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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 | Duane J. Roth
Chief Operating Officer
CONNECT | Key Note Speaker |

Coffee Break

- | | | |
|----------------|---|---|
| 1:50 pm | Gordon Brown , Moderator
Industry Outreach Coordinator
CSRC / SDSU | Panel of Industry / Academia Representatives
“Academic Preparation Science and Technology
Industries Seek” |
|----------------|---|---|

Robert Mellors
Staff Geoscientist
Department of Geological Sciences
SDSU

Bob Kain
Vice President, Engineering
Illumina, Inc.

Terie Scerbo
Academic Relations
The Learning Center
QUALCOMM, Inc.

Antonio Redondo
Division Leader
Theoretical Chemistry & Molecular
Physics Division
Los Alamos National Laboratory

Eric B. Haas
Senior Scientist/Program Manager
SAIC

Poster Presentation / Reception

- | | | |
|----------------|--|--|
| 4:50 pm | Paul Paolini
Associate Director
CSRC / SDSU | Poster Presentation Awards
&
Closing Remarks |
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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

Director Of Outreach:

Steve Napear

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, Lawrence Livermore 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

Atom Optics And interferometry With Bose-Einstein Condensates

By Martin C. Kandes, Oscar O. Salazar, Charles H. Tally IV, Spencer Williams, and Michael Bromley



One of the present technological challenges in atomic physics is to go orders-of-magnitude beyond the limits of photon-based optics by harnessing the wave-nature of dilute clouds of ultracold atoms. This requires the precision control of both the sub-microKelvin atoms and the sculpturing of magneto-optical fields to trap and manipulate them. We present the results of our computational studies into various aspects of atom optics. These include examining the performance and stability of propagating and colliding Bose-Einstein condensates (BECs) in micron-scale circular waveguides to perform matter-wave interferometry, the harnessing of BEC-based solitons in waveguides, through to the study of photon-matter interactions between BECs and Ince-Gaussian laser beams for the coherent transfer of orbital angular momentum between them for possible use in quantum information and quantum computing type applications.

Linguistic Analysis Of Unknown Metagenomic Sequences

By Victor Seguritan, Anca Segall, Robert Edwards, and Forest Rohwer



A small percentage of genomic and metagenomic sequence data are significantly similar to known sequences by homology. Sequence homology is commonly used to assign a putative function to genes from novel genomes or metagenomes. A recent functional metagenomic profiling of nine biomes, for example, generated approximately 1.4×10^7 microbial and viral sequences from which only 10 are significantly similar to sequences with known functions. A method is needed that assigns putative functions to sequence data which does not rely on sequence homology alone. The origin of this bioinformatic analysis comes from the application of linguistic methods to the analysis of DNA sequences. Linguistic elements, such as syntax, have been modeled in biological sequences data shortly after the discovery of the structure of DNA molecules in 1953. The syntax and semantics of several model proteins will be determined, including major capsid protein, DNA polymerase, and helicase. These proteins are encoded in a large number of phage genomes. The syntax of the model proteins will be represented as Context-Free Grammars (CFG), whereas the semantics of the model proteins will be represented as Latent Dirichlet Allocations (LDA). The CFGs and LDAs of model proteins will be used to identify the presence of sequences that encode model proteins from the unknown metagenomes. In doing so, putative functions may be assigned to unknown metagenomic sequence data in a manner that is similar to understanding the meaning of language through syntax and semantics.

A Multinomial-Dirichlet Model For Analysis Of Competing Hypotheses

By Jonathan Wilson and Kristin Duncan



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Analysis of competing hypothesis, a method for evaluating explanations of observed evidence, is used in numerous fields, including counterterrorism, psychology, and intelligence analysis. We propose a Bayesian extension of the methodology, posing the problem in terms of a multinomial-Dirichlet hierarchical model. The yet-to-be observed true hypothesis is regarded as a multinomial random variable and the evaluation of the evidence is treated as a structured elicitation of a prior distribution on the probabilities of the hypotheses. This model provides the user with measures of uncertainty for the probabilities of the hypotheses. A simple example involving the stadium relocation of the San Diego Chargers is used to illustrate the method. Several extensions of the model are also developed, enabling it to handle special types of evidence, including evidence that is irrelevant to one or more hypotheses, evidence against hypotheses, and evidence that is subject to deception.

ADAPTdb/ADAPT - A Framework For The Analysis Of ARISA Data Sets

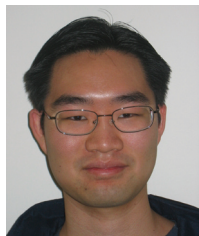
By Robert Schmieder, Matthew Haynes, Forest Rohwer, and Robert Edwards



A goal of microbial community profiling projects is to understand the influence of environmental changes. Here, we present a computational system for the analysis of Automated Ribosomal Intergenic Spacer Analysis (ARISA) data sets. ARISA is a method for analyzing the composition of microbial communities and is both faster and cheaper than other community profiling techniques. ARISA relies on the analysis of intergenic regions called Internal Transcribed Spacers (ITS), which are located between the 16S and 23S rRNA genes. ARISA data analysis steps include profile filtering, data transformation, database search, value calculation, and sample comparison. Previously all data analysis was a manual endeavor. The database ADAPTdb was created to store and maintain ITS regions along with information about their source organisms. The data stored in ADAPTdb is retrieved from different data resources, such as the SEED and NCBI sequence databases. The program ADAPT was developed to taxonomically characterize ARISA data sets using the data in ADAPTdb. The additional organism information for each ITS region in the ADAPTdb database is used by ADAPT for pathogenic and autotrophic/heterotrophic comparisons of organisms among different ARISA samples. The program is publicly available through a user-friendly web interface, which allows onsite analysis of ARISA data sets and computation of the output. The interactive web interface facilitates navigation through the output and export functionality for subsequent analysis.

