therapy (ART), there is no cure for HIV, in part due to establishment of latently infected cells, which often result in viral rebounds (VR) after the therapy is stopped. However, recent studies suggest that some patients, depending on latent reservoir size and the strength of the cellular immune response, can maintain viral load below the detection limits even after the treatment termination, exhibiting post-treatment control (PTC). Importantly, both latent reservoir size and cellular immune response are highly affected by the presence of drugs of abuse. In this study, we develop a mathematical model to study how the presence of drugs of abuse (morphine) can influence the post-treatment dynamics of HIV. Our model predicts that morphine conditioning can make it more likely a patient will undergo VR by increasing the immune strength required to maintain PTC. Using our model, we also identify that the time to VR is significantly decreased by the presence of morphine in the body.

This research is supported by a STEM scholarship award funded by the National Science Foundation (DUE- 1259951), National Science Foundation funds (DMS-1616299 and DMS-1836647), the Computational Science Research Center at San Diego State University, and the Department of Mathematics and Statistics at San Diego State University.

An Explicit High Order Stochastic Semi-Lagrangian Method

By: Hareshram Natarajan
Advisor: Gustaaf Jacobs

An explicit high order stochastic semi-Lagrangian method based on a discontinuous spectral element method for solving transport equations is developed. This will be used to simulate chemically reactive turbulent flows. Particles are seeded at the Gauss quadrature collocation nodes within each element. The position of the particles is considered stochastic. A stochastic differential equation is solved using a Euler-Maruyama scheme to obtain the advected particle position. An interpolant is constructured that fits sampled advected positions with a least squares method. The interpolant maps the function back to the Gauss quadrature nodes. With the stable explicit time restrictions particles cannot leave the element's bounds. The method is hence local and parallel.

This research is supported by AFOSR funds (FA 9550-16-1-0008) and the Computational Science Research Center at San Diego State University.

Quality of Experience Sensitive Pricing Framework for Wireless Multimedia using Stackelberg Game

By: Krishna Murthy Kattiyan Ramamoorthy
Advisor: Wei Wang

User satisfaction is one of the major concerns for wireless carriers and content providers in wireless networks. Traditionally, user satisfaction was measured objectively in terms of throughput and latency. However nowadays the user satisfaction is measured using subjective metrices such as Quality of Experience (QoE). Recently, Smart Media Pricing (SMP) was conceptualized to price the QoE rather than the binary data traffic in multimedia services. In this research, we have leveraged the SMP concept to chalk up a QoE-sensitive multimedia pricing framework to allot price, based on the multimedia quality achieved by the mobile user. The utility maximization problem between the content provider (sells multimedia content), wireless carrier (provides transmission service) and the mobile user (requests data) is modeled using the proposed framework. We begin with defining the utility equations for the provider, carrier and the user. Then we translate the interplay into a two stage Stackelberg game and find the solution using backward induction method. A global searching algorithm has also been developed to implement the proposed scheme and determine the Nash Equilibrium. Simulation results indicate that all three parties can achieve higher profits by adopting the proposed model. Finally, the proposed smart pricing scheme was tested against the traditional pricing method and results suggest a significant boost in the overall utility achieved by the mobile users.

This research is supported by National Science Foundation funds (1744182) and the Computational Science Research Center at San Diego State University.

Simulating Internal Tides Travelling Through a Submarine Canyon

By: Sidney Arthofer, Randy Bucciarelli, Mariangel Garcia, and Manuel Valera
Advisor: Jose Castillo

Submarine canyons play an important role in adding to the global energy budget of the ocean and the mixing of nutrients from the deep ocean and coastal shelf which allows ecosystems to thrive. Most global ocean models are unable to accurately model submarine canyon processes because their problem grid sizes are not fine enough. The non-hydrostatic General Curvilinear Coastal Ocean Model (GCCOM) is aimed to address some of these issues in coastal ocean modeling by using fully 3D curvilinear grids and subgrid scale resolution. This project focuses on using GCCOM to numerically simulate an internal tide travelling in the La Jolla Canyon. Simulating internal tides and their interaction with canyon walls will provide insight about physical processes in this submarine canyon.

This research is supported by a STEM scholarship award funded by the National Science Foundation (DUE- 1259951), the Computational Science Research Center at San Diego State University, and the Department of Mathematics and Statistics at San Diego State University.

