Friday, March 28, 2014
12:00 pm - 5:00 pm
SDSU’s Parma Payne Goodall Alumni Center

12:00 pm  Registration / Buffet Lunch
1:00 pm  Stanley Maloy, Dean
College of Sciences
San Diego State University

Morteza Monte Mehrabadi, Dean
College of Engineering
San Diego State University

Welcome / Opening Remarks

1:10 pm  Jose E. Castillo, Director
Computational Science Research Center
San Diego State University

Computational Science at SDSU and ACSESS Program

1:20 pm  John Matze, Chief Executive Officer
BridgeSTOR

Key Note Speaker
How Big Data is Impacting Business

1:50 pm  Panel Discussion

Mary Thomas, Moderator
Assistant Research Professor
Computer Science
San Diego State University

Shelton Darenburg
Cybersecurity Project Manager
ViaSat, Inc.

Chris Armijo
Director of Engineering
Illumina

Gregory D. Gargas
Senior Vice President, Commercial (Mast Therapeutics)
Director (Theragenics, Inc.)

Chris Chen
Intellectual Capital
SDG&E, Sempra Energy

Mark Pfleger
President & Scientist
Source Signal Imaging, Inc.

3:00 pm  Poster Presentation / Reception
4:30 pm  Paul Paolini
Associate Director
Computational Science Research Center
San Diego State University

Poster Presentation Awards
&
Closing Remarks
Welcome to the CSRC at SDSU

The Computational Science Research Center (CSRC) was established in 1999 within the College of Sciences at San Diego State University (SDSU) as an outgrowth of the Interdisciplinary Research Center. Its mission is to promote development and advancement of computational science by bringing together researchers in different areas who have a common interest in modern scientific computation.

The CSRC is thus envisioned as the coordinating body of a partnership involving several participating departments, although it is housed in the College of Sciences, it seeks interactions with any interested department on the SDSU campus, as well as those from other California State University campuses.

The CSRC is engaged in a number of initiatives aimed at fostering interdisciplinary, computationally oriented scientific research -- from providing computing infrastructure and support for students, to developing educational programs and industrial interactions. It is the aim of CSRC to function as an independent, self-sustained unit. therefore, its operation crucially depends on extra-mural funding.

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.

Executive Board

Program Director:
Jose E. Castillo

Associate Directors:
Andrew Cooksy
Paul Paolini
Satchi Venkataraman

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Gary Fogel
Natural Selection, Inc.

Richard Greenblatt
Source Signal Imaging, Inc.

Bill Bartling
SR2020, Inc.
**Quantifying Disease Severity of Cystic Fibrosis using Quantile Regression Methods**  
*By Kameryn Denaro and Barbara Bailey*

Cystic fibrosis (CF) is a genetic disease that dramatically decreases life expectancy and quality. Currently, the average life span for people with CF who live to adulthood is approximately 37 years. The disease is characterized by polymicrobial infections which lead to lung remodeling and airway mucus plugging. In order to model the severity of the disease, quantile regression methods are implemented. This paper presents a new approach to describing disease severity by extending traditional quantile regression to include the estimation of quantile regression rankscores and the corresponding normalized ranks. These ranks make use of the conditional distribution of the response across the quantiles of the entire distribution. The distribution of normalized ranks can be used to quantify disease severity and will be compared with the severity index based on expert opinion.

*This research is supported by the Department of Mathematics and Statistics at San Diego State University and the Computational Science Research Center at San Diego State University.*

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**Regularization of Singular Sources for PSIC Computations of Particle-Laden Flows with Shocks**  
*By Jean-Piero Suarez and Gustaaf Jacobs*

We propose a high-order regularization technique with optimal scaling for time-dependent singular Dirac-delta sources in the numerical solution of hyperbolic conservation laws. In one dimension, the regularization is based on a class of compactly-supported piecewise polynomials that approximates the Dirac delta distribution with the desired order of accuracy away from the singularity. The overall accuracy is controlled by the number of vanishing moments and smoothness of the piecewise polynomials plus the support length (optimal scaling). We have developed a theoretical criterion for the optimal scaling that leads to optimal order of convergence in the numerical solution of a linear and a nonlinear (Burgers) scalar hyperbolic conservation law with a singular source, as well as the nonlinear Euler equations with singular sources, a system of hyperbolic conservation laws governing compressible fluid dynamics with shocks and particles. A Chebyshev collocation method (spectral) discretizes the spatial derivatives in the scalar equation tests. A high-order high-resolution multidomain hybrid WENO-spectral method discretizes the Euler equations. We aim to the development of a two-dimensional extension of the high-order regularization and the hybrid WENO-spectral scheme in order to improve the accuracy in the simulation of particle-laden flows with shocks using the particle-source-in-cell (PSIC) method.

