# ACSESS

Seventh Annual

**Friday, March 26, 2010**
**12:00 pm - 5:00 pm**
**SDSU's Parma Payne Goodall Alumni Center**

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

CSRC — gateway to the future — an interdisciplinary

SAN DIEGO STATE UNIVERSITY

**Registration / Buffet Lunch**

**1:00 pm** — **Stanley Maloy**, Dean, College of Science, SDSU — Welcome / Opening Remarks

**1:10 pm** — **Jose E. Castillo**, Director, CSRC, SDSU — Computational Science at SDSU and ACSESS Program

**1:20 pm** — **Susan M. Baxter**, Executive Director, CSUPERB, SDSU — Key Note Speaker

**1:45 pm** — **Coffee Break**

## "Training the Scientific Workforce of the 21st Century"

**1:50 pm**

**Victor Pereyra,** Moderator
Chair, CSRC Industry Advisory Board
Weidlinger Associates Inc., ACSESS Partner

**Bill Bartling**
President/COO
SR2020 Inc.

**Jeff Southerton**
Director of Global Programs
Pfizer

**Kevin Clancy**
Senior Staff Scientist
MBR Informatics & Bioinformatics
Life Technologies

**Terie Scerbo**
Academic Relations
Learning & Development
QUALCOMM, Inc.

**Gordon Brown**
Industry Outreach Coordinator
CSRC / SDSU

**Antonio Redondo**
Division Leader
Theoretical Division
Los Alamos National Laboratory

**3:00 pm** — **Poster Presentation / Reception**

**4:30 pm** — **Paul Paolini**, Associate Director, CSRC, SDSU — Poster Presentation Awards & Closing Remarks

**Adjournment**

# Computational Science Research Center

## 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

**Industry Projects Coordinator:**
Gordon Brown

**Associate Directors:**
Andrew Cooksy
Eugene Olevsky
Paul Paolini

## Scientific Advisory Board

**Chair:** Antonio Redondo, Theoretical Division
Los Alamos National Laboratory

Steve F. Ashby, Pacific Northwest National Laboratory

Victor Pereyra, Weidlinger Associates

Horst Simon, Lawrence Berkeley National Laboratory

## Industry Advisory Board

**Chair:** Victor Pereyra, Weidlinger Associates

Richard Greenblatt, Source Signal Imaging Inc.

John Newsam, fqubed, Inc.

Antonio Redondo, Theoretical Division
Los Alamos National Laboratory

### *Computational Study of TTQ Reaction Kinetics*

***By Kirsten Ivey, Belynda Sanders, Chris Estela, & Andrew Cooksy***

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Among the simplest electrobiochemical pathways to characterize experimentally is a series of electron transfer reactions that provide the mechanism for dehydrogenation of methylamine. We describe a computational investigation of the chemical reaction mechanisms for the enzyme activity of methylamine dehydrogenase, focusing on the activity of the cofactor tryptophan tryptophylquinone (TTQ). The free energies, reaction rate constants, and related effects of temperature, pH, and isotopic substitution are being computed for comparison against experimental observations. Electronic structure calculations are carried out by density functional methods shown to be effective in the study of simpler chemical systems involving the dynamics of conjugated pi-electron systems. The COSMO-RS model will be applied to account for the considerable solvent effects in ion-mediated reaction dynamics, and will allow determination of the influence of pH on the reaction system.

### *Distribution Frequency of PBP2a Encoding Methicillin Resistance Genes in Metagenomes*

***By Victor Seguritan, Molly Schmid, Robert Edwards, and Anca Segall***

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Human infections caused by antibiotic resistant microbes are on the rise and spreading globally. According to the CDC, Methicillin Resistant Staphylococcus Aureus, or MRSA, infects close to 100,000 people and is responsible for 19,000 deaths annually. Methicillin resistance is encoded and spread by the horizontal transfer of mecA, the gene that encodes the protein Pbp2a. Pbp2a is an analog of the protein Pbp2. Both proteins function to build bacterial cell walls and can be inactivated in the presence of methicillin, leading to cell death. Resistance is conferred by the presence of Pbp2a because this isoform has much lower affinity for methicillin than its analog, Pbp2. Metagenomic data have been obtained from a multitude of different environments. We are interested in discovering the frequency of occurrence of the mecA gene in metagenomes based on the extent to which mecA like genes occur in environmental samples. To do so we have determined the frequencies of mecA genes calculated in over 200 metagenomes. The frequency with which the gene occurs in the metagenomes was obtained by counting the best BLAST alignments and normalizing to the total number of sequences in each metagenome. Generally the frequencies of mecA-like genes in the metagenomes are very low. The highest frequency occurs in wastewater environmental samples, followed by human and marine metagenomes. Zero occurrences were observed in coral, fish, freshwater, and deep-water marine samples. Frequencies are clustered by Self-Organizing Maps (SOM) and visualized by Principle Component Analysis (PCA) to determine the relationships of metagenomes in terms of the frequency of mecA gene occurrence. Our analyses were done using the BLAST algorithm and Matlab built-in functions. Environmental samples constitute a reservoir of mecA genes, and understanding the distribution, dynamics and evolution of mecA-like genes will provide insights into the development of antibiotic resistance.

