# 10th Annual ACSESS

Friday, March 1, 2013
12:00 pm - 5:00 pm
SDSU's Parma Payne Goodall
Alumni Center

## For Applied Computational Sciences and Engineering & Computational Science Curriculum Development

**12:00 pm** **Registration / Buffet Lunch**

**1:00 pm**

**Cathie Atkins**
Associate Dean
College of Science
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 Newsam**
Chairman & CEO
Tioga Research, Inc.

Key Note Speaker
"Building Industrial-Academic Bridges"

**1:45 pm** **Coffee Break**

**1:50 pm**

### "Industry-Academia Interaction"

**Steve Ouellette**
Senior Director
Engineering Learning and Development
QUALCOMM, Inc.

**Paul Kukuchek**
United Technologies Corporation
Aerospace Systems

**Antonio Redondo**
T Division
Los Alamos National Laboratory

**Satchi Venkataraman, Moderator**
Faculty
Aerospace Engineering & Engineering Mechanics

**Carlos Bazan**
Faculty, Scientific Visualization Coordinator
Computational Science Research Center

**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

gateway to the future
CSRC
an interdisciplinary

SAN DIEGO STATE
UNIVERSITY

# 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

**Industry Projects Coordinator:**
Carlos Bazan, *a.i.*

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Bill Bartling
SR2020, Inc.

### *Feedback Interaction Network Between the microRNA miR-124 and the Notch Signaling Pathway*

***By Jerry S. Chen, Joyce Tang, Abygail Gumbayan, and Robert Zeller***

The nervous system-enriched microRNA miR-124 is necessary for proper nervous system development, although the mechanism remains poorly understood. Here, through a comprehensive analysis of miR-124 and its gene targets, we demonstrate that, in the chordate ascidian Ciona intestinalis, miR-124 plays an extensive role in promoting nervous system development. We discovered that feedback interaction between miR-124 and Notch signaling regulates the epidermal-peripheral nervous system (PNS) fate choice in tail midline cells. Notch signaling silences miR-124 in epidermal midline cells, whereas in PNS midline cells miR-124 silences Notch, Neuralized and all three Ciona Hairy/Enhancer-of-Split genes. Furthermore, ectopic expression of miR-124 is sufficient to convert epidermal midline cells into PNS neurons, consistent with a role in modulating Notch signaling. We demonstrate that miR-124 is activated downstream of a series of proneural basic-helix-loop-helix transcription factors, suggesting that these genes operate collectively in a feedback regulatory network. Finally, we have developed a mathematical model which quantitatively explains how this feedback interaction network governs Ciona PNS formation. Interestingly, the genes encoding all of the factors in this network have recently been demonstrated to convert human fibroblasts into neurons. Our results thus provide important functional insight into how miR-124 promotes neuron differentiation, and should motivate future studies on this important microRNA.

***This research is supported in part by NSF funds.***

### *Ab initio Many-Body Calculations of the 4He Photo-absorption Cross Section*

***By Micah Schuster***

Working within the no-core shell model approach with a similarity renormalization group (SRG) evolved two- and three-nucleon (NN NNN) Hamiltonian, we compute the dipole strength function of 4He, using the Lorentz integral transform (LIT) method to obtain the continuum response. We then compute the total photo absorption cross section of 4He. We pay particular attention to the convergence of the total strength and of the LIT of the dipole response as we increase the size of the harmonic oscillator basis. IMRR: LLNL-ABS-609699

***This research is supported in part by U. S. DOE/SC/NP (Work Proposal No. SCW1158 and grant DE-FG02-96ER40985) funds.***

### *Tools for Fast Sequence Alignments*

***By Sajia Akhter and Robert A. Edwards***

Metagenomics or random community genomics is a rapidly emerging field in microbiology that uses the latest low-cost high-throughput sequencing technologies to sequence the whole community DNA from the environment without isolating individual microbes. Analyzing and annotating these data requires sequence alignments to compare them with genes, proteins and genomes in different databases. Sequence alignments (either DNA/protein level) are also necessary to make a similarity profile between many metagenomes from different environments. Moreover, to study the common bacterial or viral population within several metagenomes, sequence alignments are the first step.