*This research is supported in part by AFOSR, NSF funds and the Computational Science Research Center at San Diego State University.*
Mixed Effects Modelling Long-Term Human Immunodeficiency Virus Dynamic Models with Application to Acquired Immune Deficiency Syndrome Clinical Study
By Lingjun Anna He and Jianwei Chen

Human immunodeficiency virus (HIV) is the etiologic agent of acquired immunodeficiency syndrome (AIDS), a disease that disables the human immune system (HIV) through the destruction of CD4+ helper T cells, leaving the body susceptible to life-threatening opportunistic infections. Mathematical modeling of the HIV dynamics has played an important role in AIDS research. Deterministic dynamic models have been developed to study the viral dynamic process for understanding the pathogenesis of HIV type 1 infection and antiviral treatment strategies. Chen (2010) developed a multistage estimation procedure to estimate both constant and time varying parameters in a long-term HIV dynamic model, generating effective and reasonable estimation results to individual AIDS clinical trail data. However, HIV clinical trail data for each individual may be too sparse at times. Consequently, the estimation procedure which only focus on each individual data may lose validation of certain statistics. Therefore, a model with estimation methodology that can analyze the observations from all participating patients in the study is desired. In this study, we adopt the idea of this multistage estimation procedure, and extending it to a mixed-effects model for clustered AIDS clinical data. A really application to HIV clinical trail data is presented to illustrate the utility of the proposed method.

This research is supported by the Department of Mathematics and Statistics at San Diego State University and the Computational Science Research Center at San Diego State University.

Scattering and Leapfrogging of Vortex Rings in Bose-Einstein Condensates
By Jake Talley, Ronald Caplan, Ricardo Carretero, and Panos Kevrekidis

The dynamics of vortex ring pairs in a Bose-Einstein condensate is studied. The scattering behavior of rings with parallel axes and opposite charge undergoing collision is numerically investigated yielding a surprisingly simple result for the scattering angle as a function of the initial vortex ring parameters. We also study the leapfrogging behavior of coaxial rings with equal charge and compare it with the dynamics from the ensuing reduced equations of motion from a fluid model derived using the Biot-Savart law.

This research is supported by NSF funds.

Structure and Rheological Properties of Self-Associating Polymer Networks
By Mark Wilson, Arlette Baljon, and Avinoam Rabinovitch

Systems of associating polymers possess the ability to span a large spectrum of material properties, from fluid-like viscosity to near solid-like elastic dynamics. Relatively small changes in external parameters can result in large transitions in this behavior. In the following, numerical simulations of associating polymers are utilized to study viscoelastic behavior. A hybrid Molecular Dynamics, Monte Carlo (MC) algorithm is employed. Polymer chains are modeled as a course grained bead-spring system. Functionalized end groups, at both ends of the polymer chains, can form reversible bonds according to MC rules. At high temperatures the system is shown to behave as a fluid. Decreasing the temperature below the micelle transition results in a self-assembly of the system, forming a network that is transient in time. The nodes of this network consist of aggregates of end groups, while links between aggregates are formed by one or more bridging polymer chains. We report on the microstructural changes in a polymer network that arise in response to an oscillatory shear. The stress response has been obtained as a function of the oscillatory frequency and amplitude in both the linear and nonlinear regimes. Data are correlated with observed changes in the network structure. For instance, a reduction in the number of links is observed at large amplitude or low frequency. This is partly due to an increase in the number of loops (chains that have both ends connected to the same aggregate). The secondary cause is a tendency of the chains to form additional bridges between the same sets of aggregates. We have also studied the lifetime of aggregates and found that the lifetime is shortest near the walls that bound the system. Finally, we report on very intriguing transient phenomena in the moduli, as well as the structure and dynamics of the networks.

This research is supported by NSF, DOD DURIP funds, and the Computational Science Research Center at San Diego State University.
The Dynamics of Coupled Spin-Torque Nano Oscillators
By James Turtle

In this work we explore the use of Spin Torque Nano Oscillators (STNOs) to produce a spintronics voltage oscillator in the microwave frequency range. STNOs are quite small – on the order of 100 nm – and frequency agile. However, experimental results to date have produced power outputs that are too small for practical use. We attempt to increase power output by investigating the dynamics of a system of electrically-coupled STNOs. The Landau-Lifshitz-Gilbert model with Slonczewski term is modified to include electrical coupling of N-STNOs. We then examine two new coordinate systems to improve numeric integration and reduce the model dimension. Transverse Lyapunov exponents are used to quantitatively measure the local stability of synchronized limit-cycles. The synchronized solution is found to be stable for a large region of two-parameter space. However, a two-parameter bifurcation diagram reveals a competing out-of-phase solution, indicating bistability. For more robust description of existence and stability of non-synchronous solutions, we examine the normal form of Hopf bifurcations within the appropriate symmetry group representation.

