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<th>Time</th>
<th>Event/Activity</th>
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<tr>
<td>12:00 pm</td>
<td>Registration / Buffet Lunch</td>
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<tr>
<td>1:00 pm</td>
<td>Stanley Maloy, Dean</td>
<td>Welcome / Opening Remarks</td>
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<td>College of Science</td>
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<td>San Diego State University</td>
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<td>1:10 pm</td>
<td>Jose E. Castillo, Director</td>
<td>Computational Science at SDSU and ACSESS Program</td>
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<td>Computational Science Research Center</td>
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<td>San Diego State University</td>
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<td>1:20 pm</td>
<td>Gail K. Naughton, Dean</td>
<td>Key Note Speaker</td>
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<td>College of Business Administration</td>
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<td>1:45 pm</td>
<td>Coffee Break</td>
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<td>1:50 pm</td>
<td>“Industry Academic Interaction”</td>
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<td>Terie Scerbo, Academic Relations</td>
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<td>Learning &amp; Development</td>
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<td>QUALCOMM, Inc.</td>
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<td>Bob Kain, Vice President, Engineering</td>
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<td>Illumina, Inc.</td>
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<td>Victor Pereyra, Chair, CSRC Industry Advisory Board</td>
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<td>Weidlinger Associates Inc., ACSESS Partner</td>
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<td>Gordon Brown, Industry Outreach Coordinator</td>
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<td>Computational Science Research Center</td>
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<td>Carlos Bazan, Moderator, Computational Science</td>
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<td>Research Center</td>
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<td>3:00 pm</td>
<td>Poster Presentation / Reception</td>
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<td>4:30 pm</td>
<td>Paul Paolini, Associate Director</td>
<td>Poster Presentation Awards &amp; Closing Remarks</td>
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<td>Computational Science Research Center</td>
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<td>San Diego State University</td>
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<td>5:00 pm</td>
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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—ranging from providing computing infrastructure and support for students, to developing educational programs and industrial interactions. It is the aim of CSRC to function as an independent, self-sustained unit. Therefore, its operation crucially depends on extra-mural funding.

Mission Statement

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

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

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

Executive Board

Program Director:
Jose E. Castillo

Industry Projects Coordinator:
Gordon Brown

Associate Directors:
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Eugene Olevsky
Paul Paolini

Scientific Advisory Board

Chair: Antonio Redondo, Theoretical Division
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Richard Greenblatt, Source Signal Imaging Inc.

John Newsam, Windhover Ventures LLC

Antonio Redondo, Theoretical Division
Los Alamos National Laboratory
Featured Posters

Geographical Impact on Metagenomes
By Daniel Pick, Nao Hisakawa, and Forest Rohwer

Many metagenomic data sets biologists have collected in recent years have become publicly available at archives such as MGRAST, http://metagenomics/nmpdr.org, and CAMERA, http://camera.calit2.net. These specimens have been annotated with the geographical coordinates where the samples were taken, enabling them to be integrated with digital map data obtained from geographic information systems (GIS). Recently, Parks et al.1 developed GenGIS, an open source geospatial information system for genomic data, precisely for the purpose of generating and testing new hypotheses regarding global biodiversity. In this study, we are searching through a wide variety of maps available from ArcGIS, http://www.arcgis.com/, for meaningful correlations to metagenomes available from public databases. In Dinsdale et al2, it was shown that metagenomic analysis can explain the variance among and within environmental samples, and in Willner et al.3 it was shown that dinucleotide composition defines a metagenomic signature which can explain up to 80% of the variance between biomes.

We hypothesize that there are previously undiscovered correlations between such geographical features as sea surface temperature, UV light, organic pollution, and calculated metagenomic characteristics such as dinucleotide ratios and hits to metabolic subsystems. We are using a variety of computational tools to curate the data, compute meaningful statistics, and summarize the results. Data from the public repositories has been cleaned with PRINSEQ, a publicly available tool for this purpose developed by the Edwards lab at SDSU. We are using the R open source language to calculate the correlations between geographical features and dinucleotide ratios and metabolic subsystem hits.