### *General Curvilinear Ocean Model: Next Generation*

***By Mohammad Abouali, Torres C., Hernandez-Walls R., & Castillo J.E.***

GCOM-NG is a non-dimension Ocean Model. It uses three-dimensional primitive Navier-Stokes equation in General Curvilinear Coordinate system. Pressure is treated non-hydrostatically and density is calculated using the UNESCO equation of state. Temperature and Salinity are active scalars, as they change the density and Density is present in Buoyancy term in the momentum equation.

### *Investigating the Structural Dynamics Implication of Flexible Resilin Joints on Dragonfly Wings*

***By Joseph Marrocco, Luciano Demasi, and Satchi Venkataraman***

The practical application of relatively small, light weight micro air vehicles by biomimicry is of great interest to the engineering community. The goal of this research project is to improve the understanding of the structural construction of insect wings. A dragonfly insect has been chosen, as it has a very revealing structure and is an insect that has unique flight capabilities. Dragonfly wings are able to withstand the forces imposed upon them by the surrounding air, inertial forces caused by acceleration and decelerating their own weight. The basic design of a dragonfly wing is a pleated membrane stiffened by tubes at the apexes of the pleats, forming a particularly rigid and strong structure. This tubular pleated membrane provides a stiff structure along the length (span wise) direction of the wing and a flexible structure along the width (chordwise direction) of the wing. The tailoring flexibility in the wing is essential as it can play significant role in the aerodynamics wing airfoil shape it can achieve, in addition to the benefits of gust alleviations, and damage tolerance.The investigation into the material composition and architecture on the dragon fly wings revealed that while a large part of the wing structure is made of chitin protein, there is a regular pattern of joints on the wing made of less stiffer resilin protein. The focus of this effort is to understand the effect and implications of the resilin joints on the structural dynamics of the wing. To achieve this goal a finite element structural analysis tool has been used and a detailed model of the dragonfly wing was created. Main focus of the present analysis is to understand how the presence of flexible resin joints affects the natural vibration and mode shapes of the dragonfly wing.

### *Real-Time Metagenomics*

***By Daniel Cuevas, Robert Edwards, and Joshua Hoffman***

Real-Time Metagenomics (RTMg) is a three-pronged project that delivers metagenome annotation services to biologists across several platforms. The first branch, RTMg.web, performs annotations of fasta-formatted DNA sequences within minutes. Mobile Metagenomics (RTMg.mob) delivers metagenome annotations to the Android cellphone platform for as-you-go analysis. OpenSocial Metagenomics (RTMg.os) delivers the service to social networking sites for sharing data and analysis with colleagues and friends. Using RTMg.web, the sensitivity and specificity of the instantaneous annotations provided by the real-time server were compared to those generated by BLAST to reveal strengths and weaknesses of both approaches. RTMg.mob allows streaming data analysis with fully interruptible processes; users can take calls, browse the web, and send/receive SMS messages during annotation. The application implements the Android standard "Share" feature, which allows for users to email their data to other phone or computer users, and to access the data via RTMg.os. OpenSocial Metagenomics stores metagenome-annotated data on a server and allows users of the social network to access and share this information with their friends. All metagenome annotation and analysis has been designed in a portable, open, exchangeable format that allows the easy extension of the RTMg suite of applications with new tools as they become available.

### *Adaptive Ajax-Based Streaming Video for the Irobot Create Platform for Use in Buildings with Infrastructure Mode 802.11 Networks*

***By Sudha Natarajan and Christopher Paolini***

An adaptive, Internet streaming video service for use in consumer grade Web-enabled telerobotic systems is presented. The system, based on the FFMPEG multimedia framework, is designed to stream video at different dynamically controlled frame rates and video quantizer scales as a function of current wireless data rate. Video is captured from an onboard camera connected to an embedded single board computer (SBC) through an IEEE 1394 (Firewire) serial interface, all set within the robot's payload bay. As a mobile robot engages in indoor tasks that span long distances in corridors on multiple floors within buildings with integrated 802.11 infrastructure mode wireless service, different signal strengths may be observed by the robot's wireless transceiver due to free space path loss and attenuation from building infrastructure, which effectively varies the WLAN data rate. In the 2.4 GHz band used by 802.11b and g, path loss from drywall can be 4 dB, brick wall 8 dB, and concrete wall 10-15 dB. An 802.11 transceiver will step down its data rate as signal strength decreases. As a result, the rate and quality of real-time transmission of video frames from a mobile robot must adapt to a changing signal strength to prevent jitter and packet loss which is undesirable in mobile telerobotic systems, as it is essential for the human controller to have an accurate picture of the robot's position and orientation at all times to avoid collision. In this paper, we present an adaptive system that varies the frame transmission rate, the quantizer scale, or both, in real-time, as a function of the robot's current WLAN transceiver data rate. The numerical method employed is based on acquiring the effective data rate required to stream video frames from 3 to 30 fps at different quantizer scales, fitting this data to a polynomial model, and using an iterative Newton-Raphson solver to solve the inverse problem to perform rate adaptation. Performance results based on variable frame rate at a fixed quantizer scale and variable quantizer scale at a fixed frame rate are presented.