Data Mining Analysis Of HIV-1 Protease Crystal Structures

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



A data mining study has been done using HIV-1 protease crystal structures complexed with FDA approved HIV-1 protease inhibitor drugs. Quantitative Structure-Activity Relationship (QSAR) descriptors has been computed for the binding pocket of each crystal structure, yielding approximately 500 constitutional, topological, geometric, electrostatic, and quantum mechanical descriptors for each structure. Several supervised (hybrid binary particle swarm optimization/artificial neural network, random forest) and unsupervised learning (Locally Linear Embedding) techniques have been explored for feature selection to determine a QSAR model containing the most relevant descriptors needed to cluster each crystal structure according to their bound ligand. This method of computational modeling and screening process would aid in the understanding of the effect HIV mutations have on the binding affinity of various present and future HIV-1 protease inhibitors due to structural changes arising from the mutations.

Computational Investigation Of The Reaction Thermochemistry And Kinetics Of TTQ Co-factor

By Belynda Sanders, James Hart, Chris Estela, and Andrew Cooksy



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 mechanism for the enzyme activity of methylamine dehydrogenase in converting methylamine to ammonia and formaldehyde, focusing on the activity of the co-factor 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 reaction energies of several reaction steps have been mapped along selected reaction coordinates, and additional reaction steps are currently being probed to determine the minimum energy path. The most stable molecular geometries are calculated at the beginning and end of each step in the reaction, to find the reactant and product energies. Using the program Cosmo-thermx, the COSMO-RS model will then be applied to account for the considerable solvent effects in ion-mediated reaction dynamics. This will allow determination of the influence of pH on the reaction system.

Sansalvamide A Binds To HSP90 And Disrupts IP6K2 Binding

By Robert C. Vasko, Rodrigo A. Rodriguez, Chung-Mao Pan, and Shelli R. McAlpine



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Sansalvamide A is a cytotoxic molecule that works via binding to heat shock protein (HSP90), disrupting a key protein-protein interaction between HSP90 and inositol hexakisphosphate kinase 2 (IP6K2). Hsp90 is an anti-apoptotic protein that is up regulated in a majority of cancers and is responsible for modulating many signal transduction proteins. IP6K2 is in a family of enzymes that generates inositol pyrophosphate 7 (IP7), which mediates apoptosis. Hsp90 binds to IP6K2 in cells preventing it from causing apoptosis. Thus, San A has the ability to bind to Hsp90, allowing the release of active IP6K2, which initiates apoptosis. This makes San A an excellent lead for further development of chemotherapeutics that interact with this novel protein-protein interaction, as well as a lead molecule for further exploration of the ability to disrupt other signal transduction proteins that bind to Hsp90.

Cooling Of Superconducting Strange Stars

By Rodrigo Negreiros and Fridolin Weber



Quarks are the building blocks of protons, neutrons and heavier particles known as Hyperons. In the ultra-high dense environment of neutron stars (up to 20 times more dense than ordinary nuclear matter), these particles might be squeezed together so tightly that they overlap and ultimately melt, forming a new state of matter called strange matter. This state is composed of a mixture of up, down and strange quarks and the stars made up of such matter are known as strange stars. The nature of the interaction of the quarks allows them to form a superconductor, a state characterized by having zero electrical resistance. The thermal characteristic of this superconducting strange matter is drastically different than non-superconducting matter and even more different than ordinary nuclear matter. Because of this, the cooling of superconducting strange stars is unique and might be of key importance to determining whether or not these objects really exist in the universe. In this work we thoroughly investigate the cooling of superconducting strange stars by considering the most sophisticated models which account for all of the thermal properties of such an exotic state of matter. Special attention is paid to the phenomena known as the Meissner effect, in which magnetic field lines are expelled from a superconductor. We will show that the magnetic field in superconducting strange star is trapped in rotationally induced vortices and expelled from the star, depositing some energy on its surface. By taking this into account when simulating the cooling of the stars we obtain a very good agreement with observations of compact objects known as Soft Gamma-Ray Repeaters (SGRs) and Anomalous X-ray Pulsars (AXPs), and thus reconciling the theory of strange stars with observations of compact stars.

Influence Of Spatial Dependence On The Eigenvalue Spectrum Of Complex Networks

By Joris Billen, M. Wilson, A.R.C. Baljon, and A. Rabinovitch



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Many real life networks are known to exhibit a spatial dependence (SD), i.e. the probability to form a link between two nodes in the network, inversely depends on the distance between them. We investigate the influence of SD on the eigenvalue spectrum of networks. By increasing the SD in Erdos Renyi (ER), scalefree, and small-world networks we find that the eigenvalue spectrum becomes asymmetric, as a result of the increased clustering in the system. We quantify this asymmetry by the skewness, kurtosis, and the change in highest and lowest eigenvalues of the spectrum as a function of SD. Our results show that the eigenvalue spectrum can be used as a tool to detect SD in real-life networks. We illustrate this ability for the eigenvalue spectrum of a spatial dependent polymeric gel.