Mimetic Finite Difference Methods: An Application in Modeling Geological Sequestration of Carbon Dioxide
By Eduardo Sanchez and Christopher Paolini

Mathematical models of continuum mechanics phenomena are usually described by boundary value problems, expressed as a system of partial differential or integral equations. Particularly, in modeling geologic CO₂ capture and sequestration (CCS), given the necessity of accounting for diffusive and advective fluxes, as well as kinetic and equilibrium reactions, a particular form of the conservation of mass equation is of special interest. To facilitate the numerical solution of partial differential or integral equations, discretization can be achieved using any one of a large number of techniques including finite difference, finite element, or finite volume methods. Often, these conventional methods are applied by discretizing the considered system of equations directly but, although these methods are useful and relatively simple, one disadvantage of employing such methods is that the selected discretization scheme may have little connection to the underlying physical problem. Mimetic methods, on the other hand, begin first by discretizing the continuum theory underlying the problem. These methods initially construct a discrete mathematical analog version of the considered phenomena which constrains the structure that the discrete mimetic operators will have. After mimetic operators are constructed, operators can be substituted into the system of partial differential or integral equations, yielding a mimetic discretization for the considered problem which automatically satisfies the discrete version of the studied physical law. As a result, discretizations obtained using mimetic methods tend to better replicate the behavior found in the actual continuum problem. In this paper, we compare the use of mimetic methods against those methods traditionally used for CCS simulation. Specifically, mimetic operators are constructed in a way that yield comparably higher order approximations at, or near, the boundaries of a defined reservoir. These techniques are applied in the study of one dimensional horizontal advective-diffusive flow of CO₂ charged water through a sandstone based reservoir. Results are then compared in terms of efficiency, accuracy, and required computational effort.

An ANFIS-Based Multi-Sensor Structure for a Mobile Robotic System
By Jake Taylor, Abraham Gallardo, Christopher Paolini, and Gordon K. Lee

The control of a nonlinear system is a challenging problem particularly when the system has some uncertainty or there are imperfections in the model dynamics. One approach that has gained some success employs a fuzzy structure in concert with a neural network (ANFIS); the fuzzy component compensates for the uncertainty while the neural network component models the underlying system dynamics. This paper presents a system architecture for a mobile robotic system that employs an ANFIS controller for path tracking, a virtual field strategy for obstacle avoidance and path planning, and multiple sensors (an ultrasonic array, a thermal sensor, and a video streaming system) to obtain information about the environment. Simulation results and preliminary evaluation show that the proposed architecture is a feasible one for autonomous mobile robotic systems.
Phage-Detector: A Novel Algorithm for Finding Prophages in Microbial Genomes that Combines Similarity-Based and Composition-Based Strategies

By Sajia Akhter, Ramy K. Aziz, and Robert A. Edwards

Prophages are bacteriophages that cause temporarily non-lethal bacterial infections, resulting in their DNA being stably maintained in the cell and replicated along with their unwilling hosts. These mobile elements have tremendous impact on their host’s genomes and phenotypes, leading to strain emergence and diversification, increased virulence, or antibiotic resistance. However, finding prophages in microbial genomes remains a problem with no definitive answer. The majority of existing tools rely on detecting genomic regions enriched in proteins with known phage homologs, which hinders the de novo discovery of phage regions. In this study, a weighted phage detection algorithm, Phage-detector was developed based on seven distinctive characteristics of prophages i.e. protein length, transcription strand directionality, customized AT and GC skew, the abundance of unique phage words, phage insertion points and the similarity of phage proteins. The first five characteristics are capable of identifying prophages without any sequence similarity with known phage genes. Phage-detector locates prophages by ranking genomic regions enriched in distinctive phage traits, which leads to the successful prediction of 92 of prophages (including 33 previously unidentified prophages) in 95 complete bacterial genomes with 8 false negative and 18 also positive.

Smart Slice Prioritization in H.264 AVC

By Seethal Paluri, Sunil Kumar, and Barbara Bailey

H.264 is the newest video coding standard from ITU-T Video Coding Experts and ISO/IEC Moving Picture Experts Group. Its enhanced compression performance and “network-friendliness” makes this standard very popular. When the compressed video data is transmitted over a wireless channel it is highly susceptible to channel errors. It is therefore important to prioritize the compressed data so that good perceptual video quality can be maintained at the receiver even during unreliable channel conditions. Therefore, we consider the problem of predicting slice loss visibility using a Generalized Linear Model (GLM). We model the distortion caused due to the loss of a single slice by using various features of the video that are extracted while the video is being encoded. Subsequently, a higher priority can be assigned to slices that contribute to higher distortion. This will support in improving video data quality.