### *Modeling Throughput and Delay for a Hybrid Channel Access Scheme for QoS Support in WLANs*

***By Rohitha Vakamudi, Mahasweta Sarkar, and Christopher Paolini***


This work analyses a hybrid medium access control (MAC) scheme which alternates between a contention based and a polling based scheme in an infrastructure mode wireless local area network (WLAN). The scheme can be thought of as a standard 802.11 channel access scheme operating both in the Distributed Co-ordination Function (DCF) and Point Co-ordination Function (PCF) mode for enhanced Quality of service (QoS) performance. An analytical model has been proposed for such a hybrid MAC and dimensionless expressions depicting throughput and delay for such a MAC has been derived. MATLAB simulations showcasing throughput and delay characteristics of the hybrid MAC as a function of packet collision probability are presented. Furthermore, a QualNet based simulation result is used to validate the feasibility of the analytical model. In addition, discussions on the effects of various system parameters like the duration of DCF and PCF mode, packet collision probability, and superframe partition size are also presented,along with graphical analysis.

### *Gene Expression Profiling of Neonatal Rat Cardiomyocytes in Response to Rosiglitazone*

***By Daniel Pick, Kirubel Gebresenbet, Xian Zhang, & Paul Paolini***


The drug rosiglitazone, a thiazolidinedione, has been prescribed for diabetes patients, but chronic treatment with the drug has raised concerns of its effects on the cardiovascular system. In this experiment we aimed to identify the 20 genes most significantly expressed in the heart after treatment with rosiglitazone. Neonatal rat cardiomyocytes were isolated, cultured, and exposed to the drug. RNA was extracted and plated on Illumina RatRef-12 gene expression microarrays. Expression data were normalized, and statistically analyzed via t-test. Fold changes were computed, and a cluster analysis performed. Over 3,000 genes of the 22,518 genes studied had statistically significant expression levels with p values less than 0.5, 310 of which had p values less than 0.0001. Six of the genes computationally found to be the most significantly expressed were selected for validation via quantitative real-time PCR, and the expression levels found were in good agreement with computational analysis. We identified 20 genes differentially expressed by neonatal rat cardiomyocytes exposed to the drug rosiglitazone. The most significantly expressed genes occurred for the PPAR signaling pathway, consistent with the drugâ?Ts known behavior as a PPAR agonist.No genes in the calcium signaling pathway were found to be among the most significantly expressed. The Illumina RatRef-12 chip microarray is not sufficiently sensitive to detect the relatively weak expression levels of the genes in the calcium pathway, but shows exceptional reproducibility for high expressors.

### *Experimental and Theoretical Modeling of Mitochondrial Inner Membrane Conformation: Electron Microscope Tomography and Thermodynamics*

***By Mariam Ghochani, J. D. Nulton, P. Salamon, T. G. Frey, A. Rabinovich, & A.R.C. Baljon***


Electron tomograms have revealed that in normal mitochondria cristae membrane self-assembles into a complex structure that contains both flat lamellar and tubular components that are connected to the inner boundary membrane through crista junctions. This Structure is believed to be essential to the proper functioning of mitochondria. To better understand the underlying features of this structure, we propose a free energy model for this configuration in an effort to use the observable geometrical features to predict thermodynamic properties of the system such as surface tension and pressure difference that are not directly observable. The model assumes that mechanical forces act on the membrane, which we believe to be exerted by proteins. To that end, a set of geometric measurements from the structural features of mitochondria were obtained. Structural features were measured from 3D electron tomograms of mitochondria. These tomograms were obtained by collecting tilt series of 300nm sections of mitochondria, aligning the projection images of each tilt series to a common origin, and applying a filtered backprojection algorithm to the aligned tilt series to calculate tomograms of mitochondria in each section. Full tomograms were obtained by joining the reconstructions of up to four serial 300nm sections. From the measured structural features, measurements of other features of cristae membranes are extrapolated computationally. Geometric measurements predict linear relations between lamellar radius versus radius of the cristae membrane (modulated by the number of tubes), and the number of tubes versus radius of the cristae membrane describing the geometric constraints within the structure of the normal mitochondria. The free energy model combined with the geometric measurements predicts that tubular structures are stabilized by tensile forces of 10-20 pN, comparable to those typical of motor proteins. It also predicts the pressure differences of 0.01-0.1 atm across crista membrane and surface tensions of less than 0.2 pN/nm, the point at which a membrane ruptures. From the behavior of the tensile forces which stabilize the cristae structure in our model, we are gaining insights on how the proteins exerting such forces are involved with biological processes such as fission/fusion and apoptosis and the consequent thermodynamic variations in mitochondria through such processes.