Comparing Load Paths Definitions For Describing Alternate Load Paths In Structures

By Kun S. Marhadi and Satchi Venkataraman



Structural design falls under two broad categories, namely fail-safe design and safe life design. In a safe life design, the structure is designed in such a way that it will not develop any catastrophic damages during its service life. In fail-safe designs, the structure is designed such that the structure is damage tolerant and damage will only grow in a stable and predictable manner. Currently, designing damage tolerant structures are based on known or worst case scenarios. As a result, the structure is only optimum for certain damage conditions, and may be sensitive to other damage scenarios. The probabilistic nature of damages makes designing and optimizing structures for damage tolerance under various unforeseen damages to be computationally challenging.

Redundant structures are often considered to be more damage tolerant because its redundant structural members can create alternate load paths after damage. Thus they can perform their basic function even when their primary load paths are destroyed. The structural mechanics community has developed several methods to identify and visualize load paths in structures. These different methods can provide different results and lead to different interpretations. As a result there is no unified approach to characterize, quantify and visualize load paths. Our work compares the different methods already developed and investigates the effectiveness of these methods to characterize load paths. The goal is to identify suitable methods to identify alternate load paths and their effects on damage tolerance in structures.

Mathematical Modeling Of Cystic Fibrosis Ecology

By Sara Zarei and Peter Salamon



Cystic fibrosis is an inherited chronic disease that affects the lungs, digestive system and even circulatory system of CF patients. Children with Cystic Fibrosis are all born with this disease; they carry a defective gene that cause the body to produce unusually thick, sticky mucus that leads to clogging their lungs and thereby making it susceptible to lung infections. Understanding the CF patient's lung and airway as an ecosystem is a novel and powerful point of view. There are many different microbes in CF lungs that no one has ever cultured and the chronically colonized CF airways represent a complex and diverse ecosystem. Once we understand the CF lung in terms of its community and evolutionary ecology, we can then better understand the disease progression and the influence of different treatments on CF patients. Approaching the CF chronic airway infection as a community that follows specific ecological principles will allow us to find out whether there are better times to introduce specific antibiotics or whether this therapy should be cycled and if so at what periods should such cycling occur?

A complete mathematical model of CF would need equations that follow the concentrations of all different kinds of bacterial and phage species in each compartment. That means we should have different equations that can represent all different microorganisms that can be found in CF patient's lungs, airways, intestine as well as circulatory system and pancreas. This type of encyclopedic model is impossible to build in one go, therefore we can start with simple models that only look at one phage-host interaction. The choice of good model requires finding the important controlling variables in the set of equations. As part of our modeling efforts, we expect to figure out which variables are the most important using the metagenomic data currently being prepared by San Diego State University Phage group. Metagenomic methods collect and analyze genetic material recovered directly from environmental samples.

By surveying literature about predator-prey models of Phage-host interactions we found a number of papers that present mathematical models of phage-bacterial interaction. In the absence of abundant data from CF patients, these models are the only possible models that we can implement and analyze. In addition we need to consider the fact that none of these already formulated models were formulated specifically for the Cystic fibrosis ecosystem but instead were all intended to model different microbiomes.

Experiences Using The Pylons Web Framework For Science Gateways

By Sudhir Balasubramanian, Naveen Kumar Reddy Nandipati, and Mary Thomas



Science portals and gateways can be built using a variety of tools ranging from very elementary customized tools to existing frameworks that bring both greater capabilities (authentication, account management, interfaces, logging etc) and more complexity (resulting in long learning curves and complex code bases). For gateways, it is important to identify frameworks that can be easily adapted to the specialized environments needed for accessing the required cyberinfrastructure. In this paper we present our experiences in developing a prototype gateway for the General Coastal Ocean Model (GCOM) using the Pylons Web Framework and other Python tools including pyWSRF (python-Web Services-Resource Framework) and pyGlobus based web services, SciPy, and various Google code tools. We have found that the Pylons framework, which utilizes the WSGI (WS-Gateway Interface), is easy to use and learn, is very flexible and has the ability to dynamically reload services without restarting the server, which dramatically reduces development and testing time. Additionally, Pylons components can be published as services, widgets and gadgets, and desktop applications.

Evolution Of Spatial Structures In The Dynamics That Produce Epidemics Of Severe Dengue Across Thailand *By Karen M Campbell*



Dengue epidemics in Thailand are often considered to arise from dynamics that are focal in nature as indicated by local outbreaks linked with neighborhood schools or homes in Thai villages. Outbreaks separated by only a few kilometers are often associated with different dengue serotypes and therefore separate transmission networks. However, 264-month long incidence time series analyzed for the 72 Thai provinces indicate that local transmission dynamics are part of a much broader evolving regional pattern in the dynamics that regulate the recurrence of epidemics. Multi-year periodic cycles in incidence of dengue hemorrhagic fever were found to evolve systematically in space and time over 2 decades. The changing periodicity in incidence reveals spatial structures in the dynamics that generate dengue epidemics. Population dynamics indicate that the age of infected individuals is transitioning from young children to adults. The force of transmission as indicated by estimates of the basic reproductive rate for dengue was found to exhibit a 3-fold variation geographically. The dynamics of serotype mixing are systematically regulated by population and transmission dynamics and are not homogeneous across Thailand. The dynamics of dengue transmission in Thailand are systematically changing.