In the Sequence Read Archive at NCBI, there are about (up to May, 2012) 2500 publicly available metagenomes that were generated by different technologies and of different read lengths. Because of the recent advances in sequencing technologies, the number of metagenomes has been increasing each year, and consequently there is a demand for faster sequence alignment algorithms. The goal of this proposal is to develop a local sequence alignment tool for both DNA and protein sequences, which will work faster than existing tools but will give the same or better accuracy compared to other tools.

***This research is supported in part by NSF funds.***

### *Publicly Available Web-Solver for the Vibrational Schrödinger Equation: islands.sdsu.edu*

***By Peter Zajac and Andrew Cooksy***

A web-based service for predicting molecular vibrational properties has been developed and made available to research groups around the world. The service uses the finite element method to integrate the vibrational Schrodinger equation on arbitrary potential energy surfaces of up to three dimensions. Calculation of the vibrational eigenstates is important not only in predicting the experimental spectra of molecules but also for predicting their thermodynamic properties. FEMvib has the capability of treating strongly anharmonic and strongly coupled vibrational motions with a minimum of user input, in contrast to typical approaches which require the user to tailor the solver to a particular molecular structure.

***This research is supported in part by Computational Science Research Center, the Department of Chemistry, Army Research Office (57989-CH), and an equipment grant from the NSF (CHE-0947087) funds.***

### *Unbiased Variable Importance Rankings for Correlated Survival Data, with Applications to Tooth Loss*

***By Melodie J. Hallett, Juanjuan Fan, Xiaogang Su, Martha E. Nunn, and Richard A. Levine***

Oral health is a significant issue for adults because of its relationship to quality of life, as well as systematic health and well being. Impaired oral health can lead to significant health problems, such as pain and infection. In this paper, a new random forest method is proposed for correlated survival data using the VA Dental Longitudinal Study. This new method aims to remove the bias of the traditional random forest variable selection, which favors input variables with more categories, as shown by Strobl (2007). The multivariate exponential tree algorithm of Fan and Su (2009) is used to build trees, as it has proven superior prediction accuracy and computational efficiency compared to marginal and semiparametric frailty model based trees. Simulation studies for assessing the proposed tree and variable importance methods are presented. To limit the final number of meaningful prognostic groups, an amalgamation procedure is used to develop tooth prognostic groups from a forest of trees. The resulting prognosis rules and variable importance rankings may be used in clinical practice to increase tooth retention and establish rational treatment plans. By ranking the relative importance of various clinical factors for tooth loss, we are able to provide clinicians with critical information so they can develop and implement a treatment plan

***This research is supported in part by private funds.***

### *A Model to Identify Organisms Present in Metagenomes Based on Codon Usage*

***By Genivaldo Gueiros Zacarias Silva and Robert A. Edwards***

One of the major goals in metagenomics is to identify the presence of organisms in the microbial community from a huge set of unknown DNA sequences; this profiling has valuable applications in multiple important areas of medical research such as disease diagnostics. Nevertheless, it is not a simple task, and many approaches that have been developed are slow and depend on the read length of the DNA sequences. Here we introduce FOCUS, an innovative and agile stochastic model to profile and report organisms present in metagenomic samples based on codon usage without sequence length dependencies. The program was tested with simulated metagenomes, and the results show that our approach has 90 accuracy at inferring the organisms in random communities. The algorithm presented will help biologists explore the microbes present in their samples, and identify which organisms are present. A web-server and the project implementation in python are available at http://edwards.sdsu.edu/focus.

***This research is supported in part by NSF funds.***

### *DLOOP: A Flash Translation Layer Exploiting Plane-Level Parallelism*

***By Wei Wang, Tao Xie, and Abdul R. Abdurrab***

A flash translation layer (FTL) is a software layer running in the flash controller of a NAND flash memory solid-state disk (hereafter, flash SSD). It translates logical addresses received from a file system to physical addresses in flash SSD so that the linear flash memory appears to the system like a block storage device. Since the effectiveness of an FTL significantly impacts the performance and durability of a flash SSD, FTL design has attracted significant attention from both industry and academy in recent years. In this research, we propose a new FTL called DLOOP (Data Log On One Plane), which fully exploits plane-level parallelism supported by modern flash SSDs. The basic idea of DLOOP is to allocate logs (updates) onto the same plane where their associated original data resides so that valid page copying operations triggered by garbage collection can be carried out by intra-plane copy-back operations without occupying the external I/O bus. Further, we largely extend a validated simulation environment DiskSim3.0/FlashSim to implement DLOOP. Finally, we conduct comprehensive experiments to evaluate DLOOP using realistic enterprise-scale workloads. Experimental results show that DLOOP consistently outperforms a classical hybrid FTL named FAST and a state-of-the-art page-mapping FTL called DFTL.

