9th Annual ACSESS

Friday, March 23, 2012
12:00 pm - 5:00 pm
SDSU's Parma Payne Goodall Alumni Center

For Applied Computational Sciences and Engineering & Computational Science Curriculum Development

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

1:00 pm — **Stanley Maloy**
Dean
College of Science
San Diego State University
Welcome / Opening Remarks

1:10 pm — **Jose E. Castillo**
Director
Computational Science Research Center
San Diego State University
Computational Science at SDSU and ACSESS Program

1:20 pm — **Bill Bartling**
President and Chief Executive Officer
SR2020 Inc.
Key Note Speaker

1:45 pm — **Coffee Break**

1:50 pm — **"Industry Academic Interaction"**

Maritza Borunda
Academic Relations
Learning & Development
QUALCOMM, Inc.

Camille Nebeker
Principal Investigator
Research Ethics Initiatives
San Diego State University Research Foundation

Hai Ah Nam
Computational Scientist
Oak Ridge National Laboratory

Carlos Bazan
Faculty, Scientific Visualization Coordinator
Computational Science Research Center

John Fish
Airframe Design, Test Verification & Flight Operations
Lockheed Martin Aernautics

Satchi Venkataraman, Moderator
Faculty
Aerospace Engineering & Engineering Mechanics

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

4:30 pm — **Paul Paolini**
Associate Director
Computational Science Research Center
San Diego State University
Poster Presentation Awards
&
Closing Remarks

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 the aim of CSRC to function as an independent, self-sustained unit. therefore, its operation crucially depends on extra-mural funding.

Mission Statement

The mission of the Computational Science Research Center (CSRC), located at San Diego State University, is to promote development and advancement of the interdisciplinary subject of computational science. This is accomplished by fostering research, developing educational programs, and promoting industrial interaction, outreach, and partnership activities.

The Computational Science Research Center provides an excellent environment for scientific research at SDSU. The center facilitates the interaction between applied mathematics, computer science, and the sciences by providing the necessary infrastructure for productive research efforts.

Real world applications are the focus of the projects undertaken by the faculty and students of the center. Such projects provide a significant educational opportunity for our students to hone their industrially relevant computational skills.

Executive Board

Program Director:
Jose E. Castillo

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

Associate Directors:
Andrew Cooksy
Eugene Olevsky
Paul Paolini

Advisory Board

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T12 Division
Los Alamos National Laboratory

Victor Pereyra
Weidlinger Associates

Steve F. Ashby
Pacific Northwest National Laboratory

Horst Simon
Lawrence Berkeley National Laboratory

Featured Posters

Parallelization of the 3D Unified Curvilinear Ocean Atmospheric Model

By Mary Thomas and Jose Castillo

The Unified Curvilinear Ocean Atmospheric Model (UCOAM) is a Large Eddie Simulation (LES) CFD model capable of running both ocean and atmospheric simulations. It is the only environmental model in existence today using a full, 3D curvilinear coordinate system, which results in increased accuracy, resolution, and reduced times to solution. UCOAM is a petascale model: resolving sub-km scale fluctuations requires large arrays (1010 elements); the curvilinear system requires large number of arrays (~100); communication occurs along all 3 axes; and full simulations generate TBytes of data. Consequently, this model requires parallelization. To facilitate our computations and data management, we have developed a Computational Environment (CE) based on the Cyberinfrastructure Web Application Framework (CyberWeb). In this poster we discuss our approach and challenges associated with parallelizing this new model and the design of the computational environment. We will present results from scalability studies of this new parallel model.

This research is supported in part by NSF, DOE, and COAST funds.

The microRNA miR-124 Specifies the Ciona Peripheral Nervous System by Regulating Notch Signaling

By Jerry Chen, Robert Zeller, Matthew San Pedro, Arra Revilla, and Joseph Mahaffy

The nervous system enriched microRNA miR-124 is necessary for proper nervous sysem development, although the mechanism remains poorly understood. Here we discovered that extensive feedback interaction between miR-124 and Notch signaling regulates the epidermal-peripheral nervous system (PNS) fate choice in the tail midline cells of Ciona intestinalis. Notch signaling silences miR-124 in epidermal midline cells, while in PNS midline cells miR-124 silences Notch, Neuralized and all three Ciona Hairy/Enhancer-of-Split (Hes) genes. Also, ectopic expression of miR-124 is sufficient for converting epidermal midline cells into PNS neurons, consistent with a role in modulating Notch signaling. Furthermore, 3'UTR conservation analysis reveals that miR-124 targeting of the Notch pathway appears to be Ciona-specific, highlighting a unique and important role of miR-124 in regulating cell fate during embryonic development. We are currently using a mathematical modeling approach to elucidate the precise dynamics between miR-124 and Notch signaling in Ciona.