Biomimetic Design Of A Flexible Airfoil

By Joseph Marrocco, Satchi Venkataraman, and Luciano Demasi



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The practical application of relatively small, light weight micro air vehicles by biomimicry is of great interest to the engineering community. Innovative and interesting approaches to solving this problem are currently being addressed. However, the goal of this research is to investigate if flexible wing joints in an airfoil improve the flight capabilities and maneuverability of dragonfly wings. 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. As well as achieve an assortment of different flight patterns such as gliding, synchronized-stroking, phased-stroking, and the very efficient counter-stroking. The wing's basic design is a pleated membrane stiffened by tubes at the apices of the pleats, forming a particularly rigid and strong structure. This tubular pleated membrane, responds similarly whether loaded from above or below, deforming with the increase in horizontal or vertical forces. Unlike many man made airfoils which are designed to resist all aerodynamic forces they encounter, dragonfly wings have developed to yield briefly, without damage, and to recover immediately. These ultra light flexible airfoils perform all of these roles extremely well, despite the fact that they are largely passive flight structures. The dragonfly wing's innate ability to deform is generated by an elastomeric protein. It is located in specialized regions of the cuticle that require flexibility. It is these flexible regions or joints that have become a particular interest to this study. As part of this work, a computational method will be used to mimic the flexible wing design of a dragonfly. A general purpose finite element program is used to model the flexible wing joints in a standard airfoil design, under externally applied loading. In combining span wise rigidity under normal conditions with the ability of yielding reversibly under excessive loads, the pleated, and veined wings of Dragonflies demonstrate an elegant solution to insects' requirements for stiff, durable, ultra-light aerofoil for high-performance flapping flight.

DCT: Distributed Coupling Toolkit To Couple Multi-Resolution Models

By Dany De Cecchis, Leroy A. Drummond, and Jose Castillo



Due the increase of the capabilities of the high performance computing, it is possible to formulate and handle more complex physical models. Enabling very high resolution model runs improves the physical phenomena approximation, and our ability to study interactions between different physical processes at different scales. The DCT is an user friendly coupling library that promotes a purely distributed computational environment, which can easily scale both the model complexity and number of processing elements.

Changes In Calcium Pathway Gene Product Levels Caused By Rosiglitazone Treatment In Neonatal And Adult Rat Isolated Cardiocytes

By Kirubel Gebresenbet and Paul Paolini



Cardiovascular failure is the number one risk factor in diabetes and the leading cause of death among diabetics. Earlier studies have shown that, rosiglitazone (Avandia®, GlaxoSmithKline), a widely prescribed anti-diabetic drug, can improve heart performance. Recent studies reported the uncertainty of the drug's effect (Diamond et al., Ann. Int. Med. 147, 2007). To further investigate the underlying cellular basis for heart failure, we have analyzed the metabolic pathways involved in calcium signaling in the heart cell, and their links to gene expression. Studies using microarray analysis of the rat genome due to rosiglitazone effects over a 48 hour period on calcium regulation in rat ventricular myocytes during excitation-contraction calcium transient decay rates and SERCA2 gene expression level showed that this drug makes contraction of the cardiomyocytes faster and stronger (Shah et al. Cell. Physiol. Biochem. 15: 41-50; 2004).

Primary ventricular cardiomyocytes were harvested from neonatal or from adult rats and plated out in culture media. The RNA of the cells was extracted, purified, and hybridized with cDNA probes. An initial list of about 10,000 genes was reduced to a manageable set of a few important genes involving the calcium signaling pathways at tested time intervals (1, 2, 24 and 48 hours).

We have used RT-PCR and western blot analysis to validate results from the microarray study. Western blot analysis for the SR SERCA pump (Atp2a3), ryanodine (Ryr2) and NCX (Slc8a) genes to demonstrate up-regulation of these genes as the source of enhanced contractility accompanying rosiglitazone treatment. The current study focuses on the correlation and validation of the microarray and quantitative PCR RNA expression levels with protein product levels. Neonatal and adult cardiomyocytes treated with antibodies for the SERCA 2 calcium-ATPase, the ryanodine channel, and the sodium-calcium exchanger, NCX, have been analyzed to see which genes are turned on and off in response to rosiglitazone treatment time points (1, 2, 4, 24, and 48 hours).

Sintering With COMSOL

By Cristina Garcia Cardona, Mohammad Abouali, Sajia Akhter, and Brent Runyan



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Sintering is a methodology where the fluid-like behavior of powders is exploited to build arbitrarily complex shapes. A piece molded from powders is subjected to a firing process that leads to its densification and strengthening, but also causes volume shrinkage and deformation. In order to control the production of the part, it is necessary to be able to predict the final shape given an initial configuration. This can be

accomplished through a simulation of the physical phenomena associated with sintering. This poster describes the utilization of COMSOL, a software based on Finite Element Methods, to study the changes occurring to a specimen while being sintered.

