Fifth Annual

ACSESS

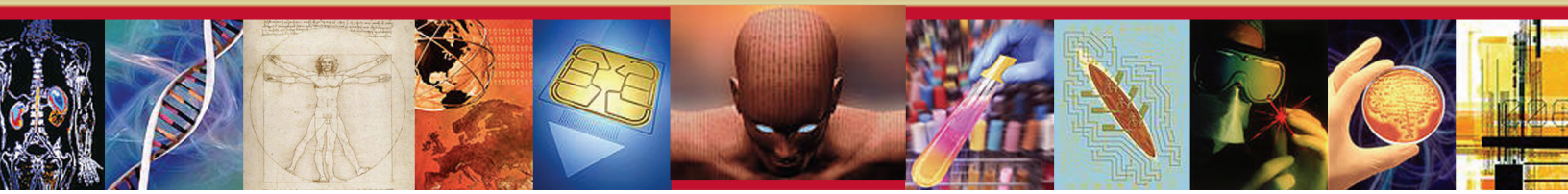
For Applied Computational Science and Engineering

&

Computational Science Curriculum Development

Monday, March 3, 2008
12:00 pm - 5:00 pm
SDSU Montezuma Hall

Program



12:00 pm		**Registration / Buffet Lunch**
1:00 pm	**Nancy A. Marlin**, Provost Division of Academic Affairs, SDSU	Welcome / Opening Remarks
1:10 pm	**Jose E. Castillo**, Director Computational Science Research Center, SDSU	Computational Science at SDSU and ACSESS Program
1:20 pm	**Michael Rondelli,** Director Technology Transfer Office SDSU Research Foundation	Working Together: Successful Collaboration Between SDSU and Industry
1:40 pm		**Coffee Break**
1:50 pm	**Gordon Brown**, Moderator CSRC Industry Outreach Coordinator, SDSU	**Panel of Industry / Academia Representatives**, "Academic Training for a Productive Workforce"
	Tyrone L. Hardy, President Medical Instrumentation and Diagnostics Corp.	**Charles Hoelzer**, Geoscience Technology ExxonMobil Corp.
	Robert Mellors, Staff Geoscientist Department of Geological Sciences, SDSU	**John M. Newsam**, President and Managing Director fqubed, Inc.
	Juan Meza, Department Head High Performance Computing Research, Lawrence Berkeley National Laboratory	**Victor Pereyra**, Chair, CSRC Industry Advisory Board Weidlinger Associates Inc., ACSESS Partner
3:00 pm		**Poster Presentation / Reception**
4:50 pm	**Paul Paolini**, Associate Director Computational Science Research Center, SDSU	Closing Remarls
5:00 pm		**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

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

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Jose E. Castillo

Director Of Outreach:
Steve Napear

Industry Projects Coordinator:
Gordon Brown

Associate Directors:
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Victor Pereyra, Wedlinger Associates

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Chair: Victor Pereyra, Wedlinger Associates

Richard Greenblatt, Source Signal Imaging Inc.

John Newsam, fqubed, Inc.(a Nuvo Research company)

Antonio Redondo, T12 Division, Los Alamos National Laboratory

Three-Dimensional Modeling of Receiver Functions in the Peninsular Ranges and Gulf Extensional Province

By Christopher Lynch

Broadband teleseismic data is used to obtain estimates of crustal thickness in southern California and northern Baja California [e.g. Ichinose et al., 1996; Zhu and Kanamori, 1999; Lewis et al., 2000, 2001]. Data recorded at individual seismic stations from earthquakes at teleseismic distances are analyzed using the receiver function method to estimate the depth to the Moho in the vicinity of each station [e.g., Langston, 1979; Owens et al., 1984; Ammon et al., 1990]. The receiver function method provides point estimates of Moho depth [Zhu and Kanamori, 1999]. Knowledge of crustal structure is critical for estimating seismic hazards, and for understanding the dynamic processes that shape the Earth. Most conventional receiver function modeling assumes a flat planar Moho and does not include effects due to 3D structure. A 3D, finite difference, staggered-grid, elastodynamic seismic wave propagation code [e.g. Graves, 1996] is being used to investigate the effect of 3D structure on receiver functions. This code has been modified to produce a plane wave that is obliquely incident on various material interfaces and the free surface. Further insight regarding the use of teleseismic data to estimate crustal structure can be obtained by generating synthetic seismograms for different 3D models. Synthetic seismograms have been produced for various 3D geometries representing the Moho structure underlying northern Baja California, (Baja California Norte, Mexico). The ratio of SH, SV and P waves generated by P waves at oblique incidence on a geometrically complex solid-solid material interface will also be investigated. The synthetic seismograms generated are being used to generate receiver functions which can then be used to help constrain crustal structure in the Peninsular Ranges and Gulf Extensional Province.

Mitochondria Stereology by Way of Maximum-Likelihood Method

By Daniel Flynn, Arlette Baljon, James Nulton, Peter Salamon

When the mitochondrial network within the cell is in a fragmented state, it resembles a spatial distribution of prolate spheroids of various shapes, sizes and orientations. The cell is studied by making electron micrographs which amount to a series of planar slices through that spatial distribution. These micrographs exhibit sections of individual mitochondria, which have roughly elliptical shape. This paper uses a maximum-likelihood scheme to infer the distribution of spheroidal shapes, sizes and orientations from the observed distribution of elliptical sections.