A Computational Study of Shear Banding in Reversible Associating Polymers

By Joris Billen, Joris Stegen, and Arlette R. C. Baljon

A novel hybrid MD/MC simulation technique is employed to study the rheological properties of telechelic polymers. When enough polymer end-groups aggregate together, a reversible gel is formed. The aggregates form crosslinks to each other as the polymer chain acts as a bridge between them. At low temperature or high concentration, the unsheared system is arrested. After application of a uniform shear, it yields and subsequently flows. Two shear bands are observed in the flow profile, a phenomenon also observed in recent experimental studies. The stress fluctuates erratically over time. These macroscopic observations are correlated with changes in the microstructure. The simulation allows us to investigate such changes between the two shear bands, and between the sheared and the unsheared system. We report on differences in topology, chain orientation, radius of gyration, and the occurrence and spatial distribution of multiple bridges between aggregates.

This work is supported by the NSF under Grant No. DMR0517201.


The Aggregation Kinetics of a Simulated Telechelic Polymer

By Mark Wilson, Arlette Baljon, and Avinoam Rabinovitch

We investigate the aggregation kinetics of a simulated telechelic polymer gel. In the hybrid Molecular Dynamics (MD)/ Monte Carlo (MC) algorithm, aggregates of associating end groups form and break according to MC rules, while the position of the polymers in space is dictated by MD. As a result, the aggregate sizes change every time step. In order to describe this aggregation process, we employ a master equation. It defines the change in the number of aggregates of a certain size in terms of reaction rates. These reaction rates indicate the likelihood that two aggregates combine to form a large one or that a large aggregate splits in two smaller parts. The reaction rates are obtained from the simulations at several temperatures of the gel. Our results indicate that the rates are not only temperature dependent, but also a function of the sizes of the aggregates involved in the reaction. Using the measured rates, solutions to the master equation are shown to be stable and in agreement with the aggregate size distribution, as obtained directly from simulation data. Furthermore, we show how variations in these rates give rise to the observed changes in the aggregate distribution that characterizes a gel transition.
**Incorporation of New Web-Based Technology to Expand the Accessibility and Flexibility of RTM Software for Use in Modeling CO$_2$ Sequestration**

*By Christopher Binter, Tony Park, and Christopher Paolini*

The advancements of mobile technology allow Internet access in more places than ever before. However, there has always been a tradeoff between mobility and speed. The computational power required to run most geologic modeling software requires it be done on desktop or server computers, thus limiting mobility. This paper demonstrates how emerging new Internet technologies can be incorporated with complex CCS modeling software. This incorporation bridges the gap between personal Internet devices and powerful servers. A novel new AJAX-based Web application has been developed that allows a user to define, run, and view simulations of Reaction-Transport modeling (RTM) software on any computer with Internet access using a standard Web browser. Computationally intensive CCS simulations are carried out on a server, allowing complex simulations to be run, regardless of the user’s mobile device speed. Another advantage of such a design is that the user can run and view simulations on a range of computers without having to save and manage CCS configuration or output files. This allows a user to quickly modify resident and injectant water compositions, lithological characteristics, and simulation parameters all from a Web browser. Two CO$_2$ sequestration scenarios were modeled using this Web interface and RTM software. The first situation modeled was 1D horizontal injection of CO$_2$ rich waters with CO$_2$ aqueous concentrations ranging from 0.1M to 1.0M being injected for 5 years at seepage velocities of 100, 300, and 500 [cc/(cm$^2$ yr)]/$\rho$ through a homogenous sandstone formation. The Web application allows easy configuration and viewing of results which show the transport of tracer ions along the injection front and dissolution-precipitation of minerals. The second scenario modeled was 1D vertical diffusion of CO$_2$ through sandstone and a shale cap rock. Simulations modeling 5 years of vertical diffusion show no CO$_2$ leakage through the cap rock and little change in porosity and permeability. The Web interface/RTM software coupling presented in this paper is not only useful in modeling CO$_2$ sequestration, but also in providing never before seen accessibility and flexibility in managing large CCS datasets.

**Computational Modeling of Quenching**

*By Matthew San Pedro and Gustaaf Jacobs*

In metallurgy, quenching is typically used to harden materials. Quenching cools metals rapidly which prevents certain phase changes that reduce the strength of a material. If a metal is quenched in water, three distinct cooling processes occur. First, film boiling dominates as a vapor envelope is formed between the hot surface of the specimen and the quench medium. Once a transitional temperature is achieved, the vapor envelope begins to collapse as the quench enters the nucleate boiling phase. The nucleate boiling regime is characterized by a high heat transfer coefficient of approximately 100 times greater than the film boiling phase. Once the temperature of the specimen is below the boiling point of water, a slow cooling quench continues by convective heat transfer.

Considering the number of conditions introduced, experimental testing is necessary to reach desired quenching rates. This often involves repeating a number of tests, which demands intensive labor and costs. Computational models are providing a good alternative. Not only are they less expensive, computational results provide more detail. In this poster, we show initial analyses towards the computational modeling of the three cooling phases of aluminum quenching in water.