Regulation Of Gene Expression By The microRNA miR-124 In The Developing Nervous System Of Ciona Intestinalis

By Jerry Chen and Robert Zeller



Small regulatory molecules called microRNAs are vital to normal tissue differentiation and development. Using the ascidian *Ciona intestinalis* as a model organism, we wish to study the role of microRNAs in the differentiation and development of neurons. Ascidians, more commonly known as seasquirts, are invertebrate marine animals that have a simple nervous system ideal for studying the physiology of neuronal development. Our lab has begun identifying the network of genes and transcription factors involved in neuronal differentiation in *C. intestinalis*. My work will involve identifying and elucidating the role of specific microRNAs within this regulatory network. Specifically, I will be focusing on genes immediately downstream of miR-124, which has been shown to promote the expression of pro-neural genes in other organisms by de-activating relevant gene repressors. miR-124, which is expressed in the human nervous system as well, may be a major player in the regulatory network controlling the differentiation of a cell into a neuron. My studies will hopefully give us some insight into the molecular basis of neural developmental disorders.

Deviation Of Amino Acid Utilization And Correlation With G C Composition In Bacterial Genome

By Sajia Akhter, Barbara Bailey, Peter Salamon, and Robert Edwards



Amino acid content in a genome may reflect lifestyle restrictions of an organism and may also be predictive of coding potential. To compare the amino acid composition for each of the complete bacterial genome sequences Kullback-Leibler divergence was calculated from the mean amino acid content as a measure of how much each genome deviates from the standard. We demonstrate that (i) there is a significant difference between amino acid utilization in different phylogenetic groups of bacteria; (ii) the bacteria with the most skewed amino acid utilization profile are endosymbionts or intracellular pathogens; (iii) the skews are not restricted to one or a few metabolic processes but are common across all genomic subsystems; (iv) the amino acid utilization profiles strongly correlate with the genomes percent G C composition even for different subsystems (except secondary metabolism). (v) Using genomes percent G C composition, a better prediction for amino acid utilization in bacterial genome is possible.

Microbial Complexity In Dental Specimens of Patients With Periodontal Disease: A Pyrosequencing And Phylogenetic Approach

By Lena D. van der Stap, Sergey Gazarov, Scott T. Kelley, and Roberta A. Gottlieb



Periodontal disease (PD) is associated with risk of a number of systemic diseases - including atherosclerosis in adults. However, younger individuals who do not have heart disease can still show signs of reduced endothelial function that could be due to PD. The central hypothesis of this study is that clinical intervention by treating PD will normal-

ize vascular endothelial function. To test this hypothesis: 1) We will determine the relationship between gum disease and heart disease in adults with PD by determining if they show early signs of endothelial dysfunction. The immunological profile (level of antibodies to virulence factors associated with bacteria in PD) will be determined using a saliva based diagnostic test. 2) We will characterize the oral microbial community in dental specimens and draw a correlation with vascular dysfunction. Preliminary Results: Dental calculus samples from 10 individuals with gum disease were analyzed for bacterial diversity following 16S rDNA isolation and subsequent 454 pyrosequencing (Roche). Analysis of this level of microbial complexity requires simultaneous detection of species followed by multivariate statistics. A total of 492 unique bacterial species were detected in the samples. Species richness varied from patient to patient. Overall, types of bacteria did not correlate with the level of immune response. Common aerobes Streptococcus and Neisseriales (associated with endocarditis), anaerobes Capnocytophaga, Porphyromonas, and Prevotellaceae, as well as Campylobacteraceae, Filifactor alocis, Propionibacterium, TM7-3, Suttonella ornithocola, and Actinobacterida, known to be linked to PD, were present in all or most samples. Patients with the most severe gum disease reflected by high salivary antibodies were distinguished by absence of Fusobacterium. Future studies will determine the association between types of bacteria found in patients with PD and those in patients who show signs of atherosclerosis. This association could point towards the etiology of vascular dysfunction. In the future, viruses and bacteria found in patients with both PD and vascular dysfunction will confirm the hypothesized specific disease-associated species.

Full Three-Dimensional General Curvilinear Ocean Model

By Mohammad Abouali, Carlos Torres, Rafael Walls, German Larrazabal, Malgorzata Stramska, Dany De Cecchis, and Jose Castillo



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General Curvilinear Ocean Model (GCOM) is a full threedimensional curvilinear coastal ocean model developed by Carlos Torres Et Al over the last 10 years., which uses a direct numerical simulation (DNS) approach to solve the primitiv Navier-Stoke's equations for the ocean.

GCOM uses boundary fitted/Curvilinear coordinate; therefore, it is possible to use GCOM in various topography and meshes. GCOM will be coupled with full thermo dynamical sets of equation. GCOM is going to be designed in a modular fashion, which makes it able to easily be connected to other biological model to study different phenomenon, such as red tides. Furthermore, in a separate project an Atmosphere-Ocean Interaction model is developed, which will be coupled later to GCOM.

Existence Of Steady State Bright Vortex Solutions To The Cubic-Quintic Nonlinear Schrodinger Equation

By Ronald Caplan and Ricardo Carretero



We study the existence of steady state bright vortex solutions to the Cubic-Quintic Nonlinear Schrodinger Equation. Through asymptotic assumptions and a variational approach, we derive different analytical descriptions of the vortex profiles. We then describe a numerical nonlinear optimization scheme which we use to refine our analytic profiles into numerically-ex-

act solutions. Our main result is that we show that the previously held existence region (parameterized by the wavefunction's complex frequency) for the vortex profiles is incorrect, and in fact, it is equivalent to its one dimensional counterpart. This has relevance to the azimuthal modulational stability regions of the vortices, and could imply that stable vortices of higher charge (previously thought not to exist) do in fact exist.