This research is supported in part by NSF funds.

Sagnac Interferometry with Bose-Einstein Condensates in a Uniformly Rotating Ring Trap

By Martin Kandes, Michael Bromley, and Ricardo Carretero

We present the results of numerical simulations studying a novel scheme to perform Sagnac interferometry with Bose-Einstein condensates in a uniformly rotating ring trap. The proposed scheme involves determining the relative phase shifts between two counter-propagating condensate wave packets as the angular velocity of the ring is varied. Analyzing the interference patterns obtained from the simulations, we find that the phase shift response of closely follows that predicted by the Sagnac effect, even when the nonlinear mean-field interaction of the condensate is large. However, we also find, unexpectedly, that the linear accumulations of the relative phase shift with respect to time manifests itself as step-like phase jumps during the collisions of the wavepackets, with the magnitude of the phase jumps being linearly dependent upon the angular velocity of the rotating ring trap and the angular momenta of the wave packets. We provide details of the proposed scheme and discuss some of the advantages this unexpected behavior in the phase shift response may offer in performing Sagnac interferometry with Bose-Einstein condensates in the near future.

This research is supported in part by ARCS and SDSU/CSRC funds.

Host Prediction for Viral Metagenomes Using Oligonucleotide Profiles

By Michiyo Wellington-Oguri, Robert Schmeider, Robert Edwards, and Bastiaan Dutilh

Metagenomic sequencing of virus-like particles has identified large numbers of viral sequences with no known homologs. The role of these viruses remains elusive, especially in environments where many potential hosts co-occur. Here, we use a Random Forest to classify viral sequence fragments by host based on the frequency that oligonucleotide sequences appear in the genomes. Our approach classifies viral sequences with a 11 o 91 recision rate, depending on the sequence length, sequencing error rate, and confidence requirements. We use this tool to analyze viral gut metagenomes and compare the predicted host distributions with the corresponding bacterial metagenomes.

This research is supported in part by NSF funds.

NLSEmagic: Nonlinear Schrödinger Equation Multidimensional Matlab-Based GPU-Accelerated Integrators Using Compact High-Order Schemes

By Ronald Caplan and Ricardo Carretero

We present a simple to use, yet powerful code package called NLSEmagic to numerically simulate the nonlinear Schrödinger

equation in multi-dimensions. NLSEmagic is a high-order finite-difference code package which utilizes graphic processing unit (GPU) parallel architectures. The codes running on the GPU are many times faster than their serial counterparts, and are much cheaper to run than on standard parallel clusters. The codes are developed with usability and portability in mind, and therefore are written to interface with MATLAB utilizing custom GPU-enabled C codes with a MEX-compiler interface. The packages are freely distributed, including user manuals and set-up files.

This research is supported in part by NSF and SDSU/CSRC funds.

Anisotropic Energy Transfer in Neutron Stars

By Omair Zubairi and Fridolin Weber

All the heat stored in the core of a neutron star and eventually irradiated away from its surface by photons has to be transported through the crust. In the absence of rotation and magnetic fields, this transport in the crust is spherically symmetric. This is expected to be different if magnetic fields are present, in which case the heat transport may become anisotropic and the heat conductivity becomes a tensor whose components perpendicular and parallel to the magnetic field lines depend on the electric conductivity of the stellar matter. As a result heat flows preferentially along the magnetic field lines. This effect may be amplified at the surface of a neutron star by anisotropies in the envelope. The bottom line of all this is that the transport of heat in the crusts of magnetized neutron stars is non-spherical, which causes significant differences in the surface temperature distributions. By obtaining a set of equations (in the frame work of general relativity) that describe anisotropic heat transfer in rotating neutron stars, one can then build numerical models which will simulate the thermal evolution of these objects. Such simulations are key for our understanding the thermal evolution of compact stars. In this poster, we present the equations required along with the numerical techniques needed to construct these simulations.