In a first analysis, the water flow dynamics and heat transfer over an aluminum cylinder are modeled. A steady state two-dimensional framework is considered. The temperature of the specimen is initialized below the boiling point of water and the slow cooling quench is analyzed. Buoyancy flows are modeled according to Boussinesq approximations. The flows are computed with Fluent, a commercial Computational Fluid Dynamics software. Grid convergence is established by comparing computational result with three grids of successive refinement. It was found that the thermal boundary layer is thin if only convections transfers heat from the metal to the water and the heat transfer rates are hence high.

In future analyses, the effect of the film and nucleate boiling phases by adding complexity to the model such as evaporation, boiling, bubble formation, and mass flow will be considered.

**Comparing Hartree-Fock and Random Phase Approximation Calculations of Atomic Systems**

*By Micah Schuster and Calvin Johnson*

The atomic many-body problem has many approximations that allow for the computation of atomic spectra without full diagonalization. Three such methods, Hartree-Fock, projected Hartree-Fock and random phase approximation are compared to full CI while using the same input parameters for each method. The atomic one- and two-body interactions, used as input, are computed analytically using slater-type orbitals, STOs. This gives a direct comparison between methods.
Utilization of Reaction-Transport Modeling Software to Study the Effects of Reservoir Temperature and Seepage Velocity on the Sweep-Diffusion Front Displacement Formed after CO₂-Rich Water Injection

By Christopher Binter, Tony Park, and Christopher Paolini

The storage of carbon dioxide underground has been proposed as a method to reduce CO₂ concentrations in the atmosphere. The effects of CO₂ injection on subsurface lithologies and formation waters are complex and highly variable. With Reaction-Transport Modeling (RTM) software it is possible to quickly and easily model a range of injection scenarios and simulate the subsurface response, limiting costly and time intensive field experiments. In this work, RTM software has been used to simulate short term effects arising from the injection of CO₂-charged water in saline sedimentary basins, similar to the sandstone lithology of the Frio Formation, a regional brine and oil reservoir along the U.S. Gulf Coast. 1D horizontal simulations were run with CO₂ aqueous concentrations of 0.5M being injected for 5 years at seepage velocities of 300-355 [cc/(cm² yr)]/φ with reservoir temperatures ranging from 60° to 140°C. Simulation results presented in this paper show that, in particular, a moving volume of water with a relatively high concentration of H⁺ ion forms from the hydration of CO₂ that occurs when the injectant water mixes with the reservoir formation water. Results show that the diffusion driven mass transport of H⁺ throughout the reservoir sandstone occurs at a faster seepage velocity than the injectant-water velocity or sweep velocity. For these simulations, the diffusion and sweep front reaches a maximum separation of 35-40 m at 60°C and a minimum separation of 15m between 90°C and 120°C. Variations in the sweep velocity had little effect on the front separation. Bright spots on seismic surveys have been used to monitor the movement of injected CO₂ through formations. However, if an acidic front develops ahead of the CO₂ injectant front, as our simulations show, this could lead to degradation of seals far from where the injectant is believed to reside. Thus, when evaluating and monitoring CO₂ injection, it is important to consider the acidic front that can develop ahead of the CO₂ plume and its effects on reservoirs and seals.

Amplitude-Symmetric Sagnac Interferometry with Bose-Einstein Condensates in a Ring Trap

By Marty Kandes and Michael Bromley

We present the results of numerical simulations studying a scheme to perform Sagnac interferometry with dilute atomic gas Bose-Einstein condensates in a rotating simple harmonic oscillator ring potential. The proposed scheme involves determining the relative phase shifts observed in the interference patterns created during the collisions of two counterpropagating, amplitude-symmetric condensate wavepackets confined within the ring. In particular, we investigate on howthe condensates' nonlinear, mean-field interaction impacts the interferometric sensitivity and stability of the interference process during these collisions. Under the amplitude-symmetric regime, we find that there is little, if any, deviation in the observed phase shift response from what is predicted by the well-known (linear) Sagnac effect, even when highly nonlinear conditions are considered. However, while the Sagnac phase shift response remains linear, the interferometric visibility is observed to degrade as the number of atoms in the system is increased. Further limitations of the proposed scheme are also discussed as well as recommendations to help guide future research on this topic.