This research is supported by NSF funds.

Virtual Screening for Novel HIV-1 Integrase Drug Candidates
By Gene M. Ko, Rajni Garg, Barbara Bailey, and Sunil Kumar

HIV-1 integrase protein is a novel target in the design of new HIV-1 inhibitor drugs. Quantitative structure-activity relationship (QSAR) models play an important role in the drug design and discovery process by providing an understanding of inhibitor-protein binding interactions. We developed QSAR models using three approaches (multiple linear regression, partial least square, and extremely randomized trees) to analyze the inhibitor-protein interactions. These models were used to virtually screen the National Cancer Institute database of 265,242 compounds to identify potential novel drug candidates towards HIV-1 integrase inhibition. This study identified six compounds which are predicted to be highly active (pIC50 > 6). These compounds have similar structural features as FDA approved integrase inhibitor drugs and may form potential novel leads in the design of future HIV-1 integrase inhibitors.

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

SubFlow – An Open-Source, Object-Oriented Application for Modeling Geologic Storage of CO2
By Johnny Corbino and Christopher Paolini

The capture of carbon dioxide for its subsequent storage in brine-saturated reservoirs or depleted oil fields has become a significant part of US energy policy. In this work, we focus on the design and development of a novel CCUS application to model carbon dioxide injection in brine-saturated reservoirs. SubFlow is written in C++ and uses a relational database to store user session and simulation parameters such as mineral, solute, kinetic reaction, lithology, formation, and injection water data. SubFlow is capable of 3D real-time visualization, distributed-parallel execution on massively parallel processor (MPP) systems using OpenMP and MPI, and features an intuitive user interface developed through Qt. Currently, SubFlow uses either a finite-volume method (FVM) or a mimetic discretization method (MDM) for solving conservation of solute mass, energy, and momentum, and the finite-element method for solving the pressure and rock stress field. The FVM is second order accurate while the MDM is capable of fourth order accuracy. OpenGL is used to render pressure, temperature, stress, velocity, and solute concentration fields on a 3D mesh that represents a reservoir. Results from selected simulations are compared with those produced by TOUGHREACT and STOMP.

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

Wireless Video Quality Enhancement through Optimal Prioritized Packet Fragmentation and FEC
By Seethal Paluri, Kashyap K. R. Kambhatla, and Sunil Kumar

The quality of compressed video delivery is affected by packet losses over time-varying wireless channels. To improve the received video quality, we propose a cross-layer joint optimization of video priority-adaptive fragmentation at the medium access control layer and forward error correction (FEC) at the physical layer. Priority is determined from the cumulative mean square error (CMSE) contributed by the video slices. Higher priority slices cause more distortion. Compressed slices in each priority class are aggregated to form corresponding prioritized packets supported by the network. More protection is provided to higher priority packets in terms of smaller fragment sizes and lower FEC rates at the expense of discarding some lower priority packets. Simulation results show that priority-aware packet fragmentation and FEC improve the received video quality as compared to priority-agnostic schemes.

This research is supported by Air Force Research Laboratory funds and the Computational Science Research Center at San Diego State University.
Higher-Order Mimetic Finite Differences to Simulate Carbon Dioxide Geologic Storage Scenarios
By Eduardo Sanchez, Christopher Paolini, and Jose Castillo