Investigation of the Limiting Energy Density of Compact Stars

By Oliver Hamil, Fridolin Weber

This research is an attempt to find the limiting energy density for compact stars using a variational ansatz for the unknown equation of state of ultra-dense nuclear matter. The Harrison Wheeler/Negele-Vautherine equation of state is used for the outer/inner crust regime of compact stars up to nuclear density, and is assumed to be the valid equation of state for this region. Beyond nuclear density, the equation of state is almost completely unknown and is thus created using a variation ansatz. The equations of state generated from this ansatz are constrained by causality (in the high pressure regime), and microscopic stability (Le Chatelier's principle). We also assume that Einstein's theory of General Relativity is the correct theory of gravity. The equations of state generated from the variational ansatz are used to generate stellar sequences of compact stars in order to investigate energy density limits for stars of given masses. From this data, conclusions can be drawn about phase transition regions within compact stars at certain densities. Also, knowing the mass limit for compact stars is of key importance for estimating the number of low-mass black holes in Galaxies.

LDPC Decoder with a Limited-Precision FPGA-based Floating-Point Multiplication Coprocessor

By Raymond Moberly, Michael O'Sullivan, Khurram Waheed

An Implementation of the sum-product algorithm in an FPGA considers tradeoffs between computational precision and computational speed. The probabilistic algorithm is used for iterative soft-decision decoding of LDPC codes. Our FPGA-based coprocessor (design) performs computer algebra with significantly less precision than the standard (e.g. integer, floating-point) operations of general purpose processors with comparable iterative convergence. Using synthesis, targeting a 3,168 LUT Xilinx FPGA, we show that key components of a decoder are feasible and that the full single-precision decoder could be constructed using a larger part. Soft-decision decoding by the iterative belief propagation algorithm is impacted both positively and negatively by a reduction in the precision of the computation. Reducing precision reduces the coding gain, but the limited-precision computation can operate faster. A proposed solution offers custom logic to perform computations with less precision, yet uses the floating-point format to interface with the software. Simulation results show the achievable coding gain. Synthesis results help theorize the full capacity and performance of an FPGA-based coprocessor.

Practices in Seismic Modeling for Oil Exploration

By German Larrazabal

In this work, we present some practices in seismic modeling for oil exploration. We have developed a computational tool for 3D synthetic modeling, 3D ray tracing, 2D acoustic wave propagation and 2D depth migration based on reverse time migration technique. The 3D modeling includes creation of the terrain, interface, topography, elastic properties, etc. The ray tracing module has implemented two ray tracing algorithms based on bending technique. The implementation is done in parallel using MPI library. The wave propagation and migration module use a 2D velocity map to compute snapshots, synthetic seismogram and seismic image. In this case, the parallelism is exploited on the shots line for the wave propagation and the domain decomposition for the depth migration. The results show some details of the computational tool and a real study case in Venezuela. This work has been supported by Sun Microsystems Inc. and INTEVEP PDVSA, Venezuela.

In Search of a Practical Non-Invasive Method for Contractility Measurements in Rat Cardiocytes

By David Torres-Barba

Background: I have developed a convenient method for measuring contractile responses of both adult and neonatal mammalian cardiocytes. These methods can be employed to quantify pharmacologic effects of drugs on myocytes. 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 (to measure the increase in cell elevation as the cell contracts), and typically interfere with simultaneous optical recording of cell signals such as the calcium transient. Methods: Optical digital images are first obtained from a CCD camera mounted on an inverted phase contrast microscope. The video images are later analyzed frame by frame using functions available in Matlab's Image Processing Toolbox. Image optimization techniques were applied to a sequence of frames depicting a contracting neonatal myocyte, focusing in intracellular fine structure details, specifically by monitoring the area of small inclusions within the cell thought to be protomyofibrils. The application of image analysis tools with this software allows measurement of the adult cardiocyte's area and optical density in each frame for corroboration purposes. Results: Application of this measurement technique produces contraction vs. time records virtually identical in time course and shape to records obtained by cell boundary tracking procedures when applied to the study of adult cardiocytes. Contraction curves generated from neonatal cells exhibit the same profile and time course. Adult cardiocyte analysis of the area of the cardiocyte in each frame yields a graph depicting sarcomere shortening versus time. The neonatal cardiocyte method utilizes phase contrast images showing inclusions that change their phase contrast image appearance (including inclusion size). The contractility graphs created by the two methods are consistent with the expected results and graphs created by more complicated existing methods. Conclusions: This new methods for myocyte contractility quantification will be helpful in the analysis of the contractile dynamics in the presence of drugs. The adult myocyte method has been found to be successful and valid. The new neonatal method has so far provided promising results, although it is still under analysis and we are considering strategies to validate the method with independent measurements of microforce or protomyofibrillar shortening by the application of high resolution imaging.

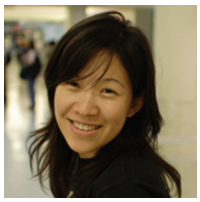
Shadow Structures to Standardize GoogleRanks© Between Disconnected Components

By Kristen Mecadon, Annalinda Arroyo, Peter Salamon, Karl Heinz Hoffman

Google© Technology allows us to define ranks for states of a random walk. If the states are disconnected we have a decomposable walk. The shadow graph can be used to make connections and compare the GoogleRanks© in different components. The biological example of interest is the graph derived from the distance matrix on phage proteins with the shadow graph linking all proteins in the same phage.

Global Gene Expression Profiling in Neonatal Rat Myocardium in Response to the Anti-diabetic Agent Rosiglitazone

By Chao-Jen Wong, Elliot Kleiman, Jerry Chen, Paul Paolini



Rosiglitazone is an anti-diabetic agent and a high-affinity ligand for peroxisome proliferator-activated receptor gamma (PPAR gamma), which functions as a central regulator of adipogenesis and lipid metabolism. Studies have shown that rosiglitazone enhances insulin-mediated glucose uptake at the whole-body level. However, the fact that the results of several research studies and meta-analyses examining the relationship between rosiglitazone and cardiovascular death have so far been conflicting means that the safety of the drug is yet to be determined. The work presented here is the first step toward discovering the molecular events that lead to association of rosiglitazone and the increased risk of heart failure. To this end, we have employed Illumina's BeadArray technology to examine the time course gene expression of ventricular myocytes in neonatal rats under the treatment of the drug and identified the differentially expressed genes and relevant over-expressed biological processes and pathways.