Quasi-Dynamical Symmetries in Ab Initio Beryllium Nuclei

By: Ryan Zbikowski
Advisor: Calvin Johnson

Nuclear many-body systems at low excitation energy contain a copious variety of behaviors and structures. One usage of this vast numerical information is to decompose nuclear wave functions according to irreducible representations of symmetry groups. This process gives rise to recognizable and persistent patterns over many states. These quasi-dynamical symmetries are particularly pronounced along rotational bands of odd mass nuclei. I apply these decompositions to first principle calculations of Beryllium nuclei.

Recent results suggest group theoretical decompositions represent an additional means of characterizing nuclear wave functions, expanding understanding of nuclear anatomy, and the possibility of compact symmetry-adapted many-body bases for future calculations.

This research is supported by U.S. Department of Energy funds (DE-FG02-96ER40985 and DE-AC02-05CH11231), and the Computational Science Research Center at San Diego State University.

A Real-Time, Distributed, Directional TDMA MAC Protocol for QoS-Aware Communication in Multi-hop Wireless Networks

By: Shivam Garg and Sushma Kuchipudi
Advisor: Sunil Kumar

The TDMA (time division multiple access)-based schemes are widely used in literature for directional nodes since they can provide a conflict-free transmission schedule. However, the existing directional TDMA-based schemes introduce significant overhead and delay, and cannot adapt to topology changes in real-time in a multi-hop network. These schemes also incur considerable overhead and delay in order to support the QoS (quality of service) traffic. In this poster, a novel, real-time, distributed, and directional TDMA MAC scheme is presented for multi-hop wireless networks. This scheme adapts to the topology changes and/or flow requirements in real-time, and facilitates QoS-aware communication with no notification overhead. In our proposed scheme, 1-hop neighborhood of every node is divided into fully connected 1-hop neighborhoods, which allows the node to intelligently serve multiple routes without requiring a globally converged scheduling solution. This feature allows the use of a rank-based mechanism to obtain a distributed, real-time transmission schedule for a multi-hop topology. The following new features are also added in the proposed scheme: (i) REQ period which reduces slot wastage, (ii) throughput scaling which ensures fairness, and (iii) piggyback reservation period which increases the spatial reuse and adapts to the dynamic requirements of multiple flows in real-time. The control-period overhead in our scheme is low and linearly changes with the number of nodes in a fully-connected 1-hop neighborhood. Simulation results show that our scheme provides high throughput for real-time traffic when one or more multi-hop flows pass through a node. The proposed scheme also provides superior performance for different QoS schemes, including the strict priority and weighted fair queue.

This research is supported by AFRL funds (FA8750-14-1-0075), the Graduate Research Fellowship Program (1321850), and the Computational Science Research Center at San Diego State University.

Casual Effect Random Forest of Interaction Trees for Observational Study Data

By: Luo Li, Kelly Spoon, and Richard Levine
Advisor: Juanjuan Fan

Estimating causal treatment effects especially individualized treatment effects (ITE) using observational data holds great interest in various research fields. Many of the recent endeavors are under the framework of counterfactual model, in which treated and untreated outcomes are estimated separately using available data, then the ITE is estimated by the differences between the two outcomes. In this study, we propose using propensity score to expand Random Forest of Interaction Trees (RFIT) (Su, 2009 & 2017) to Casual Effect RFIT (CERFIT). As opposed to the methods mentioned above, RFIT estimates treatment effect in one model using all of the data. Each interaction tree recursively partitions the data into two subgroups with greatest heterogeneity of treatment effect. By integrating propensity score into tree growing process, subgroups in CERFIT not only have maximized treatment effect differences, but also similar baseline covariates. Thus it allows for estimation of ITE using observational data. In addition, CERFIT allows us to measure the treatment effect variable importance directly, which cannot be achieved using models under counterfactual framework. Simulation studies for accessing estimation accuracy and variable importance ranking are presented. Then the method is illustrated via analysis of an educational dataset from a large public university.

This research is supported by National Science Foundation funds (1633130), the Computational Science Research Center at San Diego State University, and the Department of Mathematics and Statistics at San Diego State University.