The authors present the Mimetic Methods Toolkit (MTK), an API implementing mimetic finite differences for use in simulating carbon storage in geologic media. Mimetic methods are numerical discretization methods designed to preserve important properties of the commonly known differential operators gradient, divergence, curl, and Laplacian. A main objective of mimetic finite differences is the creation of discrete differential operators that mimic their continuous counterparts. Since the creation of these operators is achieved through the requirement that they satisfy an extended version of Gauss’ Divergence Theorem, they tend to yield numerical solutions that outperform those from other methods such as FDM, FVM, and FEM. Because of this, the solution to conservation equations, such as those modeling solute concentration profiles in carbon storage, benefits greatly from mimetic methods. In addition, the authors have developed a new method to construct higher-order accurate mimetic operators, as well as more computationally efficient methods to implement higher-dimensional mimetic operators. Second, with the objective of improving a parallel implementation of diffusive-advective-reactive solvers, the authors have developed a storage semantic based on block-defined, sparse matrices, for the parallel global solution (BloGS) of all solutes in a given simulation, using any arbitrary discretization method. One of the main advantages of the BloGS storage semantic is that it can be implemented using multiple common matrix formats, such as CRS or CCS. Furthermore, the BloGS algebraic properties are independent of the selected matrix format. In this work, we explore the solution to diffusive-reactive as well as advective problems, in one and two dimensions, through an implementation of BloGS made within the MTK, using higher-order mimetic finite differences. We discuss the advantages of such approach, in terms of achieved numerical accuracy and stability, due to the implementation of mimetic finite differences. We also show attained speedup and efficiency results from simulating injection into a deep brine saturated sandstone formation on massively parallel processor (MPP) systems. Finally, we discuss the usability of the API in the context of simulating other carbon storage injection scenarios.

This research is supported by US Department of Energy funds and the Computational Science Research Center at San Diego State University.

Geometry of Basins of Attraction for a Coupled Bistable System
By Daniel Lyons, Joseph M. Mahaffy, Sara Wang, and Antonio Palacios

Models for the coupled core fluxgate magnetometer (CCFM) demonstrated interesting dynamics. Bifurcation diagrams for this nonlinear dynamical system show a variety of behaviors. Our work provides a detailed geometric analysis of how the transitions occur in a smooth manner to the different dynamical behaviors by illustrating the evolution of the basins of attraction.

This research is supported by the Department of Mathematics and Statistics at San Diego State University and the Computational Science Research Center at San Diego State University.

An MTD-Array Based Flash Storage Framework: New Hope for Data-Intensive and Mission-Critical Mobile Applications
By Deng Zhou, Wei Wang, and Tao Xie

Emerging data-intensive and mission-critical mobile applications like wireless healthcare and 3-D digital cameras are increasingly demanding a high-performance, reliability-aware, and large-capacity embedded NAND flash memory based storage system. However, manufacturers are aggressively scaling up flash density in order to increase capacity and reduce the cost per gigabyte. Metrics like reliability, endurance, and performance are all declining. Even worse, all present embedded flash storage systems can support only one MTD (Memory Technology Device) device, which results in a poor I/O performance and an inadequate level of data reliability. Thus, developing a high-performance and highly reliable embedded flash storage system based on current single-MTD architecture on top of increasingly large but infrequent flash memory becomes a great challenge. To solve this challenge, in this paper we design and implement an MTD-array based embedded flash storage system framework called MD (multiple devices), which enables an existing embedded flash file system to access multiple MTD devices in parallel to boost performance and reliability. To verify its effectiveness, we incorporate UBIFS, one of the best contemporary embedded flash file systems, into MD in Ubuntu 13.04 with 3.8.0 kernel. Experimental results demonstrate that MD-UBIFS improves I/O performance by up to 1.9X while its mounting time is less than 120 ms and its RAM usage is no larger than 2.5 MB. Further, when it is configured in a mirroring format, on average its read performance can be improved by 73% while its write performance is similar to UBIFS.

This research is supported by NSF funds.
Creating Synthetic Muscle Using Dielectric Elastomer Actuators
By John Waynelovich

Dielectric elastomer actuators are a class of electroactive polymer based devices which contract or expand as external voltages are applied. The actuator’s contractile motion compares well with human muscle tissue and is capable of generating large strains, making them good candidates for a host of biomimetic applications such as prosthetic devices, robotics and mechatronics. Using polymers that are biocompatible should allow for the development of actuators suitable for transplantation into humans and animals.

Actuators are fabricated by coating a thin elastomer layer with conformal conductive coatings on both sides. By applying a voltage to the conductive surfaces, charges of opposite sign build up on the parallel surfaces in a manner similar to a capacitor. However, because the material separating the charged surfaces is elastic, the Maxwell forces acting on the system cause a contraction along one axis while expanding along the other two. This elongation/contraction closely resembles the action of a human muscle and consequently hold promise as a suitable replacement for damaged or destroyed muscle tissue.

With the exception of the polymer itself, there are no moving parts in the system. Layers are simply stacked in order to generate greater stresses. Due to the simplicity of the design, synthetic muscles are easily scaled down and can be utilized in micro applications such as microfluidic devices, microelectromechanical systems (MEMS) as well as novel applications such as muscles for insect-sized robots.

Despite their obvious potential, utilization of dielectric elastomers has been limited due to their high failure rate. Currently available polymers require driving voltages in the kilovolt range and generate high surface stresses by nature of their design. Issues of reliability and robustness will need to be addressed before commercial applications become feasible.