Fourier Analysis of Time Course Microarray Data and Its Relevance to Gene Expression Dynamics

By Jerry Chen, Faramarz Valafar, Paul Paolini

The overall aim of our biological research is to supplement traditional experimental techniques with computational and engineering methodologies for gaining more insight into gene and protein interaction networks and gene expression dynamics. The following study demonstrates the effectiveness of using a signal processing technique called the Fast Fourier Transform (FFT) on time course microarray (TCM) data for finding genes whose expression oscillates over time. Using FFT on previously published yeast TCM data, we find that 313 genes show periodic expression. Interestingly, there are four dominant periodicities, one of which matches the yeast cell cycle. The biological processes underlying the remaining three periodicities remain unknown. Gene annotation and GO functional analysis verify the presence of periodic cell cycle genes within the set of 313 genes found. Thus, Fourier analysis is a valuable tool for understanding gene expression dynamics.

Development of a Computer Program to Analyze the Renner-Teller Effect in NCO

By Chris Estela, Andrew Cooksy

The NCO free radical is an important molecule to study because its linear conformation allows us to create a simple effective Hamiltonian describing the most prominent contributing factors, but still allows us room to take into account the abundance of smaller interactions taking place on the molecular level. Among the most important factors yielded by examining NCO is the Renner-Teller effect. Our computational study is part of an ongoing project to simultaneously analyze the lowest energy vibronic quantum states of NCO, using existing, high-resolution spectroscopic data. These vibronic states are grouped into "unique" states, which are obtained by specific vector combinations of the electronic and vibrational angular momenta, and the more complicated "non-unique"states, for which there are two different vecotr sums that yield the same overall vibronic angular momentum. Presently, the unique v2=0 2-Pi, v2=1 2-Delta, and v2=2 2-Phi vibronic states and non-unique v2=1 2-SigmaÎ£state have been analyzed and fit to experimental data with high precision. This study now aims to develop the computer code for analyzing data from the non-unique v2=2 2-Pi, v3 = 1-0 band of NCO. The non-unique states are split by a combination of spin-orbit and Renner-Teller coupling, and this requires a more general labeling scheme for the eigenstates of the Hamiltonian matrix than has previously been implemented. Additional terms in the effective Hamiltonian may also have to be derived by perturbation theory in order to fit the data to the experimental precision, and the program will then be applicable to a variety of free radical systems.

Use of Bayesian Learning versus Scaled Conjugate Gradient Method in ANN QSAR Models for HIV Proteases

By Akmal Aulia, A. Srinivas Reddy, Rajni Garg, Sunil Kumar

Recently, there have been numerous findings on the developments of new HIV drug candidates with various inhibitory activities. These activity variation correlates to structural changes among the drug candidates. Studies involving constitutional, electrostatic, geometrical, quantum, and topological descriptors correlated with the activity are called Quantitative Structural Activity Relationship (QSAR). The large number of both the drug candidates and the associated descriptors makes it difficult for the traditional regression techniques to handle the data accurately in QSAR. Thus, it is necessary to use other methods to gain insights about these relationships. The use of machine learning techniques for structure-activity correlation has vastly increased over the past few years, due to the high accessibility of biological data and the increasing demand for more accurate and interpretable models for pharmaceutical development. This poster aims to present QSAR study on a class of HIV protease inhibitors utilizing evolutionary computation (Genetic Algorithms) and machine learning techniques (Neural Networks). In this study, comparison studies were performed, applying two different learning schemes for Neural Network training, namely Bayesian regularization and scaled conjugate gradient. Our results illustrates that, although the Bayesian regularization has more time complexity, it has better accuracy than the results obtained using scaled conjugate gradient.

Shannon's Uncertainty and Kullback-Leibler Divergence in Microbial Genome and Metagenome Sequences

By Sajia Akhter, Robert A. Edwards

All genome sequence data contains inherent information in it. Shannon's uncertainty theory can be used to measure of how much information a sequence has. Here we show that the amount of information in a sequence correlates with the similar sequences that will be found in the database using search algorithms (BLAST). Hence, a sequence with more information (higher uncertainty), has a higher probability of being significantly similar to other sequences in the database. Measuring uncertainty maybe a rapid way to screen for sequences likely to be similar to things in the database, and also show which sequences with no known similarities are likely to be false negatives. Here, we also present some work on amino acid composition for each of the complete bacterial genome sequences. We show that (i) there is a significant difference between amino acid utilization in different phylogenetic groups of bacteria; (ii) that the bacteria with the most skewed amino acid utilization profile are endosymbionts or intracellular pathogens; and (iii) the skews are not restricted to one or a few metabolic processes but are across all subsystems.

A Numerical Study of Low Reynolds Number Stratified Flow Past a Sphere

By Dany De Cecchis, Carlos Torres, German Larrazabal, Jose E. Castillo

We model the flow past a sphere in a viscous, incompressible low Reynolds number stratified fluid. The flow has uniform velocity and linear stratification. The governing set of equations, Navier-Stokes, describing the above flow were numerically solved by direct integration using boundary-fitted coordinates and a Pressure Correction Method with finite-difference approximations. In order to solve the pressure linear system with high accuracy we use the BiCGstab method. Numerical experiments are performed for different flow conditions by varying the Reynolds number. Results are presented for density and velocity fields. Simulated sphere drag is also compared to the classical drag curve cited in the literature.