***This research is supported in part by NSF funds.***

### *A Hybridized Evolutionary Algorithm for Feature Selection of Chemical Descriptors for Computational QSAR Modeling of HIV-1 Integrase Inhibitors*

***By Gene M. Ko, Rajni Garg, Sunil Kumar, Barbara A. Bailey, and Ahmad R. Hadaegh***

Feature selection is an important aspect in the development of quantitative structure-activity relationship (QSAR) models. As the number of chemical descriptors for each compound ranges from hundreds to thousands, an efficient algorithm which can identify an optimal subset of descriptors is highly desired. Existing evolutionary algorithms for feature selection suffer from slow rates of convergence and convergence to a local optima. We have developed a novel hybridized differential evolution-binary particle swarm optimization (DE-BPSO) algorithm for feature selection which aims to overcome these performance issues. DE-BPSO was observed to outperform genetic algorithms (GA) and binary particle swarm optimization (BPSO) using a test dataset of HIV-1 integrase inhibitors. We plan to use the DE-BPSO algorithm to further develop QSAR models as virtual screening tools for the identification of novel HIV-1 integrase inhibitors from large chemical databases.

***This research is supported in part by NIH funds.***

### *Numerical Simulation of Poroelastic Pressure Diffusion in $CO^2$ Sequestration*

***By Jonathan L. Matthews, Jose E. Castillo, and Christopher P. Paolini***

$CO^2$ sequestration in underground aquifers shows significant potential in reducing greenhouse gas emissions. However, rock fractures, formed during injection, may release toxic species into the water table and release $CO^2$ back into the atmosphere. Because rock fractures develop as a result of stresses, a model to compute the internal stresses induced by the injection of $CO^2$-rich water was developed. A pore pressure diffusion module has been implemented into a reactive transport modeling application to simulate effects of fluid gain stresses on rocks caused by $CO^2$-rich water injection. The theory of poroelasticity relates the pore pressure to fluid gain in rock, and stresses and strains imposed on rock. In this work, a poroelastic model for the one-dimensional case was developed for an existing reactive transport modeling application to calculate the pressures induced by the injection of $CO^2$ into a geologic sandstone formation. In this one-dimensional case, pore pressure is decoupled from stress, fluid gain, and strain. The decoupled pressure follows a diffusive process that is a function of the fluid source and the poroelastic properties of the rock formation. In this one-dimensional case, the induced mean stresses are a linear function of the pore pressure. The pore pressure module has been used to approximate formation pressure during injection of $CO^2$ rich water into the Oligocene Frio Formation along the Texas Gulf Coast, with simulation parameters derived from the Frio Test Pilot Experiment. Simulation results were compared to bottom-hole pressure data obtained from an observation well 30 meters away from the injection well, during a 35-day injection phase.

***This research is supported in part by DOE funds.***

### *Nesting ROMS and UCOAM: A Case Study in Monterey Bay*

***By Mary Thomas, Dany De Cecchis, Paul Choboter, and Jose E. Castillo***

The Regional Ocean Modeling System (ROMS) is a hydrostatic free-surface ocean model ideally suited to simulate medium to large-scale coastal ocean processes. The Unified Curvilinear Ocean Atmosphere Model (UCOAM) is a non-hydrostatic LES model designed specifically for high-resolution simulations, and is capable of accurately reproducing the interaction of currents with steep bathymetric features. In this paper we present our efforts to nest the parallel, non-hydrostatic UCOAM within a parallel ROMS model, using the Distributed Coupling Toolkit. The nested model is used to study realistic currents in Monterey Bay.