This research is supported in part by NSF funds.

Implementation of the Helgeson-Kirkham-Flowers (HFK) Model to Calculate Reservoir Temperature Evolution During Injection of CO2-rich Water in Deep Brine Aquifers

By Christopher Binter, Anthony Park, Jose Castillo, and Christopher Paolini

The storage of carbon dioxide underground has been proposed as a method to reduce atmospheric CO2 concentration. The effects of CO2 injection on subsurface lithologies and formation waters are complex and highly variable. With Reaction-Transport Modeling (RTM) it is possible to model a range of injection scenarios and simulate the subsurface response, limiting costly and time intensive field experiments. One commonly used modeling application is TOUGHREACT, developed at Lawrence Berkeley National Laboratory. TOUGHREACT simulates non-isothermal multiphase fluid flow through porous and fractured media. Simulating CO2 sequestration under non-isothermal constraints results in a changing temperature evolution which, in turn, causes kinetic rate constants that govern mineral precipitation and dissolution to vary. One of the main drawbacks of TOUGHREACT is that diffusion coefficients are assumed to be the same value for all solute species. Diffusion coefficients are solute specific functions that vary with temperature. The assumption of a constant diffusion coefficient when modeling solute transport can fail to adequately capture certain transport phenomena during CO2-charged water injection, in particular, the variation in displacement between the effluent and an acidic diffusion front of H ions. In this work, an RTM application developed at San Diego State University named WebSimC that calculates solute specific diffusion coefficients has been expanded to compute temperature evolution. This is accomplished through the implementation of the Helgeson-Kirkham-Flowers (HKF) model to calculate charged solute heat capacity and enthalpy values that are used to determine the change in temperature during each time step by integrating an ordinary differential equation that governs temperature. This improved application is used to simulate short-term effects arising from the injection of CO2-charged water in saline sedimentary basins. Results show that the diffusion driven mass transport of H ions throughout the reservoir sandstone occurs at a faster seepage velocity than the injectant water velocity. This separation between the H front and the effluent front is shown to vary with temperature. The acidic front that develops ahead of the injectant front, a result of differences in solute diffusivity, could have complex effects on lithologies and seals.

This research is supported in part by DOE and NETL funds.

A New Shanon Sampling Theory: From a Circle to a Sphere

By Julien Pierret

Shannon Sampling Theorem can perfectly reconstruct a bandlimited continuous signal from a finite sampling on a circle, but can the same be done on a sphere? This extension has numerous applications of sampling on a sphere, such as numerical climate modeling and network design for climate observations, and is a cutting-age mathematics research topic. In this poster, we show that we can go from spatial to spectral and back to spatial, but with some errors due to the poles.

This research is supported in part by SDSU/CSRC and Mathematics and Statistics funds.

Non Linear Aeroelastic Analysis of Joined Wing Configuration

By Rauno Cavallaro

The main objective of this research is the study of the aeroelastic behavior of unconventional configurations, with a major focus on joined wing vehicles. Civil transport aircraft of the future are requested to improve their performances and to achieve a significant reduction of Direct Operating Costs, noxious emissions and noise. The problem of reducing Direct Operative Costs will not be solved without a significant improvement of aircraft efficiency, which can be hardly obtained by an optimization of conventional aircraft. Hence, new non-conventional aircraft layouts configurations provide an attractive alternative. As pointed out by different leading aeronautical industries (such as Boeing, Lockheed Martin, Airbus, etc), one of these configurations is the joined wing. The main potential benefits range from a reduced induced drag to a more efficient structural design. Other interesting advantages are expected for the flight mechanics/dynamics behavior and capabilities, for engine integration possibilities, and for the operational impact. One of the most advanced and relatively unexplored fields is the aeroelasticity of joined wings airplanes. Nowadays, the aeroelastic response has not yet been well understood and, therefore, represents an interesting phenomenon to be further explored. The particular wing layout of joined wings is responsible for strong structural geometric non linearities, which are relevant even for small angles of attack and attached flows. More in detail, this research aims to analyze the static (divergence) and dynamic (flutter) aeroelastic instabilities and investigate the post-critical behavior with particular emphasis on the so called limit cycle oscillation (post-flutter analysis). The analysis will be conducted for realistic wing box configurations, represented with high fidelity structural models. Aeroelastic tailoring by means of composite materials will be also investigated.