Hopping Behavior And Effects Of Noise In Cellular Pattern-Forming Systems

By Joan Manuel Martinez, Peter Blomgren, and Antonio Palacios



We study the effects of multiplicative noise on a spatio-temporal pattern-forming nonlinear Partial Differential Equation (PDE) model for premixed flame instability, known as the Kuramoto-Sivashinsky equation, in a circular domain. Modifications of a previously developed numerical integration scheme allow for longer time integration in

the presence of noise. In order to gain additional insight, we focus on a region of parameter space where hopping patterns of the deterministic system arise as well as the region of parameter space where the transition between a single ring to multiple rings of cells appears. We discuss the numerical challenges in the integration of the Kuramoto-Sivashinsky equation in polar coordinates with the addition of the noise term. We also study the effects of additive and multiplicative noise on the normal forms or amplitude equations that describe the dynamics of hopping patterns. Finally we show some results of the implementation of the numerical scheme to solve both the PDE and the normal form equations and discuss preliminary findings.

Effect Of Die Shape On Spark Plasma Sintering Of Alumina By Evan Khaleghi



Spark Plasma Sintering (SPS) is becoming a widely used process for sintering (the consolidation of powder into solid material through the application of heat) research that relies on heating powder specimens with electric current, instead of an external heating source. The advantages of the SPS method are faster heating rates, shorter holding times, and denser final materials.

Most of the current research in Spark Plasma Sintering uses a cylindrical die, with the specimen powder placed in the hollow center of the die, surrounded by punches on the top and bottom. Most of the industrial applications of sintering, however, require dies with complex shapes to produce parts, and rarely is a final product in the shape of a perfect cylinder.

To study the effects that complex shapes, and shape anisotropy, would have on SPS. We created a nearly square, non-cylindrical die to study these effects. To enhance these effects for study, we used a square die with a 15 mm side length for the specimen (30 mm outer side length) which allowed for a standard 15 mm circle to be inscribed inside the square, corresponding to a cylindrical die with a 15 mm inner diameter for the specimen. This layout would allow us to see what variations in sintering, based on final density and density distribution, occurred in the central area of the square (where the inscribed circle lies), and the corner areas (outside the inscribed circle).

Conducting many experiments with this setup has led us to conclude that the square specimen shows significant changes in density, compared to the circular specimen. Besides the density issues related to anisotropy, the grain size and grain growth are also completely different between the two shapes. Our modeling work has predicted that these discrepancies, and confirmed their location.

Simulating Performance In Baseball By Daniel Herrlin



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In this poster I will examine and attempt to predict future performance among professional baseball players. Motivation for this project stemmed from fantasy baseball, but it is fairly clear that if an accurate model can be established the results would be useful far beyond the fantasy baseball metric. A markov chain monte carlo approach to baseball production simulation will be used to predict future performance among baseball players. Bayesian updating will be used with a quadratic growth curve model in order to use prior statistics along with team data in order to predict future performance.

Structure Enhancement Diffusion And Contour Extraction For Electron Tomography Of Mitochondria

By Carlos Bazan, Michelle Miller, and Peter Blomgren



The interpretation and measurement of the architectural organization of mitochondria depend heavily upon the availability of good software tools for filtering, segmenting, extracting, measuring, and classifying the features of interest. Images of mitochondria contain many flow-like patterns and they are usually corrupted by large amounts of noise.

Thus, it is necessary to enhance them by denoising and closing interrupted structures. We introduce a new approach based on anisotropic nonlinear diffusion and bilateral filtering for electron tomography of mitochondria. It allows noise removal and structure closure at certain scales, while preserving both the orientation and magnitude of discontinuities without the need for threshold switches. This technique facilitates image enhancement for subsequent segmentation, contour extraction, and improved visualization of the complex and intricate mitochondrial morphology. We perform the extraction of the structure-defining contours by employing a variational level set formulation. The propagating front for this approach is an approximate signed distance function which does not require expensive re-initialization. The behavior of the combined approach is tested for visualizing the structure of a HeLa cell mitochondrion and the results we obtain are very promising.

Phase Separation And Dynamics Of Two-Component Bose-Einstein Condensate

By Rafael Navarro and Ricardo Carretero



We study the interactions between two atomic species in a binary Bose-Einstein Condensate to determine conditions for miscibility, oscillations between species, steady state solution and their stability. A variational approach is developed for a quasi one-dimensional, two-atomic species, Bose-Einstein Condensate.

Using a Gaussian ansatz, equations of motion are obtained for the parameters of the system: amplitude, width, position, phase, wave number and chirp. The dynamics reduce to a simple classical Newtonian system where components oscillate at a frequency that depends on the harmonic trap strength and on the inter species coupling parameter. The steady-state solution of the reduced system is used to analyze the variation of the ansatz as a function of the interspecies coupling parameter. Using the parameter that describes the position the each species, it is possible to develop an analytical condition for miscibility that can be interpreted as a phase diagram that depends on the harmonic trap's strength and on the interspecies species coupling parameter. Finally, phase separated states at small values of harmonic trap strength yields the existence of unstable excited states containing alternating bands of atomic density of the first and second species. Results are compared to direct integration of the Gross-Pitaevski equation for each component.