### *Comparing Two Haar Wavelet Transform Algorithms in Image Compression*

***By Mohammad Abouali, Sara Zarei, & Mariangel Garcia***


The performance and the cost of two methods of 2D Haar wavelet transforms, both in blocking and non-blocking mode, is compared in image compression.

### *Detection and Visualization of HIV-1 Sequences in the Human Genome*

***By Matthew Hagen, Roland Wolkowicz & Robert Edwards***

The retroviral life cycle involves the relatively random integration of a DNA copy of the virus genome into host cell DNA. Once integrated, retroviruses remain in the genomes of their hosts; there are no known viral mechanisms for their excision. Over evolutionary time scales, the retroviral genomes may disappear or change by deletions and mutations, but their footprints may remain, allowing for their detection and the analysis of their co-evolutionary history. HIV-1 is a member of the lentiviruses within the retroviridae family of viruses. Revealing genomic sequences that have been kept and sequences that have been lost will shed light on HIV-1/Homo sapiens co-evolution. The DNA sequence of HIV-1 was compared with the human genome to detect possible remains of past integration events. Through DNA homology analysis, identical matches were found in all of the human chromosomes, with sequences that are more prevalent than otherwise would have occurred by chance. Interestingly, in some cases, the occurrences are clustered. The distribution of these matches is being analyzed to detect which viral genes have "survived", and whether there is a preference for cis elements or gene products, and whether results vary within different viral strains. A tool for the visualization of the matches between the viral genome and the human genome has also been developed. In light of the high mutation rate of retroviruses, the analysis is being repeated with several HIV-1 sequences from different clades in order to increase the biological relevance of our findings. Preliminary analysis reveals, as expected, higher incidence of structural genes which are conserved among retroviridae. Interestingly some of the regulatory genes characteristic of lentiviruses were observed as well.

### *Optimization of Limited Precision Computation for a Low Density Parity Check (LDPC) Code Decoder*

***By Raymond Moberly, Michael O'Sullivan, & Khurram Waheed***

The limited-precision implementation of the sum-product algorithm involves a trade-off between computational precision and computational speed; bits of precision improve coding gain but increase iteration latency. Our effort optimizes the use of limited precision for small numbers of bits. The sum-product algorithm has been the central focus of soft-decision decoding since Gallagher's foundational work on Low Density Parity Check (LDPC) codes. This algorithm is also known outside of the signal processing community as Pearl's belief propagation. An FPGA-based implementation offers the flexibility to perform computer algebra with significantly less precision than the standard (e.g. integer, floating-point) data types and operations of general purpose CPUs, it also permits the aggregation of computational operations.

### *Identifying the Frequency of Quinolone Resistance Genes in Environmental Samples*

***By Sajia Akhter, Anca Segall, Molly Schmid, & Robert Edwards***

Quinolones are broad-spectrum antibacterial agents and their extensive use has resulted in the development of widespread resistance. The abundance of publicly available metagenome (random community genome) sequences provides a snapshot of the genetic background of quinolone resistance. For this study, the frequency of mutations that altered the quinolone target enzymes (DNA gyrase encoded by the gyrA and gyrB genes and topoisomerase IV endcoded by the parC and parE genes) were identified in over 300 metagenomes containing over 50 million nucleotide sequences. BLAST was used to find homologs, and global alignments were used to score the presence of resistance alleles in the sequences. This analysis showed that there were proportionally more resistance alleles in gyrA than parC. Almost all of the metagenomes associated with animals have gyrA resistance alleles, but not parC resistance alleles, likely reflecting the medical and veterinary history of antibiotic treatment of these animals.

### *Identification of Macrolide Resistance Alleles in Environmental Metagenomes*

***By Robert Schmieder, Anca Segall, Molly Schmid, & Robert Edwards***

Background: Macrolide antibiotics target the 23S ribosomal RNA (rRNA) component of the ribosome and inhibit protein synthesis. In particular, they target the large subunit tunnelwhere they prevent the ribosome from tunneling the growing polypeptide out of the active site. Macrolides are composed of sugars attached to a lactone ring of variable size; the most commonly used macrolides are erythromycin (14-membered lactone ring) and tylosin (16-membered). The 23S rRNA gene consists of six conserved domains, and mutations causing resistance are typically located in domain II and within the peptidyl-transferase region in domain V.