This research is supported in part by SDSU/College of Engineering funds.

Numerical Exploration of the Dynamics of Coupled Spin Torque Nano Oscillators

By James Turtle, Katie Beauvais, and Richard Shaffer

Since the discovery of Giant Magnetoresistance in the late 80s, Spintronics has become an emerging field of electronics. One critical component to modern day wireless communications is the microwave voltage oscillator. This work explores the use of Spin Torque Nano Oscillators (STNOs) to produce a spintronics voltage oscillator in the microwave range. STNOs are quite small – on the order of 10 nm – and frequency agile. However, experimental results to date have produced power outputs that are too small to be useful. To increase power output, we investigate systems of coupled STNOs. Numerical simulations indicate that n synchronized STNOs configured in series or parallel produce n2-times as much power as n uncoupled STNOs. However as the number of oscillators n increases, the regions of parameter space corresponding to synchronization tend to shrink. To set the foundation for further analysis, we consider both Spherical and Complex Stereographic coordinates for the Landau-Lifshitz-Gilbert Equation with spin torque term. Both coordinate systems effectively reduce the equation of a singleSTNO from a three dimensions to two. Further, the Complex Stereographic representation transforms the equation into a nearly polynomial form that may prove useful for advanced dynamics analysis. Qualitative bifurcation diagrams show a rich set of behaviors in the parallel and series coupled systems and serve to develop intuition in system dynamics.

This research is supported in part by NSF and SDSU/CSRC funds.

Simulations of Coupled SQUID and bi-SQUID Arrays

By Susan Berggren, Antonio Palacios, and Anna Leese de Escobar

This research focuses on conducting extensive computer simulations and analysis of the average voltage response of arrays of non-uniform Superconducting Quantum Interference Devices (SQUIDs) and bi-SQUIDs (a SQUID with an additional junction). These arrays will serve as the basis for the development of a sensitive, low noise, significantly lower Size, Weight and Power (SWaP) antenna integrated with Low-Noise Amplifier (LNA) using the SQUID technology. The non-uniformity in size of the SQUIDs (or bi-SQUIDs) in the array produces an average voltage response that has a pronounced single peak with a large voltage swing around the zero magnetic field. We develop and validate a full mathematical model for SQUID arrays, investigate the different distributions of loop sizes, do a perturbation analysis on the system of equations and compare the simulations to experimental results. The end goal is to invent a new device and systems designs capable of significantly exceeding, per size weight and power, state-of-the-art receiver system measures of performance such as bandwidth, sensitivity, dynamic range and spurious free dynamic range.

This research is supported in part by The Tactical SIGINT Technology Program and the ONR NREIP Internship Program.

High Performance Computing in Water-Rock Interaction and Reactive Transport Modeling for Simulation of Geologic Carbon Dioxide Sequestration

By Eduardo Sanchez, Christopher Paolini, and Jose Castillo

Carbon dioxide capture and geologic sequestration is a promising technology to minimize the environmental impact of greenhouse gases, whereby CO2 is separated from flue gases expelled by coal-fired power plants, compressed to a

supercritical phase, and injected into exhausted gas reservoirs or deep brine aquifers. It is believed that CO2 can remain sequestered in such formations, depending on the chemical and mechanical characteristics of the underground resident water and rock constituents. To simulate the long-term effects of geologic CO2 sequestration, numerical water-rock interaction and reactive transport models are employed. Researchers at the Computational Science Research Center at San Diego State University, along with Sienna Geodynamics, Inc., are developing a novel water-rock interaction and reactive-transport simulator called WebSymC. Traditionally, numerical codes that simulate water-rock interaction sequentially solve an elemental mass balance equation for each control volume that represents a defined lithology containing some fraction of brine with a number of charged aqueous solute species. Pressure, temperature, and solute concentrations are then solved in separate modules and coupled through an iterative process until a convergence criteria is satisfied. Coupling is achieved by iterating between the discretization of mass-transfer coefficients and solving a discretized form of elemental conservation equations and equilibrium reaction expressions. Mass-transfer coefficient matrices constructed from formation and injectant water velocities and solute concentrations, derived from the previous iteration, are constructed and solved using LU factorization. However, this formulation is not well suited for execution on many-core distributed clusters. In this work we present a numerical scheme whereby all solute concentrations in all control volumes are solved simultaneously by constructing a large block-banded sparse matrix of dimension Na x Nx, where Na is the number of diffusion, advection, and reaction terms and Nx is the number of control volumes. These very large sparse matrices are then factored using the distributed variant of SuperLU developed at Lawrence Berkeley National Laboratory. Performance metrics are presented to compare our large sparse matrix scheme against a sequential scheme on the SDSC 10K core XSEDE cluster trestles.sdsu.edu. Simulations based on the Frio Formation Test are presented with respect to achieved speedup, efficiency, and grid refinement impact.