A SOA For Distributing Science Applications Via Cyberinfrastructure

By Carny Cheng, Rob Edwards, Chris Paolini, and Mary Thomas



This research project explores a framework that allows distribution of single-threaded embarrassingly parallel applications on cloud, cluster, grid computing resources such as the NSF Teragrid and Nimbus projects. This framework provides the user a programmable web service interface based on standard SOAP protocols. Due to the increasing complexity and density of modern real-world simulations, this is an essential tool in maximizing the utility of cyberinfrastructure resources and minimizing application run time. In addition to developing a framework, we analyze the performance of our framework on the cyberinfrastructure resources mentioned above using three scientific applications -- the CHEQS chemical equilibrium application, the General Curvilinear Ocean Model (GCOM), and the Open Life Science Gateway (OLSGW). Experimental results demonstrate that our application framework noticeably improves the performance of our existing test applications.

A Free Energy Model For The Observed Morphologies Of The Crista Membrane Of Mitochondria

By Mariam Ghochani



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Electron tomograms have revealed that in normal mitochondria the crista membrane contains both flat lamellar and tubular components that are connected to inner boundary membrane through crista junctions. The entire matrix space is connected and interacting resulting in regular functions of mitochondria. We are investigating if this morphology can be obtained by minimizing the free energy of the configuration to obtain the thermodynamic state of mitochondria. To use the free energy model a set of geometric measurements from the structural features of mitochondria is obtained. Structural features are measured from 3-D electron tomograms of mitochondria each consisting of a stack of two-dimensional images of constant z . These image stack files are obtained by doing electron tomography on a 300nm-section of mitochondria, aligning the projection images of the tilt series to a common origin, and applying a filtered backprojection algorithm to the aligned tilt series. From the measured structural features, measurements of other features of cristae membranes are extrapolated computationally. The measurements are also evaluated by comparing the tomogram with the 3-D model obtained by segmenting the tomogram. Geometric measurements predict relations between crista junction radius versus tubular lengths and lamellar radius versus number of tubes that can be explained by linear fits to describe the geometric constraints within structure of normal mitochondria. Free energy model combined with geometric measurements

predicts that tubular structures are stabilized by tensile forces of 10-20 pN, comparable to those typical of motor proteins. It also reasonably predicts the pressure differences of 0.01-0.1 atm across crista membrane and surface tensions of less than 0.2 pN/nm. This work was performed in collaboration with A. Rabinovitch, T. Frey, J. Nulton, P. Salamon and A. Baljon.

Implementing Low Density Parity Check Code Decoders

By Raymond Moberly and Michael O'Sullivan



Low Density Parity Check (LDPC) decoding using the iterative sum-product algorithm can be achieved in programmable logic implementations (e.g. Field Programmable Gate Arrays (FPGA) at performance rates that outperform software-based decoders. Research among LDPC experts has shown that greater block length LDPC codes achieve better bit error rates (BER) at comparable signal to noise ratios (SNR). Software-based decoder implementations retain the most flexibility and can accommodate these necessary block lengths. A hardware / software codesign achieves the combination of hardware speed and software flexibility for the decoder system. A processor-enhanced FPGA offers a single chip solution for an implementation composed of hardware and software, allowing for tight coupling of the hardware and software pieces of the partitioned design, minimizing the overhead as probabilistic data is conveyed between the software and the hardware-based coprocessor.

Modeling The Meso-Scale Evolution Of Anisotropic Materials During Sintering

By Gordon R. Brown, Richard Levine, and Eugene Olevsky



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 material properties. Computer simulation models have been used to gain insight into phenomena associated with sintering. One of the more popular simulations is a two-dimensional Potts MC model. This research modifies the existing algorithms to simulate the evolution of granular structure with anisotropic materials. Limitations of this algorithm imposed by the underlying lattice structure are identified and analyzed. Solutions to mitigate these artifacts are proposed and implemented. Results are discussed and evaluated. The ability to incorporate anisotropic grain growth in meso-scale modeling allows the investigation of anisotropic granular development under several different situations to better understand some of the observed anisotropic phenomena.

Measuring Contractility In Cardiocytes

By David Torres Barba and Paul Paolini



We developed a convenient method for measuring contractile responses of both adult and neonatal mammalian cardiocytes. Methods of quantifying neonatal cell contraction reported in the literature have required the use of elaborate methods such as a proximity detector or an atomic force microscope (measure the increase in cell elevation as cardiocyte contracts), and typically interfere with simultaneous optical recording of cell signals such as the calcium transient that can be recorded using calcium-sensitive dyes like Fluo-3. Our new approach to contractile measurement was developed with the intention to be a practical and relatively inexpensive method. In this method, digital video images are obtained using a CCD camera mounted on an inverted phase contrast microscope. Our method uses two different image processing sequences that allow us to record the contractility of both adult and neonatal cardiocytes. In the case of the neonatal myocytes the analysis focuses on intracellular fine structure details, specifically by monitoring the area of small inclusions within the cell thought to be a result of the presence of protomyofibrils. Our other application using Matlab's Image Processing Toolbox allows measurement of the adult cardiocyte's area in each frame. Adult cardiac cell's contractility can be measured by tracking the cell's shortening, or the shortening of individual sarcomeres, the engines' of shortening and force development within the cell (Rieser et al., 1979). Application of our two dimensional quantification technique to the study of adult cardiocytes produces contraction vs. time records virtually identical in time course and shape of records obtained by traditional one dimensional, cell boundary tracking procedures (Rieser et al., 1979). The contractility graphs created by the two methods are consistent with the expected results and graphs resulting from historical studies performed on myocytes (Katz, 2001). This new practical approach to contractile quantification will be helpful in the analysis of the myocyte contractile dynamics in the presence of drugs.