***This research is supported in part by private funds.***

### *Hybrid High-Order Eulerian Lagrangian Methods for Simulations of Particle-Laden Flow with Shocks*

***By Jean Piero Suarez and Gustaaf Jacobs***

Our research is focused in the development of a Hybrid high-order Eulerian-Lagrangian algorithm to simulate shock wave interactions with particles. The algorithm enables the solution of a class of problems currently out of reach as well as improved prototyping of engineering application such as high-speed combustors, volcano eruptions, and explosion impact and mitigation thereof. The mathematical model is based on a coupled system consisting of non-linear hyperbolic balance laws with a singular source term that accounts the influence of the particles on the flow and kinematic equations, which govern the fluid flow and particle motion, respectively. The continuum balance equations solve the carrier flow with a Hybrid scheme that uses the weighted essentially non-oscillatory (WENO) method for shock capturing, and a more computationally efficient high-order scheme, including a central finite difference or spectral methods in regions where the solution is smooth. The singular source term is approximated through a regularization technique based on piecewise polynomials compactly supported. Numerical experiments shows the accuracy and computational efficiency of a parallel Hybrid WENO-Z finite difference scheme on a benchmark problem for a three-dimensional sonic flow injection in supersonic cross flow. In the numerical solution of scalar balance laws with spectral methods, the regularization technique yields to accurate approximations with a convergence order according to the asymptotic behavior of the spectral interpolation error.

***This research is supported in part by Department of Defense - Air Force Office of Scientific Research funds.***

### *Compact, Broadband, Geolocation Systems*

***By Daniel Lyons and Antonio Palacios***

There is a current need for accurate geolocation systems that can detect and track RF emitters at long range. Many of the existing geolocation technologies have an associated premium in regard to low size, weight, and power for such systems. We propose a new geolocation system that utilizes a Colpitts Oscillator with dynamic inductance. Signal direction finding occurs via calculation of the Poynting vector, while signal strength is measured via Residence Times Detection (RTD). The system generates its own bias signal, leading to reduced power consumption in the device. Numerical calculations of sensitivity and resolution suggest that the proposed device represents a significant improvement in the current state-of-the-art for extremely low magnetic field detection.

***This research is supported in part by Computational Science Research Center, the Department of Mathematics and Statistics, and Office of Naval Research funds.***

## *The Structure and Rheology of Transient Self-Associating Polymer Networks*

***By Mark Wilson, Arlette Baljon, and Avinoam Rabinovitch***

Numerical simulations of telechelic polymers have been employed to investigate the structural dynamics within the viscoelastic stress response common to triblock copolymers. A hybrid molecular dynamics, Monte Carlo (MD/MC) algorithm has been used within the simulations. Therein, functionalized end groups, at both ends of the polymer chains, form reversible bonds according to MC rules, while the spatial positions of the polymers are dictated by MD. The system is studied under an applied oscillatory shear at a temperature below the micelle transition. Hence, the chains self-assemble to form a transient network. The nodes of this network consist of aggregates of end groups, while bridges between aggregates are formed by one or more polymer chains. The structure of this polymer network changes in response to the frequency and amplitude of the applied shear strain. Our results indicate a continual restructuring throughout the material as a result of the rupture and healing of bonds between the functionalized end groups. These dynamics evolve from viscous to elastic behavior with increasing frequency. At low frequencies, the entire bulk is actively involved, where as higher frequencies lead to localized dynamics and cohesive failure. Over time, configurations slowly develop towards those including more bridges, containing a larger number of polymer chains, along with more tightly packed aggregates.

***This research is supported in part by Computational Science Research Center and NSF funds.***

## *Generalized Linear Varying-coefficient Model with Data Missing at Random*

***By Qian Xu and Jianwei Chen***

The generalized linear varying-coefficient model is an important extension of the generalized linear model. The model structure allows the coefficient to be a curve function with different time. Since local quasi-likelihood estimation is useful for nonparametric modeling in generalized linear models, we extend three estimation methods from it for the generalized varying-coefficient model when there are data missing at random: the local quasi-likelihood estimator using only complete-data, the local weighted quasi-likelihood estimator and the local quasi-likelihood estimator with imputed values. We also develop the local quasi-likelihood imputation methods for estimating the mean function of the response variable. Our simulation results show that the proposed imputation methods perform better than both the one based on complete-case only and the weighted method.