Variational Quantum Monte Carlo and Neutron Scattering off Tritium

By: Abraham R. Flores
Advisor: Kenneth Nollett

It is an paramount goal of nuclear physics to describe the collision of two nuclei in terms of the dynamics of all of the neutrons and protons involved. Thus, the collision of a 3H nucleus and a neutron is fundamentally a four-body problem. The complexity of the nuclear interaction and the fermionic many-body nature of nuclear systems has however greatly restricted the range of such 'ab initio' reaction models to a small number of favorable cases, often with simplified interactions. The variational Monte Carlo (VMC) and Green's function Monte Carlo (GFMC) -- collectively, quantum Monte Carlo (QMC), which achieved important early successes in reproducing discrete nuclear states and constraining the three-nucleon interaction. Single-channel scattering of neutrons from 4He has been successfully described with the QMC methods, but eventual application to reactions requires development of 'coupled channel' methods suitable for reactions that alter the colliding projectiles. As a first example of coupled channels, we are studying neutron scattering from tritium, in which the final states can have different total spin or orbital angular momentum from the initial state. As an initial step, we are computing wave functions and phase shifts using nuclear VMC wave functions (which will also be needed as starting points for GFMC calculations). Our calculation uses both two- and three-body terms of a nuclear Hamiltonian that describes hydrogen and helium isotopes accurately. Our solution strategy is to impose particle-in-a-box boundary conditions and use VMC/GFMC to find the energy and wave function of the lowest state in the box. Then the energy, surface boundary conditions, and amplitudes at the box surface can be matched onto scattering solutions outside the box. The main challenge for coupled channels is to generate pairs of linearly independent solutions with the same energy but different boundary conditions and read out their surface amplitudes accurately. To guide the choice of boundary conditions we constructed a phenomenological two-body potential of neutron-triton scattering to guide our variational minimization. Through VMC we will build the four-body wave functions, these wave functions will then be the first step toward extracting reaction properties using GFMC. Since the mass-four systems are computed accurately using the same Hamiltonian by other methods, this work will allow us to benchmark the accuracy of our results. It will pave the way for more complicated coupled-channels problems in which the colliding nuclei exchange particles.

This research is supported by a STEM scholarship award funded by the National Science Foundation (DUE- 1259951) and the Computational Science Research Center at San Diego State University.

Adaptive Pre-Shaping of Ultrashort Pulses in AZO/ZnO at the Epsilon-Near-Zero Spectral Point

By: Matthew Portman
Advisor: Wayne Hayes

Galaxy classification is an area of active interest with regards to cosmology and astrophysical phenomena. Existing classification systems such as the Hubble (1936) or Vaucouleurs (1959) systems however rely on subjective and qualitative information to sort galaxies by the structures they contain. In order to quantitatively compare galaxies with theoretical models or structural evolution on cosmological scales, it is important to establish a system that can be evaluated objectively.

SpArcFiRe or Spiral Arc Finder and reporter is a general automated method which takes an image of a spiral arm galaxy and uses computer vision techniques to detect segments of its arms. The code was first released in 2014 (Davis & Hayes) and managed to perform on par with results from the Galaxy Zoo project (Lintott et al. 2008, 2011). It was later used to reaffirm the Cosmological Principal of galaxy spin direction (Hayes, Davis, Silva 2017) in effect superseding the findings of the GZ1 catalog all without resorting to human supervision. As an active project, it continues to receive updates to improve its accuracy, speed, and the techniques utilized.

It is the goal of this project to continue these improvements to the code base. This primarily includes the introduction of a physics-based model that can be used to supplement the current computer vision algorithm and provide results which better describe spiral arm galaxy structure. In the future, we plan on applying the SpArcFiRe method to explore other galactic or cosmological phenomena including dark matter of which the newly implemented physics model should be of great assistance.

This research is supported by a STEM scholarship award funded by the National Science Foundation (DUE- 1259951) and the Computational Science Research Center at San Diego State University.

UAV Swarm Mobility Model for Search and Rescue Operations

By: Shreyas Devaraju
Advisor: Sunil Kumar

In recent years, swarms of micro unmanned aerial vehicles (UAVs) are being used in search & rescue, surveillance and tracking of targets, and disaster assessment. Improvement in onboard computational capabilities of these UAVs is now driving the development of autonomous UAV swarms, which are capable of self-organization for carrying out diverse missions. These swarms use the scalable and distributed architectures. In this poster, we will discuss the development and simulation of efficient 3D mobility models for fixed wing UAV swarms for search and rescue operations. We investigate the swarm coordination and mobility in order to improve search time and coverage area during search and rescue operations. In particular, we consider the combination of stigmergic models using digital pheromone maps and UAV flocking behaviors to coordinate the movement of decentralized multi-agent UAV swarms, in order to improve their operational efficiency. Since the swarm organization and mobility models also impact the quality of communication links between UAVs, our mobility models will also serve as the foundation for our future research on 3D swarm organization, and routing and transport layer protocols.

This research is supported by Air Force Research Lab funds (FA8750-18-1-0023) and the Computational Science Research Center at San Diego State University.