Methods: All sequences similar to 23S rRNA genes were identified from over 300 metagenomes, and then aligned using a global alignment. The bases at the alleles known to determine resistance to macrolides were used to calculate the frequency of sensitivity and resistance for each single metagenome.

Results: A web site has been developed to allow the easy identification of antibiotic resistance alleles in metagenomes (http://edwards.sdsu.edu/robar/). Although several key positions in the 23S rRNA gene were invariant in all metagenomes, there were differences in the closely related 23S genes, and the coverage across those genes varied for each metagenome. Moreover, the presence of resistance alleles depended on the biome from which the metagenome was sampled, and also on the geographical separation within each biome.

### *A Random Forest Model for the Analysis of Chemical Descriptors for the Elucidation of HIV-1 Protease Protein-Ligand Interactions*

***By Gene M. Ko, A. Srinivas Reddy, Sunil Kumar, & Rajni Garg***

A model for the classification of 70 HIV-1 protease crystalstructure binding pockets to one of its complexed FDA approved protease inhibitors utilizing Random Forest has been developed. 456 chemical descriptors of the binding pocket of each crystal structure have been computed and are used to develop the classification model. A computer simulation of 40,000 iterations was performed to determine the optimal Random Forest model parameters with the lowest out-of-bag (OOB) classification error. The optimal tree size was determined to be 10586 trees with an average error rate of 40.114 Several models were created using the optimal Random Forest parameters, with a minimal OOB classification error of 38.57 An implicit feature relevance measure for each of the models was analyzed using the Gini importance measure. The chemical descriptors most influential in classifying the binding pocket of HIV-1 protease with its complexed protease inhibitor were analyzed. The top ranked chemical descriptors emphasize the protein-ligand interactions between the C-N atoms, atomic connectivity, and the physical shape of the binding pocket by the volume and shadow descriptors. This study suggests the stability of Random Forest to always select for the same set of descriptors when using a large number of trees. Random Forest was determined to have suitable classification performance for this highly underdetermined dataset by being able to consistently select for the most relevant chemical descriptors while ignoring irrelevant ones in its tree building process.

### *Simulating the Nonlinear Schrodinger Equation Using the Computational Capability of NVIDIA Graphics Cards*

***By Ronald M Caplan & Ricardo Carretero***

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We describe our efforts to simulate the Nonlinear Schrodinger Equation (NLSE), using the computational capabilities of NVIDIA graphics cards. Our goal is to exploit the massive parallelism of the graphics processing units (GPU) on the NVIDIA cards to greatly reduce the computation time required for the simulations. The GPUs have the potential to speed up the simulations by a factor of over one hundred and are an extremely cheap parallel solution when compared to cost of an equivalent CPU cluster. We begin by first formulating a high-order explicit finite difference code to integrate the NLSE which includes a new Modulus-Squared-Dirichlet boundary condition. This code is then modified for use with NVIDIA GPUs using an application programming interface called CUDA. We show good speedup results for one dimensional simulations of the NLSE using CUDA, and expect even better results once the code is extended to two and three dimensions. We conclude that the advantages of using CUDA for simulating the NLSE are well worth the added development time.

### *Modeling the Meso-Scale Evolution of Anisotropic Materials During Sintering*

***By Gordon R. Brown, Eugene Olevsky, & Ricahrd Levine***

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Monte Carlo (MC) simulations are widely used for understanding a wide variety of physical phenomena including the microstructural evolution of sintering bodies. The physics of these phenomena are frequently directionally dependent in nature. Unfortunately, the models currently in use do not accommodate these anisotropic properties. With regards to sintering materials, anisotropy has a significant effect on grain growth rates which impact critical material properties. One of the more popular simulations is a Potts MC model. This research focuses on the use of a two-dimensional Potts MC model to simulate the evolution of the granular structure and modifies the existing algorithms to incorporate the effects of anisotropy inherent in the material. The anisotropy is introduced using Wolff plots to map the anisotropy in the surface energy of the grains. Limitations of this algorithm imposed by the underlying lattice structure are identified and analyzed. A novel solution to mitigate the artifacts resulting from the lattice is proposed and evaluated. This type of Potts MC model is widely used in many fields including problems in statistical physics, weather simulation, radiation damage, etc. In almost all of these applications, the artifacts resulting from the underlying lattice structure are a concern. The ability to incorporate anisotropic grain growth in our meso-scale modeling allows the investigation of anisotropic granular development under several different situations to better understand some of the observed anisotropic phenomena.