Parallel Implementation of the CCBA for Mesh Generation

By Elbano David Batista, James Otto, Jose E. Castillo

In this work we extend the CCBA to produce a parallel-iteratively mesh generator. The CCBA or Convex-Combination-Based-Algorithm (presented in ACSESS 2007) uses a mesh-size function and convex combinations on local polytopes to change the position of the nodes of an initial mesh. This process is repeated iteratively and stops when the max norm between two consecutives meshes is smaller than a given threshold. The parallelization is obtained by dividing the initial mesh into as many submeshes as processors available and dealing with each submesh in a different processor. This so-called mesh decomposition does not depend on the physical domain of the problem, which is the main difference and the main advantage over domain decomposition-like techniques for parallelization. We also present a way to reduce overhead while preserving the property of non-folding of the original sequential algorithm. Several examples of 2D meshes on complex domains show the potential of the technique for constructing non-uniform quad meshes.

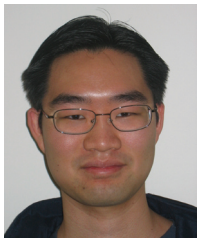
Azimuthal Modulational Instability for Vorticies in the Focusing Nonlinear Schrodinger Equation

By Ronald Caplan, Ricardo Carretero, Enam Hoq, Panayotis G. Kevrekidis

We study the azimuthal modulation instability (MI) of vortex structures, with different topological charges, in the focusing two dimensional Nonlinear Schroedinger (NLS) equation. This setting bears direct application in the realm of Bose- Einstein condensates and nonlinear crystals. The method to study the stability relies on freezing the radial direction and applying a MI analysis in Fourier space of the azimuthal modes. We find that, typically, vortices are unstable after a critical azimuthal wave number. Results are corroborated by direct numerical simulations performed on a polar coordinate finite-difference scheme. We also show how to extend the method to encompass non-local nonlinearities (ubiquitous in nonlinear crystals) that tend to stabilize solutions.

Binding Pocket Mutational Analysis of HIV-1 Protease Crystal Structures

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



Mutations that arise in HIV-1 protease after exposure to various HIV-1 protease inhibitors have proved to be a difficult aspect in the treatment of HIV. Mutations in the binding pocket of the protease can prevent the protease inhibitor from binding to the protein effectively. In the present work the mutations of HIV protease crystal structures complexed with FDA approved protease inhibitors deposited in the Protein Data Bank (PDB) were studied. The mutations of each crystal structure were determined by comparing the amino acid sequence of each crystal structure against the HIV-1 wild type strain HXB2. Any amino acid within 6Ã. of the bound ligand was considered to form the binding pocket. A mutation map has been developed, mapping the mutations for each ligand with the binding pocket highlighted. Mutation patterns for each ligand are analyzed. The determination of mutation patterns with the combination of chemical descriptors and data mining approaches may aid in the prediction of mutations that may arise in newly designed inhibitors during the drug design process.

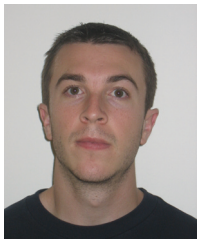
A Bayesian Network Approach to Building a Gene Regulatory Network of Plants Undergoing Cold Stress

By Jeremy Burrell, Chao-Jen Wong

Continuous abiotic stresses (such as extreme temperatures, high winds and edaphic conditions) can have adverse effects on plant life. This can become a major constraint in crop production. In order to alleviate the problems, it is important to understand the cold stress mechanisms at the molecular and cellular levels, regarding the signaling pathways from cold perception to activation of gene expression. My mentor, Dr. Joan Chen, and her lab, together with other labs, have collected a large amount of DNA microarray data involving plants undergoing cold stresses. I took a systems biology approach, aiming to build the gene regulatory network using the cold stress microarray data that have been obtained, to gain a better understanding of plant responses to cold stress at the molecular level. The results generated from this approach will be utilized to generate hypothesis which can be tested by other experimental approaches. The Bayesian Network (BN) method was chosen to build the transcription regulatory network. This work will show an implementation of Bayesian Network (BN) method and use of the R package, GeneNet, to build a gene regulatory network, which can be easily interpreted by bench scientists.

Conformational Analysis of an Antineoplastic Class of Macrocycles

By William Disman, Melinda Davis, Stephanie Lapera, Robert Vasko



Recent studies on the bio-potency of Sansalvamide A derivatives show promising properties against pancreatic, colon, breast, prostate, and melanoma cancers. Recent NCI panels have also proven potency on leukemia, thus a more detailed analysis of the structural features within the macrocycles is needed to explore further roles of the molecules. Sansalvamide A (San A) is a marine fungal product that was discovered by William Fenical. Through structural manipulation of peptide derivatives based on structure-activity relationship (SAR) and 2-D NMR, valuable trends arise to provide a systematic means of controlling bio-potency. Through the use of various biological assays as well as computational resources it is possible to analyze the effect of such conformational changes and gain insight into the development of more potent compounds. Multiple derivatives of the San A scaffold were synthesized and their activity on a pancreatic cancer cell line PL-45 and the colon cancer cell line HCT-116 is reported here. Then, using MacroModel within Maestro, we have validated the preferred conformation of many San A derivatives. Using Monte Carlo methods as well as conformational constraint and limiting electrostatic and steric qualifications, a pool of conformers was created. By arranging the lowest energy conformer within NAMFIS and using 2D NMR experiments NOESY and ROESY predictive studies of the proposed protein target of the derivatives are described. By performing pull-down assays we have determined that the protein target of these derivatives is Hsp90, and therefore computational validation combined with incorporation of the co-crystal structure of Hsp90-drug can be used to determine the active conformation of the molecule when bound to Hsp90. This crystalline matrix will then be analyzed using NAMFIS, a NMR based modeling program, to create a dynamical picture of the Sansalvamide A derivatives. Future potent derivatives can then be predicted using this hybrid computational/ experimental approach.