***This research is supported in part by Department of Mathematics and Statistics funds.***

## *Diagnosis of Glaucoma by Joint Modeling with Longitudinal Data*

***By Jeff Ledahl, Richard A. Levine, Juanjuan Fan, and Shaban Demirel***

Detection of glaucomatous progression is an important part of ophthalmologic care. Without early detection, a patient developing glaucoma may loose some or all of their vision. Glaucomatous progression is characterized, in part, by a slowly deteriorating loss of vision. As such, longitudinal measures play an important part in diagnosis. In the literature many longitudinal measures have been proposed for use in diagnosis, but as of yet none have tried to model directly the probability of glaucoma based on these measures. We introduce a joint model which allows us to directly model the probability of glaucoma based on a longitudinal measure, while accounting for the correlation between the eyes of a single patient. We also show how these models may be used to construct better methods of diagnosis which take into account additional patient information.

***This research is supported in part by Computational Science Research Center and Department of Mathematics and Statistics funds.***

## *Application of a Three-Dimensional Hydrodynamic Model for San Quintin Bay, B.C. Mexico. Calibration and Validation using OpenDA.*

***By Mariangel Garcia, Isabel Ramirez, Martin Verlaan, and Barbara Bailey***

A 3D hydrodynamic model (Delf3D) was developed for San Quintin Bay (SQB). Calibration and validations were conducted, using measured bathymetry, water surface elevation, velocities, and temperature. The calibration period was taken during the winter season of 2010. Model predictions were evaluated graphically and statistically against field observations to quantify the accuracy of model predictions and evaluate the success of model calibration. Comparisons between model predictions and field observations of water surface elevations at interior stations indicated that the model was successfully calibrated and model predictions were highly correlated with observed water surface elevations. Agreement between observed and simulated values was based on graphical comparisons, root-mean-square errors, and principal components analysis. The objective of this study was to show that OpenDA can be used to rapidly calibrate a hydrological model.

***This research is supported in part by Computational Science Research Center funds.***

## *Characterizing Unknown Genes Through Metabolomics*

***By Tiffany Y. Liang, Savannah Sanchez, Jason Rostron, and Forest Rohwer***

Viruses are thought to be the most diverse biological entities on earth. However, they are also the least characterized regarding their genetic, taxonomic, and functional diversity. In metagenomic analyses of viral communities from various environments, most sequences are unrelated to any known sequences. About 90 of the viral sequences found in marine environments are unknown. The goal of this study is to characterize the function of unknown viral genes that alter host metabolism. Open reading frames were predicted from the metagenomes and genes synthesized and cloned into E. coli [everyone knows E. coli]. The metabolites produced by the bacterial clones are then identified by gas chromatography-coupled time-of-flight (GC/TOF) mass spectrometry. In total 551 metabolites were found, however 84 of them were not identified based on their mass. We are identifying the specific metabolites produced or affected by the over expression of phage proteins to suggest the physiological roles for these proteins that could be tested experimentally. We are building a systematic analysis tool that can process any kind of matabolomics data for downstream analysis of metabolomics and related data sets.

***This research is supported in part by NSF funds.***

## *An Improved Estimation Method for Mixed-Effects Models with Applications to Health Care*

***By Lingjun Anna He and Jian Wei Chen***

Mixed-effects models arise frequently when data are collected from different clusters or from longitudinal studies. They provide investigators a powerful way to adjust for the measured and unmeasured covariates that might affect the regression function. This paper investigates an estimating method for a nonparametric mixed-effects model where we model the unknown functional using the local linear smoother. Although the proposed estimation methods are applicable for general mixed-effects models, we develop the asymptotic properties of the proposed estimators and show that it is an efficient method for estimating unknown functions and predicting random effects. Our simulation results demonstrate that the proposed estimator is outperformed without considering random effects when there are random effects in the model. A real application from the health care expenditure in China is presented to illustrate the proposed method. Furthermore, an application using mixed-effects models for HIV clinical trial data is presented.

***This research is supported in part by Computational Science Research Center and the Department of Mathematics and Statistics funds.***

## *Microbial Database*

***By Dwaine Smith and Blaire Robinson***

Technological advances in genetic research have enabled scientists to sequence and study microbial genomes. Microbial genomes provide information about specific proteins, how these specific proteins function, and how these proteins are regulated to mechanistically maintain a functioning organism. There is, however, a lack of phenotypic information associated with the microbes whose genomes have been sequenced. Phenotypic information includes: optimum pH, as well as maximum, minimum, and optimal growth temperatures at which the organisms live. Creating a database that will collect and combine phenotypic microbial data that can be utilized and accessed in a computational consumable format will help to expand the usability of microbial genomic databases. We have defined the database schema and selected organisms being studied in Edwards' lab were targeted to populate the database with phenotypic data. We are implementing community standard ontologies to facilitate data exchange with other databases. The microbial phenotype database will provide access to phenotypic data that will drive the formulation of correlations between genotype and phenotype that can be tested experimentally.