### *Predicting Glaucoma Progression Using Decision Trees for Clustered Data by Goodness of Split*

***By Lucie Nguyen, Juan Juan Fan, & Richard Levine***

Predicting who will progress has been recognized as one of crucially needed developments for glaucoma management. Unfortunately, there is currently little consistency among practitioners and researchers in the assignment of visual field progression risk factors. To this end, a decision tree procedure is proposed that deals with the correlation between the fellow eyes from the same patient through the generalized estimating equation (GEE) approach. We adopt the goodness-of-split pruning algorithm of LeBlanc and Crowley (1993) to determine the best tree size. Simulation studies for assessing the proposed tree are presented. To limit the final number of meaningful prognostic groups, an amalgamation algorithm is employed to merge terminal nodes that are homogenous in glaucomatous progression. The resulting prognosis rules and seem to offer simple yet clear and insightful interpretations.

### *Promoter Analyses Reveal Patterns of Clustered and Spatially Organized Transcription Factor Binding Sites that Distinguish Subsets of Autophagy Genes*

***By Lena D. van der Stap***

Autophagy is an intracellular pathway that is essential for cellular homeostasis and therefore has an effect longevity and health spans. The pathway is induced by a starvation or oxidative stress response and it clears misfolded proteins and malfunctioning organelles from cells. We hypothesize that composition, number and position of multiple transcription factor binding sites (TFBS) are organized into distinctive clusters conserved among functionally-related human autophagy gene promoter sequences. Fouty seven autophagy promoter sequences were analyzed with pattern detection and pattern matching algorithms. Comparisons of composition, number, and position of predicted TFBS within conserved regions in aligned human autophagy gene promoters identified distinctive patterns of TFBS clusters. Each gene's upstream 2kb flanking sequence contained 129 to 600 TFBS of which 5-30 were conserved among subsets of autophagy genes. Sp1, c/EBP alpha, and NF1 binding sites were most abundant. Distinctive clusters identified were found to be shared by several autophagy gene promoters. In some cases, multiple instances of a cluster were present in a single gene. Clusters differed among subsets of autophagy genes, suggesting differential regulation of autophagy pathway components. Functional annotation and experimental confirmation of candidate transcription factors will allow us to predict pathways and physiological stimuli that affect autophagy gene transcription. This approach can inform gene expression and systems biology studies of autophagy.

### *Improving the Performance of Thermochemical Computations Using Many-Task Computing Methods*

***By Carny Cheng, Mary P. Thomas, Robert A. Edwards, & Christopher P. Paolini***

The SDSU online Chemical Equilibrium Services perform numerical heat transfer and fluid flow computations, using the Flame3D simulator, for thousands of researchers, educators, and students. The computation is broken down into a grid of 2D or 3D control volumes, each of which runs for a few seconds, has small memory requirements (100 Bytes), is independent of its neighbors, and is submitted individually to a Web Service. The embarrassingly parallel simulation requires several hours to compute a few thousand control volumes, for 10¼s of thousands of iterations on a desktop. To improve the computational performance, a multi-task computing (MTC) approach was adopted. For this, a simple job distribution Web service framework (JODIS) was designed that distributes application workloads across hetergenous computing systems. JODIS has been demonstrated to run millions of Flame3D tasks simultaneously on a variety of resources and queuing systems. In this paper we report on the impact of JODIS on Flame3D computations, along with our experiences gained and challenges encountered when using heterogeneous computing environments, including the TeraGrid. Using JODIS, we have demonstrated a significant increase in the resolution of Flame3D (from 103 to more than 106 control volumes) and significant reduction in run times (by a factor of over 40 for a large test case of 128 processors and 107 tasks). In general, we conclude that the MTC approach can significantly improve Flame3D computational performance, but that changes need to be made to queuing/job submission systems in order to facilitate the rapid cycles needed for jobs similar to the Flame3D tasks.

### *Design and Implementation of a Rich Internet Application (RIA) for the Simulation of a Combustion Chamber*

***By Mark Patterson, Subrata Bhattacharjee, and Christopher Paolini***

The TEST web portal, www.thermofluids.net, is a comprehensive, freely accessible, thermodynamic courseware that includes a large number of Java applets, each one designed to address state evaluation and mass, energy, entropy, and exergy analysis specific to a particular class of thermodynamic systems. Use of these applets, called daemons, requires sophisticated knowledge of the system being studied. For simulating a steady-state reactor, for instance, the user must balance the reaction in the reaction panel, set up fuel, oxidizer, and products states in the state panel, and import the calculated states in the device panel where the mass, energy, and entropy equations are solved to determine the desired unknown in a well posed problem. An animation of a combustion chamber, on the other hand, can be intuitive even to a beginner. Combining the richness of an advanced programming language such as Java with the visual appeal of an animation can produce a powerful analysis tool for engineering education. A rich internet application, or RIA, has the potential to do just that. The combustion RIA presented in this work is freely accessible from http://www.thermofluids.net (click on RIAs link on the task bar) and is the first of its kind. It has a number of desired features: once the user selects a fuel and the combustion parameters, the RIA calculates reaction stoichiometry, adiabatic flame temperature or heat transfer as appropriate. Moreover, users can select probable species at the exit and a chemical equilibrium calculation in the server results in graphical display of emissions at the chamber exit. As more fuels are added to the Web Service or properties are refined, the RIA does not have to be updated as data is not hard coded in the client application but delivered through Web Services. Using this RIA as an example, the paper intends to establish RIA as an attractive and superior alternative to existing analysis tools for reacting systems for meaningful learning.