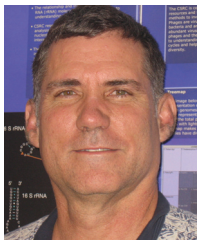
Structure and Thermal Evolution of Neutron Stars

By Rodrigo Negreiros, Fridolin Weber

Neutron stars are among the most enigmatic objects in the Universe. They possess the mass of our sun but are several billion times smaller than it. The matter in the cores of neutron stars is therefore compressed to densities that are several times higher than the density of atomic nuclei. Under such extreme physical conditions the conventional building blocks of matter as we know them (atoms, protons, electrons) give way to new and widely unexplored states of matter, such as superconducting quark matter and novel particle condensates searched for in the most powerful terrestrial collider experiments. In this paper we study the thermal evolution of neutron stars in order to explore the properties of ultradense matter and the inner workings of neutron stars. The calculations are performed in the framework of Einstein's theory of general relativity, since neutron stars curve the geometry of space-time so strongly that classical Newtonian theory of gravity fails to describe their properties.

Meso-scale Monte Carlo Sintering Simulation with Anisotropic Grain Growth

By Gordon Brown, Richard Levine, Eugene Olevsky



Although Monte Carlo (MC) simulations are widely used for understanding the microstructural evolution of sintering bodies, the models currently in use do not accommodate anisotropic material grain growth. This paper proposes and implements a two-dimensional algorithm to simulate the evolution of granular structure with anisotropic materials using a Potts MC model which incorporates the sintering mechanisms of grain growth, pore migration and vacancy annihilation. Limitations of this algorithm imposed by the underlying lattice structure are identified and solutions are proposed, implemented and tested. Even though this ability to incorporate anisotropic grain growth in our meso-scale modeling does not provide a significant direct effect on the macroscopic properties or deformation of sintered objects, it can allow us to investigate the granular development under several different situations to better understand some of the observed phenomena like patterning in sintered materials.

Computational Investigation of the Reaction Thermochemistry and Kinetics of TTQ Cofactor

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

SAN DIEGO STATE UNIVERSITY

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 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 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 COSMO-RS model will then 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.

Estimating Confidence Bounds of Reliability Estimate with Bayesian Inference of Johnson Unbounded Family Distribution Parameters

By Kun Marhadi, Satchi Venkataraman

Probabilistic analysis of physical systems (e.g. simulation for reliability estimate) requires information on the distributions of the random variables. These distributions are typically obtained from testing or field data. In engineering, where tests are expensive, the sample size of such data are small O(10). Identifying the correct distributions with such sample size is difficult. A distribution function is often chosen based on prior knowledge (experience) of the underlying distribution of the random variable. The chosen distribution is then fitted to the samples, and a goodness of fit test is performed to accept or reject the chosen distribution. When the sample size is small, the goodness of fit measures is not sufficient to discern the best distribution function. Even when a correct distribution function can be identified, fitting the distribution to small sample data creates uncertainty in the parameters of the distribution function. Thus the results of probabilistic analysis can be uncertain if the analysis uses parameters from the fitted function. In this study a Johnson unbounded (SU) family distribution function is used to identify the shape, location and scale parameters of distribution that can best fit small sample data. In order to quantify the uncertainty in the fitted parameters, a Bayesian inference procedure is used, in which the distributions of these parameters are determined. In a test case, samples from distributions of these parameters are then used to determine confidence bounds of probability of failure estimates of a system. The results show that with this method, the probability of failure of the system can be estimated with high confidence in a small interval. The advantage of this method is that using Johnson unbounded family distribution function eliminates the needs of having prior knowledge of the characteristic of the sample data.

A Comprehensive Metagenomic Approach to Determine the Relationship between Periodontal Disease and Cardiovascular Disease in Young Adults: Towards a Better Understanding of Human-Microbial Interactions and Disease.

By Lena D. van der Stap, Lesley Lee, Scott T. Kelley, Roberta A. Gottlieb

Periodontal Disease (PD) is shown to be associated with an increased the risk of a number of systemic diseases - including atherosclerosis. We are investigating a possible causal relationship in a young population of individuals with PD (ages 20-30) to determine if they show early signs of atherosclerosis. Using powerful new culture-independent molecular approaches based on pyrosequencing technology, we are conducting a comprehensive metagenomic analysis to identify, classify, and quantify bacterial species associated PD and atherosclerosis (both pre- and post- treatment for PD). This survey of microbial diversity is expected to cover between 300,000-500,000 16S sequences for 300 samples from 40 patients. The bioinformatics pipeline will include 1) databasing data sets of unique 100-250-base 16SrRNA sequences per species, 2) sequence alignment and phylogenetic analysis, and 3) computing distance metrics for differences between microbial communities (samples) at different stages of PD and with or without changes in brachial artery flow dynamics. Multivariate analyses, such as Principle Coordinates Analysis (PCoA), will be used to show the distribution of 16S community samples. Subsequently, functional annotation of the genes combined with relative abundance data for each species will allow for the prediction of important functional relationships among potential subnetworks of species that support the persistence of PD and that could be involved in the mechanism of action leading to atherosclerosis. Ultimately, this knowledge could be used to develop an effective probiotic treatment for PD.

Multimode Interferometry of Bose-Einstein Condensates in a Circular Waveguide

By Martin Kandes, Michael Bromley

Simple circular waveguides promise to be an ideal architecture for building high-precision matter-wave interferometers that exploit the coherent source of atoms provided by Bose-Einstein condensates (BECs). Using finite difference methods, we perform numerical calculations of the time-dependent Gross-Pitaevskii equation in one and two dimensions to simulate gravity-induced quantum interference for counterpropagating BECs in a circular waveguide. The aim of this work is to clearly understand the impact multimode excitations and nonlinear interactions have on the feasibility of interferometric measurements. Our results vividly illustrate many of the challenges to be expected in performing these types of experiments.