Sharp Biological Materials

By Yen-Shan Lin



Teeth represent an important natural mineral tissue composed of collagen fibrils and carbonate apatite mineral. Structure and mechanical properties of teeth of a broad range of species including shark, piranha, alligator, and hippo are investigated. Hardness test results are compared and show similar hardness values in different living species. The hardness of the enamel ranges from 1.2 to 1.7 GPa and the hardness of the dentin is about 0.2-0.5 GPa. Serrations are observed through SEM analysis for piranha and great white shark teeth with serration sizes of $25\frac{1}{4}\mu\text{m}$ and $300\frac{1}{4}\mu\text{m}$, respectively. The conducted analysis indicates that serrations are used to optimize the biting mechanism.

Mimetic Approximations On Non-Uniform Meshes

By Elbano David Batista and Jose Castillo



Mimetic operators or summation-by-part operators are approximations that satisfy discrete versions of continuum conservation laws. In 2003 J.E. Castillo and R.D. Grone developed a way of constructing high order gradient and divergence approximations with mimetic properties for one dimensional problems on uniform grids. The main attribute of Castillo-Grone operators are that they preserve symmetry properties of the continuum, they have an overall high order accuracy, and no numerical artifacts such as ghost points or extended grids are used in their formulation. In this work we show a generalization of Castillo-Grone schemes for non-uniform, one and two dimensional meshes. The technique is based on the application of local transformations and the new operators preserve the valuable attributes of the original uniform ones. We used the non-uniform mimetic operators to solve boundary-layer like problems on non-uniform meshes. Numerical results show that the implementation of the new schemes along with adaptive meshes maintains the same order of accuracy as the Castillo-Grone uniform operators, while decreasing the convergence-rate constant.

Towards A Parallelization Of The General Curvilinear Ocean Model (GCOM)

By Mary Thomas and Jose Castillo



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The General Curvilinear Ocean Model (GCOM) solves 3-D, time-dependent, curvilinear flow equations to simulate stratified flows over uneven terrains and coastal regions [1] [2]. GCOM differs significantly from traditional approaches, where the use of Cartesian coordinates forces the model to simulate terrain as a series of steps. It uses an adaptable, curvilinear grid in all 3 dimensions, and can handle both orthogonal and non-orthogonal grids. The resulting model equations are more complex than the original Cartesian ones, but the advantage is that the boundary conditions are easier to implement. Additionally, there is a one-to-one mapping between the grid points and the computational matrix, and the grid generation technique allows grid points to be clustered in any region of the computational domain. The benefits of this approach include a more efficient algorithm and increased resolution [3]. The sequential, F77-based GCOM model has been validated for several types of water bodies, different coastlines and bottom shapes, and new models are being incorporated (e.g. biogeochemical, pollution). In this paper, enhancements to the GCOM model are presented, including: migration from F77 to F90; approach to a component design; initial steps towards parallelization of the model; and development prototype system for the GCOM science gateway project [4].

Gene Expression Profiling Of Neonatal Rat Cardiomyocytes In Response To Rosiglitazone

By Daniel Pick, Paul Paolini, Denise Buenrostro, Elliot Kleiman, Chao-Jen Wong, David Torres Barba, and Frank Gonzales



A time course study of differentially expressed genes in neonatal rat ventricular myocytes responding to Rosiglitazone was performed. 21,910 genes were interrogated using the RatRef-12 BeadChip™ from Illumina, Inc. to identify the statistically significant differentially expressed genes and signaling pathways, and discover whether the drug has any significant effect on the contractile response of heart cells. Recent reports regarding a possible link between the use of the drug rosiglitazone and incidence of cardiovascular death from heart failure and myocardial infarction has created a controversy regarding this drug's safety. A number of recent and ongoing clinical data studies indicate that the link is not statistically significant (Diamond et al., Ann. Int. Med. 147, 2007). However, earlier studies from our laboratory have demonstrated a significant effect of the drug by way of the short-term calcium

signaling pathway (Shah et al. Cell. Physiol. Biochem. 15: 41-50; 2004). Our preliminary results have identified 37 differentially expressed genes under the drug treatment, and show that mono-carboxylic acid, fatty acid, lipid, and cellular lipid metabolic processes are overrepresented. Out of the 37 genes found, there was no gene detected with sufficiently high expression that was directly involved in the calcium signaling pathway. Further work to identify gene regulatory networks from time course expression data will provide a global view of transcriptional network of heart cell responses to rosiglitazone, which may also demonstrate any connection between the drug and heart failure.

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