High Order Mimetic Finite Differences on Overlapping Grids

By: Angel Boada
Advisor: Jose Castillo

We examine the viability of High Order Mimetic Finite Difference operators on overlapping grids, by solving representative PDEs problems using these operators on overlapping grids generated by Overture (a portable and flexible object-oriented framework for solving PDEs), while exploring different interpolation techniques on these grids (both implicitly and explicitly).

This research is supported by the Computational Science Research Center at San Diego State University.

Machine Learning to Classify Phage Structural Proteins

By: Vito Adrian Cantu, Anca Segall, and Peter Salamon
Advisor: Robert Edwards

Viruses, especially bacteriophages (viruses that infect bacteria), encode a large fraction of genes of unknown function. At the same time, they are proven effective agents of horizontal gene transfer, and are known to carry toxins and other virulence factors in both eukaryotes and prokaryotes. Artificial neural networks have been proven to be universal approximators of functions in Rn, including the function that maps protein sequence to gene annotation.

Our Current feed forward/back propagation neural networks is trained with ~410 features to classify viral genes into one of 11 classes (10 viral structural protein categories + “other”). It uses 25,000 known genes for training and has f1-score of roughly 0.8 for the test set of 2,000 genes. These networks can classify viral-associated genes not only in the context of viral genomes but also within host organism genomes (i.e. prophages and proviruses).

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Deep Object Tracking Localization and Mapping

By: Eric Medwedeff
Advisor: Xiaobai Liu

Machine learning and deep learning models have led to major advances in the reliability and accuracy of detecting objects. By leveraging these deep models and joining them with 3D scene reconstruction techniques, there are far more clever ways of localizing and tracking objects of interest than ever before. In this work in progress project, we attempt to create a fully functional and large-scale detection and tracking model fed by monocular video data that utilizes state of the art convolutional neural networks.

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Parallel Implementation of a PETSc-based Framework for the General Curvilinear Coastal Ocean Model

By: Manuel Valera, Mariangel Garcia, and Mary P. Thomas
Advisor: Jose Castillo

The General Curvilinear Coastal Ocean Model (GCCOM) is a 3D curvilinear, structured, non-hydrostatic, large eddie simulation model that is capable of running oceanic simulations. GCCOM is an inherently computationally expensive model: it uses an elliptic solver for the dynamic pressure; meter-scale simulations requiring memory footprints on the order of 10^12 cells and gigabytes of output data. As a solution for parallel optimization, the Fortran interfaced PETSc library was chosen as a framework to help reduce the complexity of managing the 3D geometry, to improve parallel algorithm design, and to provide a rich suite of choices to solve and precondition the related linear systems. GCCOM discretizations are based on an Arakawa-C staggered grid, and PETSc DMDA (Data Management for Distributed Arrays) objects were used to provide communication and domain ownership management of the resultant multi-dimensional arrays, while the fully curvilinear Laplacian system for pressure is solved by the PETSc linear solver routines. In this poster the framework design and architecture are described in detail, and results are presented that demonstrate both the scaling of the parallel framework to 240 cores over domains of order 10^6 cells per variable, per time step, and the correctness and performance of the model for a baseline experiment known as seamount.

This research is supported by the Computational Science Research Center at San Diego State University.

Temperature and Entropy in the Nuclear Shell Model

By: Oliver Gorton
Advisor: Calvin Johnson

Temperature is a thermodynamic property of macroscopic systems. In a 'shell model' of atomic nuclei, diagonalization of the Hamiltonian operator yields every possible state of the nucleus within that model space. Because temperature is related to the derivative of the entropy - the log of the number of states at a given energy - the temperature may be derived from the level density of the solutions. Level densities in shell model calculations take on a Gaussian form, and the width of that Gaussian represents a temperature. However, quantum information theory provides alternative definitions of entropy. The question arises whether or not we can, or rather what meaning can be derived from setting out to, define a temperature from these other definitions. We computed the temperature of shell model model systems using three different methods: from the level density, from the von Neumann entropy of the wave function, and from the proton-neutron entanglement entropy. In this work we compare the three evaluations of the temperature we obtain from the various methods.