The goal of this project is to develop a highly dependable, biocompatible, synthetic muscle. Accomplishing this requires the development of both conductive and non-conductive elastomers that are not only compatible with each other in terms of adhesion and elasticity, but also compatible with the human body. We are currently testing several promising polymers as well as prototyping a new microprocessor based driving system that can be used to evaluate new polymers.

This research is supported by student funds.

Wideband Frequency Tunable Circular Microstrip Patch Antenna with Simultaneous Polarization Reconfiguration for L-band GPS Communications
By Behrouz Babakhani and Satish K. Sharma

A wideband frequency tunable circular microstrip patch antenna with simultaneous polarization reconfiguration is demonstrated. Both frequency tunability and polarization reconfigurability are controlled by a proposed feed network. Changing the capacitance value of the varactor diodes changes the operating frequency of the antenna from 1.17 GHz to 1.58 GHz (around 30% tunability), which covers Global Positioning System (GPS) communication bands (L-band). Each set of the two varactor diodes provides vertical and horizontal linear polarizations excited using one of the feed ports at a time. Similarly, right hand circular polarization (RHCP) and left hand circular polarization (LHCP) are generated by employing all four varactor diodes and both feed ports with ±90° time phase difference. The antenna is fabricated on a 120 mil thick Arlon AD450 dielectric. The proposed feed network to control the excitation of ports for each of the polarizations is fabricated on 62mil thick FR-4 substrate material. Antenna along with feed network was manufactured inside the Antenna and Microwave Lab (AML) and consequently, was measured for the S-parameters and radiation performance in the anechoic chamber. Experimental results compared well with the simulated ones. The antenna can find applications in GPS receive communications when operated in the CP mode and for other L-band communications when operated in linear polarizations.

This research is supported by NSF funds.

Dynamics in Quasi-One-Dimensional Polariton Condensates
By Julia Rossi

We use computational methods to study polariton Bose-Einstein condensates (BECs) in semiconductor microcavities. Unlike atomic BECs that need operating temperatures close to absolute zero (of the order of nano Kelvin), polariton BECs exist at much higher temperatures making them much more experimentally accessible. Polariton BECs, consisting of short-lived exciton-photon quasiparticles, are an excellent candidate for solid-state applications in quantum computing, quantum clocks, and other high-precision devices. We study the stability and dynamics of the ground state dark solitons in the quasi-one-dimensional polariton condensate in the presence of non-resonant pumping and nonlinear damping.

This research is supported by ARCS Foundation Award funds.
MLC (multi-level cell) NAND flash memory based solid state drives (SSDs) have been increasingly used in supercomputing centers because of their merits in cost, performance, and energy-efficiency. However, as each cell starts to store two or more bits, a threshold voltage range employed to represent a state has to be continuously shrunk, and a narrowed threshold voltage range causes more bit errors. An ad-hoc solution to this problem is to apply an enhanced ECC (error correction code) scheme. Still, a comprehensive understanding of the impact of threshold voltage on MLC flash performance and reliability is an open question. In this paper, we first empirically measure the correlations between threshold voltage and program/erase (P/E) performance as well as reliability. After analyzing experimental results, we make several interesting observations: 1) a memory cell programmed to a lower threshold voltage has a faster programming speed (up to 31%) as well as a fewer number of bit errors; 2) the programming time of an MSB page is about 2 to 3 times shorter than that of an LSB page; 3) erase performance is highly correlated to threshold voltage. These new findings provide system implications for the development of a better SSD.

Further, to demonstrate how these findings can be leveraged to enhance MLC flash, we propose an approach called threshold voltage reduction (TVR), which increases programming speed and longevity by 50% and 7.1%, respectively. Finally, we conduct a study on TVR-powered SSDs. Simulation results show that overall mean response time can be reduced by up to 35%.

This research is supported by NSF funds.

Exploration and Expansion of the Projected Hartree-Fock Algorithm in a Shell Model Basis
By Joshua Staker

We have seen that the Projected Hartree-Fock (PHF) algorithm shows promise for computing nuclear spectra, especially in cases of Even-Z Even-N nuclei, when compared to the exact Configuration Interaction (CI) results. We now look to identify possible sources of error in PHF by examining the CI-PHF spectral variance with respect to the quadrupole nuclear deformation parameters, as well as examining expectation values of spin \( S^2 \) and isospin \( T^2 \) operators. Additionally, we examine the improvement to the PHF spectra when expanding the basis to include not only the global minimum Hartree-Fock Slater determinant, but local minima as well.