A Multiple Linear Regression Analysis of Extrinsic Factors Associated with the Incidence of Dengue in Thailand

By Karen Campbell

In a pattern of increasing global spread since the 1960's, dengue threatens 40% of the world's population annually. In endemic areas such as southeast Asia, hemorrhagic fever, the severe and sometimes fatal form of dengue strikes with devastating seasonal epidemics. The highest morbidity and mortality is in children. This study examined a range of extrinsic factors (climate, land use, demographic, economic) in relation to incidence of severe dengue in Thailand over space and time. Spatial and temporal autocorrelation were high and required iterative adjustments using a general linear model.

Intelligent Sensor Networks: Towards of Theory of Stochastic Resonance in Multi-Stable Systems

By John Aven, Antonio Palacios, Visarath In, Adi Bulsara

A large class of dynamic sensors exhibit nonlinear input-output characteristics, often corresponding to a bistable potential energy function. Examples include: magnetic field sensors, e.g., fluxgate sensors, ferroelectric sensors, and mechanical sensors, e.g., acoustic transducers made with piezoelectric materials. Many of these sensors have assisted mankind in analyzing and controlling thousands of functions for many decades. Computer memory has increased over many years through the use of magnetic sensors embedded in storage devices. Airplanes fly with higher safety standards because of the high reliability of noncontact switching with magnetic sensors. As new technologies emerge, however, more powerful and more efficient sensors are required. In response to this need, we present preliminary results which demonstrate that higher sensitivity, lower power-consumption, and reduced costs, can all be achieved through an integrative approach that combines a novel Intelligent Sensor Network (ISN) network architecture with a new sensing technique, the Residence Time Detection (RTD). By intelligent, we mean the following. We treat each sensor as a nonlinear dynamical system of the form dx/dt = -grad(U(x)), where x(t) is the state variable of the device, e.g., magnetization state, and U is the bistable potential function. Then the fundamental idea is to exploit the phenomenon of coupling-induced oscillations and the nonlinear characteristics of magnetic materials so that the ISN network can, intelligently, produce its own self-biasing signal and, simultaneously, achieve better sensitivity.

Bi-Objective Reliability Based Design Optimization(RBDO) Incorporating the Data Uncertainty

By Raghu R Sirimamilla

Reliability based design optimization (RBDO) is necessary for the design of complex engineering systems with quantified levels of risk. To achieve failure probabilities in the order of 10-3 in large systems such as space vehicles and aerospace structures typical component level failure probabilities have to be of the order of 10-4 to 10-7. Quantification of risk using reliability based approaches relies on availability of statistics of the random variables that affect the response. In engineering applications where extensive tests cannot be performed, we introduce uncertainty into characterization of the random variables. The uncertainty is introduced from the use of small sample sizes to estimate the distribution parameters (mean and variance â?" location and scale) of a chosen distribution function; uncertainty could also arise from the selection of an incorrect probability distribution function (PDF). Including data uncertainty introduces yet another level of complexity to the already computationally expensive problem of RBDO. Inverse reliability measures have been proposed and used in RBDO to minimize computational effort. This poster presents methods to obtain confidence bounds for the inverse reliability measure, namely the probabilistic sufficiency factor, resulting from data uncertainty. The estimated confidence bounds are them approximated using a response surface for use in optimization. A bi-objective optimization is performed to achieve a design with the greatest reliability and lowest sensitivity to data uncertainty.

Intelligent Sensor Networks: Coupled Core Fluxgate Magnetometers, a New Device Configuration

By John Aven, Antonio Palacios, Visarath In, Patrick Longhini

Here we investigate an extension to work that has been performed on a nonlinear device known as a sensor. This devices is the Coupled Core Fluxgate Magnetometer, or CCFM. This device, and others classifiable as sensors are modeled as possessing a bistable potential. Additionally, they possess a specific characteristic: in the presence of an external signal (to be detected) the signal, or evolution of the system, will spend a greater, disproportionate, amount of time in one well compared the time spent in the other well. This allows the use of a time-domain detection scheme known as Residence Time Detection. With Residence Time Detection the external signal is quantified by either the absolute difference in time that the evolution spends in one well versus the other, or by the magnitude of the maximal ratio of the times spent in the two wells. We present, in what follows, a deterministic analysis of this characteristic, as well as of the dynamics, of a new arrangement of the devices. This new arrangement cam from what one may call an experimental mishap and has lead to a scalably large increase in the sensitivity of the CCFM under the new arrangement.

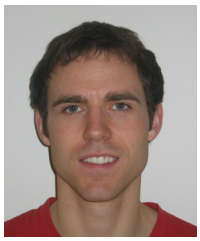
Image Smoothing and Edge Detection by Nonlinear Diffusion and Bilateral Filter

By Carlos Bazan, Peter Blomgren

In this work we propose a new image smoothing and edge detection technique that employs a combination of nonlinear diffusion and bilateral filtering. The model is based upon two very well established methodologies in the image processing community, which makes the method easy to understand and implement. Our numerical experiments show that the proposed model is capable of achieving more accurate reconstructions from noisy images, as compared to two other popular nonlinear diffusion models in the literature. We also propose a new and simple diffusion stopping criterion, based on the second derivative of the correlation between the noisy image and the filtered image. This indirect measure allows stopping the diffusion process very close to the point of maximum correlation between the noise-free image and the reconstructed image, in the absence of the former. The stopping criterion is sufficiently general to be applied with most nonlinear diffusion methods normally used for image noise removal.