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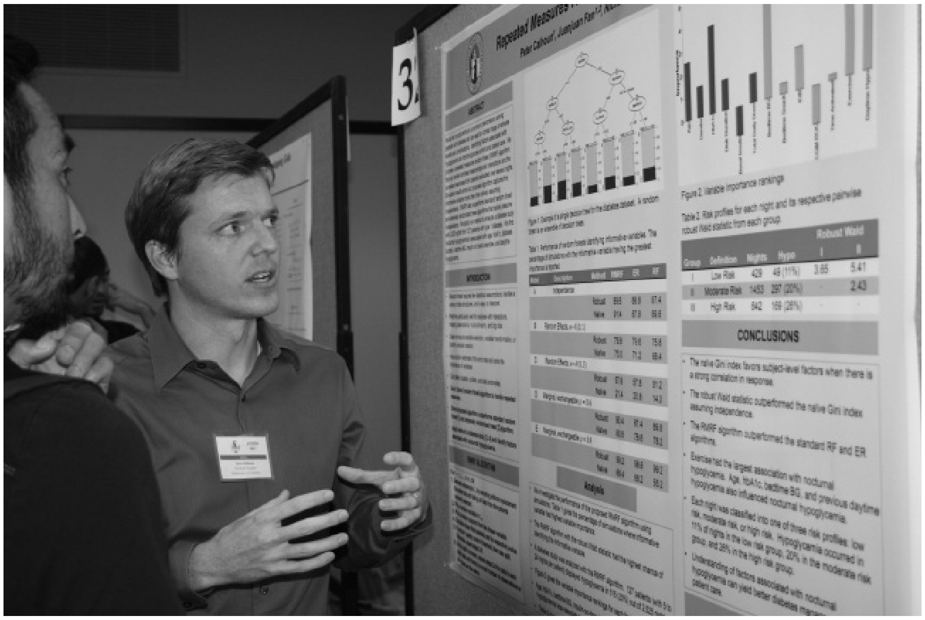

SEIR Models and the Complexity of Heterogeneity

By: Chris L. Lehnig, Karen M. Campbell, and Jose E. Castillo
Advisor: Jose E. Castillo

Compartmental models are commonly used for the mathematical modeling of infectious disease dynamics. These models divide a population into mutually exclusive compartments and use a system of ordinary differential equations to represent changes in compartment size/membership over time. The parameters influencing virus transmission are incorporated into these equations providing a means of studying parameter relationships and sensitivity. Compartmental models are thus a simple, yet powerful, tool for understanding complex dynamics in virus transmission, however, the absence of parameter heterogeneity can inhibit these models from accurately representing real-world dynamics. In this research, we explore the potential effects of heterogeneity by using a simple Susceptible-Exposed-Infectious-Recovered (SEIR) compartmental model to simulate dengue virus transmission. Cumulative infections per capita were calculated from 4,500 simulations of a single-serotype SEIR model by varying human population annual growth rate, extrinsic incubation period (EIP), and vector lifespan. Results show that higher values of cumulative infections per capita are associated with shorter EIP durations and longer vector lifespans, however, the relationship is not linear. This non-linear relationship became more apparent, and cumulative infections per capita more variable, as human population annual growth rate was increased. This analysis was repeated with a two-serotype SEIR model requiring an additional 4,500 simulations. Results from the two-serotype model are similar to that of the one-serotype model, however, the variability in cumulative infections per capita was less affected by human population annual growth rate compared to the one-serotype model. In real-world dynamics, human population growth changes from year to year and EIP and vector lifespan are influenced by environmental factors, such as weather, creating seasonal variability. The results of our analysis demonstrate that small changes in parameter values are capable of producing significantly different simulation outcomes, confirming the need for models that account for intrinsic virus heterogeneity.

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Geometric Classification of Viral Capsids

By: James Mullinix
Advisor: Antoni Luque

Early studies of viruses by Watson and Crick hypothesized that, due to the limited amount of genetic material, viruses would optimize the information needed to construct their protective shell, called a capsid, by tiling multiple copies of a single protein. The earliest hypotheses predicted 60 proteins tiled to form hexagons that create an icosahedron. Caspar and Klug expanded this theory to include tilings which had 60T proteins, where T may be certain positive integers. This method for capsid tiling strategies works for many viruses, but many virus capsids do not fit this framework. Recent work by Twarock and Luque shows that three additional lattices need to be considered: trihexagonal (3,6,3,6), snub-hexagonal (3^4,6), and rhombitrihexagonal (6,4,3,4). Twarock and Luque found that these lattices, together with hexagonal (6,6,6) and their duals, combine to generate the possible icosahedral tiling lattices, and that the known viral capsids can be unambiguously classified under this new construction. Our work here empirically tests the hypothesis that known viral capsids can be unambiguously classified under the newly expanded lattice framework, and our ongoing work is to test the hypothesis that lattice classification is linked to phylogeny.

This research is supported by a STEM scholarship award funded by the National Science Foundation (DUE- 1259951), the Computational Science Research Center at San Diego State University, and the Department of Mathematics and Statistics at San Diego State University.