### *The Physiological Model of Cystic Fibrosis*

***By Sara Zarei, Ali Mirtar, Forest Rohwer, & Peter Salamon***

Cystic fibrosis (CF) is the most common autosomal recessive disease in Caucasians with a reported incidence of 1 in 2500. It is caused by mutations in the Cystic Fibrosis TransmembraneRegulator (CFTR) ion channel gene. The defective gene causes the body to produce abnormally thick, sticky mucus that mainly affects the lungs, digestive system and even circulatory system of CF patients. CF patients face severe breathing problems, inadequate digestion and absorption of nutrients. They experience intermittent pulmonary exacerbations characterized by dyspnea, cough, sputum production and sinusitis, which result from a build-up of mucus plugs and biofilms. Over time this will cause airway scarring and lung infection and finally respiratory failure of a CF patient. The goal of this paper is to use a physiological model of CF to better understand and control the disease. This model links mucus plug/biofilm formation to lung physiology. In this research we are representing a spatially distributed physiological model that follows the rate of mucus buildup, scarring rate, and scarring threshold for irreversible restructuring. The model is based on the fractal structure of a lung and assumes that the rate of mucus accretion and scarring in an infected bronchiole are constants characteristic of the local microbial community. A preliminary version of this model is used to adjust these constants to mimic the CF patient registry's FEV1 data. FEV1 is a spirometric test that measures the volume exhaled during the first second of a forced expiratory maneuver. We were able to match our predicted results to the observed data. By using this physiological model we will be able to run in silico tests of different treatment regimens (e.g., timing of antibiotic administration, types of antibiotics, steroids, etc).

### *General Curvilinear Environmental System Coupling*

***By Dany De Cecchis, L. A. Drummond, & Jose E. Castillo***

Computer simulations become more realistic as they include interactions between different physical phenomena. The General Curvilinear Ocean Model - Next Generation (GCOM-NG) is a solid-lid ocean numerical model developed in FORTRAN 90 and uses a general curvilinear staggered mesh. The aim is to develop a library in order to provide to the GCOM-NG the capability to interact or couple with other models, components or modules. The library should be user friendly and avoid intrusive code in the models. In our understanding, the mentioned coupling mechanism is defined in a domain overlappedby the two models to be coupled, and some variables or fields are exchanged between models at predefined time intervals (i.e. weak coupling). In addition, the coupling could be with models running sequentially or concurrently. At this stage, preliminary results are shown.

### *Computational Analysis of Vortex Dynamics in One-Component Bose-Einstein Condensates*

***By Eunsil Baik***

Bose-Einstein condensates (BECs) are a quantum state of dilute atomic gases of weakly interacting bosons confined in an external potential and cooled to temperatures near absolute zero. We consider Gross-Pitaeviskii Equation (GPE), which is a variant of the Nonlinear Schoroedinger Equation (NLSE), to describe the dynamics of vortices in one-component BECs. By expressing a solution of the wave function in polar coordinate, an ordinary differential equation (ODE) is obtained, which is a well known vortex amplitude profile. This ODE is solved numerically and we use this numerically solved vortex profile to sit vortices on BECs. In order to solve GPE, we use 2nd order central finite difference scheme for spatial derivation and 4th order Runge-Kutta method to integrate in time. With different external potential, we observe different dynamics of vortices in BECs. With an infinite plane potential with a certain angle, the gradient of the field initiates vortex dynamics and a vortex moves in perpendicular to the gradient of the field. When the plane potential has no angle and have two vortices sitting on BECs, the change of phase and density difference in background initiate vortex dynamics. If they have same charge, they move around in circular motion; whereas, if they have opposite charge, they move in parallel to each other. With a magnetic trap, we use Thomas-Fermi (TF) limit (ie. Large atom number limit) to approximate the background density of the BEC. In this case, the gradient of the field initiates the precession of a vortex orbiting about the center of TF cloud. Our computational analysis observes all different vortex dynamics, and it confirms and supports theoretical analysis that has been done previously.

### *The Cosmological Constant and Compact Stars*

***By Omair Zubairi and Fridolin Weber***

In this research, a stellar structure equation known as the Tolman-Oppenheimer-Volkoff (TOV) equation is introduced in the framework of general relativity that includes the cosmological constant. Starting with Einstein's field equations, a derivation of this equation is made. Due to this additional term, different solutions are obtained by incorporating finite values for the cosmological constant in this equation. Depending on the value of the cosmological constant, stellar properties such as mass and radius may change dramatically. These changes lead to very intriguing results in which a link between compact star formation and stellar collapse in the early Universe maybe established. The result of this study elucidate the effect of the cosmological constant on the possibility and nature of the formation of compact objects in the early Universe.