ADAPTdb/ADAPT - A Framework for the Analysis of ARISA Data Sets

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



The characterization of natural microbial assemblages in community profiling projects introduces the major scientific challenges of understanding and predicting the function and response to environmental changes of microbes of an ecosystem. Here, we present a system for the automatic analysis of ARISA data sets. ARISA is a method for analyzing the composition of microbial communities, which performs faster and at a much lower cost than other community profiling techniques. ARISA relies on the analysis of intergenic regions called internal transcribed spacer (ITS), which are located between the 16S and 23S rRNA genes. 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 Entrez sequence databases. The program ADAPT was developed to taxonomically characterize ARISA data sets using 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.

Opposed-Flow Flame Spread Over Thin Films of PMMA in a Microgravity Environment - A Comparison of Experimental Results with Computational and Theoretical Predictions

By Subrata Bhattacharjee, Christopher Paolini, Kazunori Wakai, Shuhei Takahashi

Flame spread over solid fuels in a microgravity environment is an important area of research due to its fire safety implications in space crafts. Of all different configurations, flame spread over thin fuels in an opposed-flow environment is the simplest and, therefore, received most attention during the past decade of research. The problem has been studied experimentally and theoretically by different groups of researchers. Recently a theoretical study advanced closed-form formulas for spread rate over thin and thick fuels in the radiativley dominated regime of the microgravity environment. In this work we use a comprehensive computational model to numerically predict the flame spread rates over thin PMMA fuels in different ambient conditions. The results are found to agree quantitatively with the predictions of the theory as well as experimental data accumulated over three years of drop-tower experiments on flame spread over thin PMMA films, further establishing the validity of the flame spread formulas in the microgravity regime proposed by the authors. Flame shapes predicted by the computational model are also found to agree quite well with the interferometer images of the spreading flames in microgravity as well as downward configuration.

Optimizing a Coral Nerve Net

By Eugenia Chen, Klaus M. Stiefel, Terrence J. Sejnowski, Theodore H. Bullock

Electrically stimulated coral polyps form a traveling wave of contraction from the site of the stimulation. A model of a coral nerve network was optimized to match one of the experimentally observed behaviors, a constant velocity of spread of excitation. We applied genetic algorithms to increasingly more complex models of a coral nerve net. In the first stage, individual neurons were optimized to respond with a spike to multiple, but not single pulses of activation. In a second stage, we used these neurons as the starting point for optimization of a 2-dimensional nerve net. This strategy yielded a network with parameters that reproduced the experimentally observed spread of excitation.

WiBandAccelero - New Concepts in Wide Bandwidth Frequency Tunability in MEMS Accelerometers

By Amandeep Singh, Berhanu Wondimu, Sam Kassegne

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MEMS (Micro Electromechanical Systems) accelerometers continue to make inroads in such applications as airbags, navigational systems, military applications and gaming devices. The application of MEMS accelerometers is expected to enter newer areas such as mobile devices such as cell phones for both civilian and military applications. However, these new applications pose aggressive performance requirements such as tunability of frequency range over a significantly wide bandwidth. A particular example relates to the needs of the next generation of commercial as well as military hand-held devices with navigational capabilities. This research concentrates on developing an accelerometer capable of detecting a quick movement (0.5g â?" 2.5g) as well as the zooming movement (0.1g â?" 0.5g). The MEMS accelerometer is named WiBandAccelero and is tunable from tens of kHz to hundreds of kHz. The range is selected to cover tilt needs in both digital map navigational as well as mobile gaming applications. The tunability is achieved by the use of a series of embedded accelerometers of sequentially differing resonant frequency on a monolithic frame and a novel active structural re-configuration design. So far, we have accomplished the design to meet specs for mobile navigation systems. This was preceded by a large study of 50 individuals to determine statistical distribution of acceleration signatures. The study is now focusing on the design of the electronic and control systems. The extension of the tunability by 2 orders (1000is certainly very significant progress with wide ranging implications. Further, we feel that this ongoing work in wide tunable accelerometers will open up new possibilities in personal mobile device applications for both civilian and military uses by introducing much wider bandwidth tunability unavailable so far.

Scoring Amino Acid Substitutions in Phage Genomes

By Promita Bose, Robert Edwards, Peter Salamon

Substitution matrices are among the most widely used scoring techniques : BLAST, Phylip and other alignment packages, all use them. However these matrices are general, ignore organism specific properties, and do not provide customized scoring schemes. We present a phage specific Blosum matrix based on the abundances of aligned substitutions. These matrices use information from approximately five and a half million significantly similar protein alignments and over five hundred phage genomes. Our scoring matrix is significantly different from the existing PAM and BLOSUM matrices and indicate the need for similar treatments for other groups of organisms.

Fabrication and Analysis of High Sensitivity Biochemical Sensors Using PMN-PT Single Crystal Thin Membranes

By Michael Frank, Saravana Pitchaikani, Kee S. Moon, Samuel K. Kassegne

In this paper, we report the results of the HCL wet etching process to fabricate a PMN-PT single crystal piezoelectric thin membrane. A piezoelectric thin membrane can offer the ability to passively sense vibrations without power requirements. Furthermore the new generation oxide material exhibits extraordinary piezoelectric properties. The material, the single-crystal solid-solutions (1-x)Pb(Mg1/3Nb2/3)O3-xPbTiO3 (PMN-PT), has been shown to possess piezoelectric coefficients and electromechanical coupling responses significantly larger than conventional ceramics. A four-fold enhancement in piezoelectric coefficients and much higher efficiencies in electrical to mechanical energy conversions have been found. Use of a PMN-PT sensor to detect, with high sensitivity, minute amounts of waterborne pathogenic bacteria such as E. coli O157:H7 is one promising direct application. Design of a compact and portable PMN-PT sensor device used in produce packaging facilities and grocery stores is a primary focus. In this paper, we present the research results produced from the experimental work for the PMN-PT wet etching in HCL solution.