This research is supported by US Department of Energy funds.
**Fluid-Solid Interaction in CO2 Sequestration Simulation**
*By Jonathan Matthews*

Mitigating environmental impacts of fossil-fuel combustion on global warming has become a critical issue. With nearly 70% of electricity generated from fossil fuel combustion, CO$_2$ sequestration in underground aquifer-caprock systems is one solution that is a promising technology for reducing harmful CO$_2$ emissions created by coal-fired power stations. However, carbon sequestration by injection of CO$_2$-rich fluids in geologic media is not without risk. One of the primary fears is the unintentional triggering of small- to moderate-sized earthquakes as well as fracturing of the impermeable cap rock layer that can damage the seal integrity of geologic formations consisting of brittle sandstones, and thereby leak stored CO$_2$ into the atmosphere. Furthermore, the transport of toxic heavy metals and organic species into fresh water systems can occur through new fractures in caprock formed during CO$_2$ injection. Stresses resulting from CO$_2$-rich fluid injection can induce rock fracturing. We present simulation results of a mechanical-chemical-thermal-hydrogeologic model that computes averaged rock stress, using the Winterfeld-Wu model, as a function of formation temperature and pressure. This mean stress model is coupled to a heat-transfer model with a volumetric energy generation source derived from the revised Helgeson-Kirkham-Flowers (HKF) thermodynamic model for aqueous solute species. The HKF model is based on computing properties of dilute aqueous species by separately considering solvation and nonsolvation contributions. The HKF derived partial molal heat capacity and enthalpy of charged aqueous species arising from the interaction of CO$_2$-rich brine with sandstone are used in the source term of an advection-diffusion energy equation that is solved using the finite volume method. Formation pressure is computed using a poroelastic pressure-diffusion model and the finite element method. Changes in rock porosity and permeability are modeled as a function of rock stress, and are determined using the relations of Gutierrez, Rutqvist, and Ostensen. These distinct models for stress, pressure, and temperature are coupled and used to predict fracture characteristics of a shale-sandstone system that models the Oligocene Frio Formation along the Texas Gulf Coast. Simulation results are compared to bottom-hole pressure data obtained during the Frio Pilot Experiment from an observation well 30 meters from the injection well.

*This research is supported by US Department of Energy funds and the Computational Science Research Center at San Diego State University.*

**POD Decomposition of Air Particle Time Series Data to Characterize Behavior Associated with Secondhand Smoke**
*By Vincent Berardi*

Project Fresh Air (PFA) is an ongoing study that recruits households with cigarette smokers and installs real-time air particle monitors placed in them for a period of four to six months. The monitors are fit with aversive visual and auditory feedback devices that are activated once air quality exceeds a certain threshold with an aim to decrease indoor secondhand smoke (SHS) exposure throughout the household. A preliminary agent-based model (ABM), with a foundation in principles of operant conditioning, has been developed to describe participants’ interaction with the monitor feedback devices. The air particle monitor data can serve as a proxy measure for human behavior associated with SHS generating activities and can be used to validate and calibrate the ABM. A fundamental requirement for this process is the identification of discriminative characteristics of the air particle time-series data that will allow for the categorical differentiation of behavior over time. Principal orthogonal decomposition (POD) is used to achieve this task. First, the time-series data is segmented into events, each of which corresponds with an interval of elevated air particle concentrations. POD analysis is then performed on the set of events, which provides an optimal basis to decompose the data. The first three modes of this basis account for over 80% of the total variance between events and the coefficients corresponding to these modes are used to discriminate characteristics of each event. Preliminary results are described for several households and an exploration of the sensitivity of the results to various data segmentation approaches are discussed.

*This research is supported by NIH and NHLBI funds.*

**Subjective Health Across the Lifespan: Age and Gender Moderation of Genetic and Environmental Influences in the Consortium on Interplay of Genes and Environment Across Multiple Studies (IGEMS)**
*By Kelly Spoon, Carol Franz, Deborah Finkel, and Matt Panizzon*

Harmonized subjective health data across 9 studies to investigate the extent to which age and gender moderate genetic and environmental influences on subjective health across the life course in aging men and women.