This research is supported in part by NSF funds.

Detecting Bacteriophage Structural Protein Sequences Using Artificial Neural Networks

By Michael Arnoult, Victor Seguritan, Nelson Alves, and Anca Segall

Phages are adept at manipulating host populations by killing their hosts via cell lysis or conferring selective advantages to their hosts by contributing phage-encoded fitness factors. As a result, phages play a significant role in host survival and pathogenicity, and in nutrient redistribution. The discovery of phages from environmental samples may provide clues to the physiological impact of viruses on the microbial community and human health. Accurate identification of viruses would also aid in better detection and diagnosis of disease, and in vaccine development. Unlike viral structural proteins, the catalytic activity of most enzymes generally demand high amino acid conservation, which may serve as signatures that are relatively easy to detect by sequence alignment. Conversely, viral structural protein function is challenging to detect from sequence data because of insufficient experimental data, low sequence conservation, and few known conserved catalytic sites or sequence domains.

Our method of predicting phage structural protein sequences by amino acid composition uses Artificial Neural Networks (ANNs) that were trained by the Levenberg-Marquardt supervised learning algorithm with validation to avoid the effects of overfitting. The networks correctly classified 76 f test sequences with 73 pecificity and 84 ensitivity, and identified all coding sequences of the VP16T phage genome that are similar (e-value ≥ e-2$) to known phage structural proteins. Three of the ΦVP16T coding sequences detected by our ANNs were experimentally confirmed, two of which do not have similarity to known sequences. In addition, we trained ANNs to detect phage major capsid (MCP) and tail proteins. The MCP and tail ANNs were used to predict the function of phage hypothetical proteins from the Reference Sequence database. Gene constructs of the ANN-predicted sequences were expressed and visualized by transmission electron microscopy.

Therefore, our ANNs provide a new tool for identifying phage structural proteins, which are not detectable by traditional bioinformatic analysis. The networks will be valuable in situations where the genomic sequence is available but in vitro propagation of the phage may not be practical or possible. Our ANNs may also be useful for the analyses of DNA sequences that are obtained from exotic locations, or for the identification of prophages in microbial genomes.

This research is supported in part by NSF Viral Dark Matter (DEB-1046413) funds.

Projected Hartree-Fock in a Shell Model Basis

By Joshua Staker and Calvin Johnson

We implement Projected Hartree-Fock (PHF) in a shell model basis for nuclei. Starting with the deformed Hartree-Fock (HF) slater determinant, we project out states of good angular momentum in order to study the sectrum, which is then compared to the exact variational technique known as Configuration Interaction (CI). All three methods (PHF, HF, and CI) are computed using the same interaction and single-particle space, which has not been studied before. We look at spectrum comparisons for the fixed parity s-d and p-f fixed parity shells, as well as the mixed parity p-sd shell.

This research is supported in part by Department of Energy grant DE-FG02-96ER40985 funds.

Analysis of HIV-1 Integrase Inhibitors Using Computational QSAR Modeling

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

We have developed a novel differential evolution-binary particle swarm optimization (DE-BPSO) algorithm for the development of quantitative structure-activity relationship (QSAR) models to study the physiochemical interactions between 91 structurally diverse HIV-1 integrase inhibitors (β-diketo acids) and the HIV-1 virus. 387 constitutional, geometrical, topological, electrostatic, and quantum-chemical descriptors were computed for each of the 91 structures. DE-BPSO is used to search for optimal descriptor subsets for the development of multiple linear regression based QSAR models. Models satisfying predictive statistical constraints (r2 > 0.6, r2validation > 0.5, r2test > 0.5) are considered for analysis of the physiochemical features of Î²-diketo acids conducive for inhibition of HIV-1 integrase. The selected model for analysis suggests that molecular volume and electrostatic interactions of the inhibitors play a dominant role in the inhibition of HIV-1 integrase. We plan to use this model as a virtual screening tool to identify novel HIV-1 integrase inhibitors.