***This research is supported in part by private funds.***

## *Testing the Spin Cut-off Factor Parameterization of the Nuclear Level Density*

***By William Spinella and Calvin Johnson***

The spin cut-off factor is the standard parameterization of the nuclear level density. Using shell model data, we systematically examine the quality of the spin cut-off factor parameterization for a large number of light nuclei.

***This research is supported in part by Computational Science Research Center and the Department of Physics funds.***

## *Dynamics of Coupled Spin Torque Nano Oscillators*

***By James Turtle, Richard Shaffer, and Katie Beauvais***

Spin Torque Nano Oscillators (STNO) are a potential building block for a new type of electronics called spintronics. Mastery of this field, would yield a new generation of smaller, faster electronics. We attempt to create a nano-scale microwave signal generator and advance the field of spintronics by studying the dynamics of coupled STNOs.

***This research is supported in part by Computational Science Research Center and the Department of Mathematics and Statistics funds.***

### *Modeling of the Diffusion of Calcium within a Single Sarcomere of an Adult Cardiomyocyte*

***By Rosa Lemus and Amanda Brambila***

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.

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 simulation to demonstrate the calcium turnover, and the dependence upon factors like abundance and transport rates of Ryr2, SERCA and NCX channels.

We have developed an initial simulation of calcium fluxes within a single sarcomere using MATLAB™. Assuming radial symmetry in a cylindrical sarcomere, a 2-dimensional grid model accounts for calcium exchanges within the myofilament system, between the SR's terminal and longitudinal cisternae, and within the cytosol. A 2-D half-sarcomere was divided into pixels. The rate of $Ca^{2+}$ release from the terminal cisternae (TC) region was assumed to be proportional to the product of the probability of the $Ca^{2+}$ release channel being open and the difference of $[Ca^{2+}]$ between the TC and a pixel facing the TC. $Ca^{2+}$ moves from element to element by simple diffusion and is taken up by the longitudinal SR via the SERCA pump. $Ca^{2+}$ influx responsible for triggering the TC $Ca^{2+}$ release is introduced to elements at the terminal cisternae.

An animated visualization of the fluxes uses pseudocolor to represent the calcium concentration changes vs. time in the sarcomere during a single twitch. Increases in SERCA channel density caused a faster relaxation rate of the $Ca^{2+}$ transient.

Changes in number of RyR2 and NCX channels altered $Ca^{2+}$ transient amplitudes and kinetics in a manner predicted by our laboratory's gene silencing experiments. We intend to extend the 2-D model into 3-D and to add other features relating to calcium fluxes, such as a more detailed description of the $Ca^{2+}$-induced $Ca^{2+}$ release mechanism.

***This research is supported in part by Computational Science Research Center funds.***

### *Stability Analysis of Castillo-Grone's Mimetic Difference Operators*

***By Mohammad Abouali and Jose E. Castillo***

This poster shows the stability analysis of various Castillo-Grone's Mimetic (CGM) operators in one dimensional and two dimensional advective equation in conjunction with RK3 time discretization scheme. Furthermore, the effect of different interpolation schemes, including Radial Basis Function (RBF) method, on these operators is discussed.

***This research is supported in part by Computational Science Research Center funds.***

### *Propensity Score and Proximity Matching Using Random Forest*

***By Peng Zhao, Xiaogang Su, and Juanjuan Fan***

To reduce potential bias, in observational study, it is essential to have a balanced matching on all available background information between case and control. Propensity score has been a key matching variable in this area. However this approach has several limitations, such as handling missing values, categorical variables and interactions. Random forest, averaging outcomes from many classification trees, is straightforward to use and easy to handle those issues in balanced matching. Each classification tree in random forest recursively partitions the available dataset into sub-sets to increase the purity of overall tree. With this process, the case and control remaining in the same terminal node automatically becomes the best balanced match. By averaging the outcome of each individual tree, random forest can provide robust and balanced matching results.

***This research is supported in part by private funds.***