*This research is supported by NIH funds.*
**Random Forest and Variable Importance Rankings for Correlated Survival Data**  
By Melodie Hallett, Juanjuan Fan, Xiaogong Su, and Richard Levine

We have developed a permutation based variable importance ranking method based on the extremely randomized trees method (Geurts et al., 2006), for correlated censored data, which provides nearly unbiased variable selection when applied with either subsampling or bootstrap sampling. The extremely randomized trees method randomly picks a subset of m variables at each node and chooses d cutpoints for each of the m variables to find the best split. With respect to computation time, the new methodology is less expensive than the regular random forest, which considers all cutpoints of selected variables in computing the best split. In our simulation studies, the original random forest method’s variable importance rankings were affected by the number of categories of the predictor variables, which are not direct indicators of the true importance of the variable. This bias occurred regardless of whether subsampling or bootstrap sampling was applied. Through our simulation studies, we found the extremely randomized tree method to be consistently better than regular random forest procedures, in both subsampling and bootstrap sampling applications, in picking predictors without a bias towards variables with many possible cutpoints. In comparing the performance of this method to an existing method for correlated survival data, the Cox proportional hazards (PH) model with a frailty term, the extremely randomized trees method produced more accurate results compared to the Cox model. We found the extremely randomized trees method was more reliable in choosing the most important variables in particular when the model form was nonlinear or had high order interactions.

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

**Deconfined Quark Matter in High Mass Neutron Stars**  
By William Spinella, Milva Orsaria, Gustavo Contrera, and Fridolin Weber

Using a non-local extension of the Nambu-Jona-Lasinio model to describe quark matter and relativistic mean field theory to describe hadronic matter, we show that mixed phases of deconfined quark matter and confined hadronic matter may exist in neutron stars as massive as 2.35 solar masses.

*This research is supported by the Department of Physics at San Diego State University and the Computational Science Research Center at San Diego State University.*

**Changes in the Neonatal Rat Cardiomyocyte Gene Expression Caused by Rosiglitazone**  
By Esteban Vazquez-Hidalgo, Elesha Bartolotta, Paul Paolini, and Gary Hardiman

Rosiglitazone is a peroxisome proliferator-activated receptor g (PPARg) agonist with both beneficial and adverse effects on cardiac function. We investigated the effects of rosiglitazone on genome-wide gene expression over 48 hours on neonatal rat ventricular cardiomyocytes in order to identify the drug’s impact on cell signaling pathways. We examined cardiocytes subjected to the drug at 0, ½, 1, 2, 4, 8, 12, 18, 24, 36 and 48 hours of exposure compared to cardiocytes under only DMSO (carrier) exposure. A microarray experiment was performed using the Illumina RatRef-12 BeadChip™ technology; data analysis used both the standard Illumina and our own custom analysis methods we developed. Five key targets were examined by qPCR to validate the microarray data. Myocytes subjected to rosiglitazone stress exhibited a differential gene expression profile compared to control experiments. Over 3,000 genes of the 22,518 genes studied had statistically significant expression level changes with p-values < 0.5, and 310 had p-values < 0.0001. Cardiovascular system development, extracellular matrix, and immune response were represented prominently among the significantly modified gene ontology terms in the data set. Hmgs2, Angptl4, Cpt1a, Cyp1b1, Ech1 and Nqo1 mRNAs were strongly up-regulated in cells exposed to rosiglitazone. Enrichment of transcripts involved in cardiac muscle cell differentiation and extracellular matrix provides a panel of biomarkers for further analysis of adverse cardiac outcomes in humans.

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

**Modeling 2D Seismic Wave Propagation Using Finite Difference and Mimetic Methods**  
By Trevor Hawkins and Peter Blomgren

In this analysis, subsurface seismic waves on a 2D vertical half plane are propagated through a homogeneous elastic medium. Both P (primary, pressure) and SV (secondary, vertical shear) waves are modeled, which requires solving for the stresses between time steps. In order to avoid an interpolation step, the Standard Staggered Grid (SSG) is chosen, which calculates the x and z velocities on separate edges of the grid. Both standard finite difference and mimetic discretization are used to solve the elastodynamic velocity equations, and their techniques and results are compared and contrasted.

*This research is supported by the Department of Mathematics and Statistics at San Diego State University and the Computational Science Research Center at San Diego State University.*
**Mimetics and Finite Difference Approaches to Modeling the Diffusion of Calcium Within a Single Sarcomere of an Adult Cardiomyocyte**
*By Rosa Lemus*

How does free calcium ion flow occur through the sarcomere (the repeating contractile unit of myofibrils within the cardiocyte) in triggering contraction? We wanted to visualize this process in an animation to best appreciate the pattern of calcium flow within a muscle cell using mimetic methods to calculate the concentration of calcium.

We focused on the role calcium ions play during the excitation-contraction coupling process, including on the expression of genes that serve in calcium transport across cell membranes (outer membrane and the SR). We created a mathematical model to demonstrate the calcium turnover, and the dependence upon factors like abundance and transport rates of RyR2, SERCA2 and NCX channels.