This research is supported in part by NIH funds.

Measurement of Temperature Field in a Stabilized Downward Spreading Flame

By Wynn Tran, Subrata Bhattacharjee, Christopher Paolini, and Fletcher Miller

Although a downward spreading flame exhibits steady-state behavior in flame fixed coordinates, the propagating flame creates an unsteady phenomenon with respect to the laboratory frame of reference, making it difficult for field measurement. In this study, a spreading flame is stabilized by moving a sample holder upward at the rate of spread. This is accomplished by a PID controller that moves the sample holder through a stepper motor in order to maintains a constant temperature (voltage) reported by a gas phase thermocouple at the flame leading edge that is fixed to the laboratory frame. For flame spread over thin ashless filter paper, the stabilizer produced a stationary flame for a 120s duration. A thermocouple mounted on a dual-axis probe is used to map the flame temperature. Different thermocouple sizes and orientations are tested to reduce the heat loss due to radiation and conduction through the thermocouple wire. The temperature field is reconstructed from multiple experiments and compared with results of a numerical simulation.

This research is supported in part by NASA funds.

Compact, Broadband, Geolocation Systems

By Daniel Lyons, Antonio Palacios, and Robert Dickey

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

This research is supported in part by Navy STTR Phase I Contract: N68335-11-C-0426 funds.

Promoter Analysis Identifies a Regulatory Cassette that is Shared Among Autophagy Genes with a Common Function/ Subprocess

By Lena D. van der Stap, Roberta A. Gottlieb, and Kim Finley

BACKGROUND: Macroautophagy (autophagy) is one of the primary homeostatic mechanisms that the cells of organisms use to maintain energy, nutrient, and metabolic balance. The pathway shows dynamic regulation and can be rapidly enhanced under conditions of starvation, infection or stress. In addition, it has been shown that nutritional excess and enhanced insulin/ TOR signaling serve as a potent suppressors of autophagy. Autophagic defects have progressive consequences within cells. Depending on the tissue-specific requirements of the pathway, autophagy has been linked to disorders of immune, cardiac and neural systems. It is hypothesized that the position of individual transcription factor binding sites and regulatory cassettes within the promoter will be conserved between subsets of autophagy genes that are interacting partners within the pathway. These conserved sequences may be predictive of transcriptional co-regulation between autophagy components. Several computational matrix-based approaches were used to compare upstream promoter sequences of individual human and macaque autophagy genes. Both pattern matching and detection algorithms were used to identify, map, and characterize several putative cis-regulatory elements in the 5' promoter sequences of multiple autophagy genes. RESULTS: Pairwise comparisons between human and macaque promoter sequences of individual autophagy genes were performed. A substantial degree of conservation was found in the 5' sequence within 4.0kb of the genes' transcriptional start sights. On average 70-92 dentity was found between species within this non-coding sequence, and a significant degree of spatial conservation wasobserved for most binding sites. In addition, a highly conserved cassette sequence

was identified that was initially identified from BLAST-z alignments of the human Map1LC3b and Atg4A 5' promoter regions. We found that cassette number and spatial organization show considerable overlap among those pathway components that closely interact or function in concert for autophagosome biogenesis, further suggesting potential co-regulation of these genes. Conversely, cassette positions and distributions varied greatly between the promoter regions of duplicated autophagy gene paralogs such as Atg4A and Atg4D. The rVista software was used for a detailed analysis of the regulatory cassette. Multiple highly conserved transcription factor binding sites were found within the cassette, which included NRF2/MAF/TAXCREB, PITX2/CRX, PITX2/LUN1, HNF3/FOXD3 clusters. Functional analysis of cassette clusters was further broken down into five major physiological responses; 1) early development and pattern formation, 2) early immune and the inflammatory responses, 3) metabolic development and insulin and glucose metabolism, 4) visual development and circadian cycles, 5) stress responses. CONCLUSIONS: By comparing the 5' promoter sequences of human and macaque autophagy genes we identified multiple conserved cis-regulatory elements. In addition to transcription factor binding sites, we identified and characterized a unique cassette sequence that was conserved in nearly all autophagy genes but was absent in a select set of control promoters. The number and position of these autophagy gene cassettes suggested that pathway components that interact or function together at a particular point during autophagosome formation had conserved promoters. This work may also serve as a foundation for the further analysis of autophagy gene evolution. The identification of these cis-element sub-groupings will facilitate the design of experiments that examine the regulation of autophagy genes under a variety of physiological conditions, including metabolic syndrome, aging, immune dysfunction, cardiac disease, cancer, and neurodegenerative disorders.