Avian Flu Grid: International Collaborative Environment for Team Science on Avian Influenza

By Dong Xu, Rommie Amaro, Irene Newhouse, Wilfred Li

The avian influenza virus (subtype H5N1) is currently becoming the world's largest pandemic threat due to the high lethality, in birds and increasingly humans , and virulence of its endemic presence, its increasingly large host reservoir, and its significant ongoing mutations. The two surface glycoproteins, hemagglutinin (HA) and neuraminidase (NA) of influenza A virus, play an important role in the interactions with cellular receptors containing terminal N-acetyleneuraminic acid (Neu5Ac, or NANA) moieties, aka, sialic acids (http://en.wikipedia.org/wiki/Sialic_acid). The approved anti-influenza drugs oseltamivir and zanamivir inhibit H5N1 activity by targeting the NA active site. However, research has shown that antigenic drift may result in viral resistance to the abundant presence of existing NA inhibitors through the retention of NeuAc moieties by complex glycan near HA receptor binding site; and antigenic shift could give rise to new virulent subtypes of the flu virus. Thus, it is crucial to design novel HA- and NA-targeted inhibitors, which can be used in combination for optimal prophylaxis and treatment. Work has been ongoing to apply the Relaxed Complex (RC) scheme and Molecular Dynamics (MD) simulations on the two target proteins in the hope of capturing key protein dynamics information and accounting for receptor flexibility. Research is under way to take advantage of novel loop flexibilities and changing cavity shape adjacent to NA active site to discover novel NA inhibitors that may work in a way similar to the HIV integrase inhibitor, raltegravir, inspired by the RC/MD simulation procedures. Further investigation involves statistical cluster analysis for rational selection of representative HA/NA protein structure snapshots, which will be used in the virtual screening with diverse ligand libraries. Finally, the binding energies of the high scoring compounds will be re-evaluated and refined by Molecular Mechanics-Poisson Bolzmann Surface Area (MM-PBSA) approach for lead optimization. By leveraging the PRAGMA grid and high performance computing (HPC) resources, the implementation of many state-of-the-art computational techniques would be expected to greatly facilitate the drug discovery process and improve the accuracy in the search for novel avian influenza inhibitors, subsequently generate drug leads with potentials for further validation and development in biological assays and experiments.

Development of a Cyberinfrastructure Environment for the General Curvilinear Ocean Model (GCOM)

By Mary Thomas, Jose Castillo, Carlos Torres

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The General Curvilinear Ocean Model (GCOM) uses a 3-D time-dependent curvilinear ocean model to simulate stratified ocean currents over uneven terrains with irregular bottom topographies in a rotating system. GCOM solves fluid flow dynamics for open oceans or coasts, lakes, bays, and estuaries. A parallel, componentized version of CGOM is being developed that that will utilize resources and services made available via distributed cyberinfrastructure environments and computational services, all interfaced with a user portal [1][2]. [1] Torres C.R., Mascarenhas, A. S., Castillo J. E. (2004). Three-dimensional stratified flow over Alarcon Seamount, Gulf of California entrance. Deep-Sea Research II, 51, 647-657. [2] M. P. Thomas, et. Al. Grid Portal Architectures for Scientific Applications. Proceedings of SciDAC 2005, 26â?"30 June 2005, San Francisco, CA, USA. Journal of Physics: Conference Series, Volume 16, 2005.

Computational Challenges of AB Initio Nuclear Shell Model Calculations

By Hai Ah Nam, Calvin W. Johnson

A consistent microscopic theory of the atomic nucleus is necessary to explain a wide range of nuclear phenomena and to predict nuclear behavior that cannot be measured experimentally. Over the past decade, theoretical investigations have fundamentally shifted from phenomenological methods to ab initio approaches to understanding nuclei. The availability of high performance computing resources allow for the more reliable, but computationally intensive first principles methods to be tractable. The No-Core Shell Model (NCSM) is an ab initio approach that has been successful in describing light nuclei. Nuclear properties are obtained through diagonalization of the Hamiltonian matrix, which is large (dimension > 10^8) and sparse. The computational effort increases exponentially with nucleon number using a 2-body Hamiltonian, and becomes particularly difficult when including 3-body forces, as the matrix becomes less sparse. New algorithms and load balancing techniques are needed to scale this method for larger nuclei (A > 16). We analyze the computational challenges of REDSTICK, a nuclear shell model program, and implement several techniques to scale REDSTICK to investigate high p-shell and low sd-shell nuclei.

Electrically Active Microarray of 3D Carbon MEMS Electrodes for Pathogen Detection Systems

By Jiae Shin

The ability to isolate and concentrate pathogens (bacteria, virus, etc), biomolecules and any sub-micron particle is critical to many biomedical applications, including diagnosis for cancer and infectious disease (SARS, deadly flu strains, STD, etc). Conventional two-dimensional active microarrays have been used with success for the manipulation of biomolecules including DNA. However they have a major drawback of inability to process relatively â?~large-volumeâ?T samples useful in oncology and infectious disease applications. This research presents an active microarray that exploits electrokinetic (electrophoresis and dielectrophoresis) forces for its hybridization method using 3D carbon electrodes that will enable the large volume manipulation for pathogen detection. Carbon electrodes are fabricated using C-MEMS (Carbon MEMS) technology is an emerging fabrication method that enables low cost fabrication of MEMS devices exploiting fascinating physical, chemical, mechanical and electrical properties of carbon materials. The chip fabricated using C-MEMS technology is packaged and the efficiency of separation and accumulation of the 3D electrodes on the chip is tested by manipulating negatively charged polycarboxylate 2 micron beads in 50 mM histidine buffer.