The model will be solved using mimetic finite difference (MFD) methods and standard finite difference (SFD) methods with MATLAB implementations for visualization. Assuming radial symmetry in a cylindrical sarcomere, a 2D grid model accounts for calcium exchanges within the myofilament system, between the SR’s terminal and longitudinal cisternae, and within the cytosol. A 2D sarcomere was divided into computational cells. The rate of Ca2+ release from the terminal cisternae (TC) region was assumed to be proportional to the product of the number of open Ca2+ release channels and the difference of [Ca2+] between the TC and a cell facing the TC. Ca2+ moves from element to element by simple diffusion and is taken up by the longitudinal SR via the SERCA2 pump. Ca2+ influx responsible for triggering the TC Ca2+ release is introduced to elements at the level of the Z-line. Calcium buffering is not considered for simplicity of the model. We ignore calcium binding to troponin C (TnC) found on the thin myofilaments and calmodulin (CaM) found ubiquitously in the cytosol. Therefore, we consider all calcium in the cytosol as free calcium.

An animated visualization of the fluxes will use pseudocolor to represent the calcium concentration changes vs. time in the sarcomere during a single twitch. We anticipate that increases in SERCA2 channel density cause a faster relaxation rate of the Ca2+ transient. Changes in number of RyR2 and NCX channels should alter Ca2+ transient amplitudes and kinetics in a manner predicted by our laboratory’s gene silencing experiments.

Future work of a finished simulation may examine biological and mathematical modifications. Other features relating to calcium fluxes may be added, such as a more detailed description of the Ca2+-induced Ca2+ release mechanism. Calcium buffering may be explored by adding it to the model as a source term. Higher order accuracy may be implemented by the use of more points per approximation and the appropriate MFD and SFD coefficients.

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**Variations in Nuclear and Cytosolic Calcium Transient Behavior in Neonatal Cardiomyocytes**
*By Delnita Moore and Carlos Alvarez*

How do calcium transient signals from the nuclear, perinuclear (regions surrounding the nucleus) and more distant cytosolic regions of neonatal cardiomyocytes differ? Previous studies of calcium spikes have found significant differences in signal decay between regions close to and relatively distant from the nucleus. It has been observed that nuclear calcium transients are slower to occur and have broader peaks than cytosolic transients further from the nucleus. Nuclear transients overlap briefer cytosolic signals when measurements are taken close to the nucleus. In order to assess these variations, four regions of interest (ROI) in the cell were targeted: (1) ROI 1 corresponds to the region with the least amount of nuclear calcium contribution (2) ROI 2 refers to regions adjacent the nucleus where there is significant nuclear calcium contribution (3) ROI 3 refers to a measurement within the nucleus. (4) ROI 4 represents the signal averaged over the entire cell. Laser scanning confocal microscopy was employed to perform line scans through individual neonatal cardiomyocytes using Fluo3 as a calcium ion marker.

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Bose-Einstein condensation is a state of matter of boson particles at ultra cold temperatures. The Gross-Pitaevskii (GP) equation, a variant of the nonlinear Schrödinger equation (NLS) that includes the external trapping, can effectively describe the mean field dynamical properties of Bose-Einstein condensates (BECs). Experimental progress has been made to create BECs with particles with a strong dipolar moment such as in chromium. The dipole-dipole interaction adds a nonlocal term to the GP equation in the form of a convolution. On the other hand, previous work has focused on vortex nucleation in non-dipolar condensates by moving impurities at supercritical speeds in the condensate. In the case of the one-dimensional GP equation with no external potential nor dipolar effects, a critical velocity can be found analytically above which dark (grey) solitons are emitted from the moving impurity. However, the case pertaining the supercritical velocity for vortex nucleation in two-dimensional dipolar condensates has not been considered so far.

Computational work can be done in C taking advantage of the CUDA-able GPU cards to accelerate the numerical integration of the GP equation. Due to the nature of the convolution term in the dipolar GP equation, a fast Fourier transform (FFT) is performed several times. We approach the time-run of the simulation using a pseudo-spectral algorithm. The composition of time-split methods is easy to implement obtaining a high order accuracy algorithm.

For such purpose, a linear stability analysis in 1D is also studied. This approach will require the use of the FFT capabilities of the CUDA language to perform time integration as well as the calculation of the convolution term in the dipolar GP equation, expecting higher speed-ups in computation time. We hope this work will allow us to characterize the nucleation. Interestingly, since the dipole-dipole interaction is anisotropic in two dimensions, the critical speed is found to depend on the orientation of the trajectory of the moving impurity with respect to the dipolar axis.

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