This research is supported in part by NIH RoadMap Initiative award T90 DK07015 funds.

Benchmarking Approximations for the Electronic Structure of Atoms

By Micah Schuster and Calvin Johnson

A full numerical solution of the electronic structure of atoms, usually through diagonalization of the many-body Hamiltonian using configuration-interaction, is not always computationally tractable. Therefore, we benchmark three standard approximations, Hartree-Fock (HF), projected Hartree-Fock (PHF), and the random phase approximation (RPA), against 'exact' configuration-interaction (CI) using the same input parameters for all four calculations. These inputs, the atomic one- and two-body interactions, are computed analytically using Slater-type orbitals (STO). This gives a direct comparison between methods for the ground state energies, ionization potentials and electron affinities, for the atoms lithium through neon. These methods could be useful when optimizing basis sets. Obtaining exact results at the beginning of the optimization process is not necessary; therefore, a less accurate method can allow for a faster exploration of basis sets. With this motivation in mind, we perform a sample basis optimization on carbon and boron to determine which method, particularly PHF and RPA, can be used as a proxy for CI.

This research is supported in part by Department of Energy grant DE-FG02-96ER40985 funds.

Tools For Fast Sequence Alignment

By Sajia Akhter and Robert Edwards

Metagenomics or random community genomics is a rapidly emerging field in microbiology. There are more than 3,000 publicly available metagenomes in the Sequence Read Archive at NCBI. To be annotated and analyzed the metagenome sequences need to be compared with genes, proteins and genomes in different databases. To make a similarity profile between many metagenomes, sequence comparisons are necessary. Because of the recent advances in sequencing technologies, the number of metagenomes has been increasing each year, and consequently there is a demand for faster sequence alignment algorithms. In this study, we developed two exact alignment approaches, which work faster than existing tools but give the same accuracy in protein and DNA sequence alignment.

This research is supported in part by NSF funds.

Diffusion and Transport of Calcium Within a Cardiomyocyte Single Sarcomere

By Rosa Lemus

The isolated neonatal rat ventricular heart cell is a widely used model system for studying cardiac muscle contractility and the cell's behavior in health and disease states. Our laboratory has focused on the role of calcium ions in heart excitation, contraction and relaxation, including the expression of genes that serve in calcium transport across cell membranes (the outer membrane and the sarcoplasmic reticulum, or SR, that stores calcium within the cell). I have developed a computer simulation of calcium fluxes within a single sarcomere, the repeating contractile unit of myofibrils within the cardiocyte. The 2-dimensional model accounts for calcium exchanges within the (thick and thin) myofilament system, between the SR's terminal and longitudinal cisternae, and within the cytosol. The model analyzes fluxes among neighboring voxels in the sarcomere in response to a trigger calcium signal (calcium-induced calcium release). An animated visualization of the fluxes uses pseudocolor to represent the calcium concentration changes with time in the sarcomere during a single twitch.

This research is supported in part by SDSU/CSRC funds.

Vibrational Energy Levels of Acrolein Related Free Radicals Asdetermined by a Finite Element Approach

By Peter Zajac, Dong Xu, and Andrew L. Cooksy

Relocalization isomers are configurational isomers connected by a vibronic pathway that redistributes electron density, altering orbital hybridizations and molecular geometry without changing the sequence of chemical bonds. We report a computational study of the most stable acroleinyl free radicals, which exhibit potential energy surfaces (PES) with distinct, non-equivalent minima, separated by small energy barriers. A three- dimensional potential energy surface has been calculated at the explicitly correlated coupled cluster level. Unlike the HC3O radical, which we have studied previously, the distinct minima on the acroleinyl surface do not share a common electronic state symmetry, and the configurational isomerization involves a straightforward symmetry breaking. The vibrational eigenvalues and eigenvectors are solved on this surface using the finite element method, and used to predict rovibrational energies and effects of vibrational averaging that may help identify and quantify effects of the isomerization on infrared spectra.