### *Analysis of a Ring of Coupled Vibratory Gyroscopes*

***By Huy Vu, Antonio Palacios, Visarath In, & Patrick Longhini***

A Coupling Inertial Navigation Sensor (INS) system may proven to be beneficial for performance improvement, especially when the manufacturing yield is very low for meeting the specification requirement of various applications. For instance, navigation grade sensors using the current fabrication process would yield one in every few hundreds which would meet the specification requirement after careful selection process and testing. We propose to couple these sensors by putting together the ``low grade'' sensors in a small array of particular coupling topology to explore their stability properties of known parameter variations produced during the fabrication process. By coupling them in a particular way one may improve the system stability to effect the performance of the INS. Thus in this work we present a Coupled Inertial Navigation Sensor (CINS) system consisting of a ring of vibratory gyroscopes coupled through the driving axis of each individual gyroscope. Numerical simulations show that under certain conditions, which depend mainly on the coupling strength, the dynamics of the individual gyroscopes will synchronize with one another. The summed response of the synchronized state is larger than the output from a single gyroscope, and thus, in principle, it has the potential to enhance sensitivity while minimizing the negative effects of drift rate in an actual CINS device.

### *Global Identification of miR-124 Targets in Ciona Intestinalis*

***By Jerry Chen & Matthew San Pedro***

Our overall project is focused on elucidating the fundamental components of the gene regulatory network (GRN) governing neural differentiation. We are currently studying the microRNA miR-124, a post-transcriptional regulatory molecule that promotes neural differentiation. Using the invertebrate chordate Ciona intestinalis as our model organism, we have computationally identified over 800 putative targets of miR-124, and have also experimentally verified several of our targets using fluorescence assays on whole animals. Next, using bioinformatics tools, we have shown homology of one-fourth of our targets to human miR-124 targets. Finally, we are in the process of using computational gene ontology (GO) analysis to annotate our targets and find overrepresented GO terms relative to the entire ascidian genome. As the closest invertebrate relative to the vertebrate among chordates, Ciona intestinalis is an ideal model organism for understanding the mechanisms governing neural differentiation. In the future, we plan to use ChIP-SEQ to globally identify targets of key transcription factors within the neural GRN. These studies will help us understand neural development and give us insight into the mechanisms behind neural development disorders.

### *Exploring Contractility in Cardiac Myocytes: Current Methods and Future Developments*

***By David Torres Barba, Carlos A. Bazan, & Paul J. Paolini***

We have proposed two computational frameworks for the assessment of contractile responses of enzymatically dissociated adult and neonatal cardiac myocytes. The proposed methodologies are variants of mathematically sound and computationally robust algorithms very well established in the image processing community. The computational pipeline for assessing contractility in adult cardiocytes comprises the following stages: digital video recording of the contracting cell, edge preserving total variation-based image smoothing, segmentation of the smoothed images, contour extraction from the segmented images, shape representation by Fourier descriptors, and contractility assessment. For assessing contractility of neonatal cardiocytes, the stages in the computational framework consist of digital video recording of the contracting cell, signal masking, representation by polar Fourier descriptors, and contractility assessment. The physiologic applications of the methodologies are evaluated by assessing the contractions in isolated adult and neonatal rat cardiocytes. Our results have demonstrated the effectiveness of the proposed approaches in characterizing the contraction process of the cardiocytes. The proposed methods provide a more comprehensive assessment of the myocyte contraction processes, and can be utilized to evaluate changes in contractile behavior resulting from drug intervention, disease modeling, transgeneity, or other common applications to mammalian cardiocytes. We are exploring possible enhancements to our image analysis methodology, the automation of the analysis process and the creation of a comprehensive cardiocyte analysis toolbox.

### *Biomolecular Mechanism of Action of Sansalvamide A-amide and Derivatives*

***By Robert C. Vasko, Rodrigo A. Rodriguez, Christian N. Cunningham, Veronica C. Ardi, Shelli R. McAlpine, & David A. Agard***

Sansalvamide A-amide is a cytotoxic molecule that effects multiple cancer pathways via binding to the N-middle domain of Hsp90. Binding of Sansalvamie A-amide causes an allosteric change in the conformation of Hsp90 which allows the release and activation of two C-terminal pro-apoptotic proteins, whereas N-terminal client proteins are not effected. Furthermore, Sansalvamide A-amide does not have an effect upon the ATPase activity of Hsp90 as does the small molecule 17-AAG, a know Hsp90 inhibitor that is currently in phase II clinical trials for multiple cancers. Put together, this suggests that Sansalvamide A-amide is a useful tool that may be used to study C-terminal interacting client proteins of Hsp90 as well as a potential novel cancer therapeutic.

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