This research is supported in part by Army Research Office(57989-CH) and an equipment grant from the National Science Foundation (CHE-0947087) funds.

Introduction of Non-linear Elasticity Models for Characterization of Shape and Deformation Statistics: Application to Contractility Assessment of Isolated Adult Cardiocytes

By Trevor Hawkins, Carlos Bazan, David Torres-Barba, and Peter Blomgren

We are exploring the viability of a novel (and potentially unified) approach to cardiocyte contractility assessment based on bio-mechanical properties of the cardiac cells, energy conservation principles, and information content measures. All of this within a variational framework that requires the solution of nonlinear partial differential equations. We define our measure of cell contraction as being the distance
between the cell shapes, assessed by the minimum total energy of the domain deformation (warping) of one cell shape into another. To guarantee a meaningful vis-a-vis correspondence between the two shapes, we employ both a data fidelity term and a regularization term. The data fidelity term is based on nonlinear features of the shapes while the regularization term enforces the compatibility between the shape deformations and that of a hyper-elastic material. We tested the proposed approach by assessing the contractile responses in isolated adult rat cardiocytes and contrasted these measurements against two different methods in the literature. Our results show good qualitative and quantitative agreements with these methods as far as frequency, pacing, and overall behavior of the contractions are concerned. We hypothesize that this proposed methodology, once appropriately developed and customized, can provide a framework for computational cardiac cell biomechanics that can be used to integrate both theory and experiment. For example, besides giving a good assessment of contractile response of the cardiocyte, since the excitation process of the cell is a closed system, we can also attempt to infer statistically significant model parameters for the constitutive equations of the cardiocytes.

This research is supported in part by CSRC/SDSU department and NIH Roadmap Initiative award R90 DK07015 and NIH NIDDK funds.

Two and Three Bit Quantization for Decoding Low Density Parity Check (LDPC) Codes

By Raymond Moberly

Two-bit and three-bit quantizations for Sum Product Algorithm(SPA) Low-Density Parity-Check (LDPC) decoding are simulated in software to measure decoding performance and implemented in programmable logic using a Field Programmable Gate Array (FPGA). Analysis of the Sum Product Algorithm (SPA) is performed. While quantization effects are the focal point of the research, a suitable choice of the number of decoding iterations and a study of the number of bits of precision used in the decoder are both presented to substantiate the quantization experiments. The hardware design combines the parity-check and variable-node update steps into a single computational step. Hardware implementation requirements are compared to a selection of other published works, including the work of Planjery et al. Decoder performance, measured in terms of both Bit Error Rate(BER) and Frame Error Rate (FER), is tested for each two-bit and three-bit quantization over a range of Signal to Noise Ratio (SNR) values. A flexible implementation is proposed that can adapt the quantization as the channel conditions change; it outperforms a single quantization.

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Initial Results of a Parallel 3D Curvilinear, Non-hydrostatic Coastal Ocean Model

By Mary Thomas and Jose Castillo

The SDSU Unified Curvilinear Ocean Atmospheric Model is a non-hydrostatic, Large Eddie Simulation (LES) CFD model capable of running both ocean and atmospheric simulations. It is the only environmental model in existence today using a full, 3D curvilinear coordinate system, which results in increased accuracy, resolution, and reduced times to solution. UCOAM is a petascale model: it is capable of resolving sub-km scale

fluctuations requires large arrays (1010 elements; the curvilinear system requires large number of arrays (~100); communication occurs along all 3 axes; and full simulations will generate TBytes of data. Consequently, this model requires parallelization. To facilitate UCOAM computations and data management, we have developed a new parallel framework capable of distributing the computations across arbitrary 3D processor arrangements, manages the complexity of the staggered grid variables, and performs communications along all axes, including diagonal and tri-diagonal neighbors. To facilitate computations, we have developed computational environment (CE) based on the Cyberinfrastructure Web Application Framework (CyberWeb) which supports the development of web services and portals. In this paper we discuss the design and architecture of the parallel framework and supporting CE infrastructure, as well as challenges associated with parallelizing this novel model. We include the first initial parallel results for a small problem size (105 elements) 1 meter resolution seamount test case that shows scaling of the parallel model.

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