Statistical Analysis of a Novel Method to Measure Mammalian Neonatal Cardiocyte Contractility

By Esteban Vazquez-Hidalgo and David Torres-Barba

There is a need to study neonatal cardiocyte contractility in order to compare functional responses of cells relative to a wide variety of results from various pharmacological, physiological and molecular genetic assays. Current methods used to assess cardiocyte functionality include calcium transient signals, gene and protein expression, and contractility. Adult cardiocyte contractility measurements are more easily achieved since there is a measurable change in the cell’s boundary along the longitudinal axis, but there is no apparent shortening in the neonatal cell with its irregular shape. There is a need to develop a simple and practical tool to measure neonatal cell contractility. We have developed an image-based analysis method employing a Matlab-guided user interface (GUI). The GUI provides quick, quantitative analysis of neonatal cardiocyte contractility. I hypothesized that this new analysis method will provide a high degree of statistical reliability. Video images are acquired using an inverted phase microscope and a digital camera. We then extract a contractile signal from successive video frames using signal masking, total variation-based image smoothing, segmentation of the smoothed images, contour extraction from the segmented images, shape representation by polar Fourier descriptors, and assessment of the resulting “contractility” signal. When the beat-to-beat signal was normalized from 0 to 1, 0 being the peak of contraction and 1 being the relaxed state, the standard deviation was found to be 0.04. We have also implemented a series of mathematical steps to identify the onset of contraction, average the contractile signal, and detect the variability that exists in the contractile data. Using these methods we have been able to record variations that exist from beat to beat within the same cardiocyte as well as among a population of cardiocytes. We are currently developing faster and more automated software to handle the acquired contractile data. Supported by the NIH/NIGMS SDSU MARC Program 5T34GM008303 -21A1.
The real time contractile behavior of an isolated adult mammalian cardiac cell is commonly recorded as a shortening of the cell following excitation. Neonatal cardiac cells are preferred because they survive longer than adult cardiocytes. These cells do not exhibit shortening (their contractile machinery is not assembled and in place). Our laboratory has developed a neonatal cell contraction measurement based on a computational approach: digital video recording, variation-based image smoothing, segmentation, contour extraction, and shape representation of the cell by Fourier descriptors. Resultant contraction measurements can be validated by applying the technique to adult myocytes and comparing responses to cell boundary movement (shortening) records. An independent measure of the contractile potential of both adult and neonatal cells is the calcium transient that can be detected fluorescently by incubating cells in a calcium ion-sensitive dye such as Fura-2 or Fluo-3. Such dyes show a shift in their emission spectra in response to changes in free calcium ion concentration in the cytosol following excitation. Transients reveal the magnitude of the release of Ca\(^{2+}\) from the SR through ryanodine channels (RyR) and the subsequent resequestration of cytosolic Ca\(^{2+}\) by the SERCA pump and by Ca\(^{2+}\) exchange via the sarcolemmal Na\(^+\)-Ca\(^{2+}\) exchanger (NCX). We addressed three questions. (1) How consistent are calcium transient responses in a single neonatal cell, and do they provide a statistically valid measurement of contractility? (2) How variable are transients from cell to cell within the same population of isolated neonatal cells? (3) How well does this measurement of contractility agree with our new computational assay of contractility? Transients were measured on a PTI fluorescence microscopy system running Felix acquisition software. We automated the analysis of the transients, and used Excel to validate the results. Signals are averaged to improve S:N ratios. Parameters measured include the baseline (normalized to 0), amplitude (normalized to 1), intensity (signal integral), rapid (SERCA) and slow (NCX) resequestration rates, calcium release rate (Ryr), peak time, onset time, and decay time. Expressed in terms of normalized transient records, the SERCA resequestration rate was 2.37 \(\pm\) 0.30 \(\%\) per sec, while the NCX cytosolic Ca decrease rate was 0.154 \(\pm\) 0.063 \(\%\) per sec. The rate of calcium release was estimated to be 73 mM/sec, fast resequestration was 42 mM/sec and slow recovery was 0.52 mM/sec. By comparison, contractile records exhibited a 4% error, while the Ca\(^{2+}\) transient showed a 6.9% error.

We present the development of computational tools for handling and analyzing functional data of neonatal and adult cardiocytes. The motivation for our development is the need for simple and practical tools to study cardiocyte functional activities. Our methods can assist in the assessment and analysis of such data. We recently developed and published two computational frameworks to comprehensively assess contractile responses of isolated neonatal and adult cardiocytes. These recent developments and our capability to acquire calcium transients, allow us to obtain functional data from the same cardiocyte almost simultaneously. This functional data can be collected and analyzed to characterize the effects of inotropic factors in neonatal and adult cardiocytes. The developed computational tools are capable of analyzing functional responses obtained from both contractility and calcium transient measurements. We have implemented a series of mathematical methods for the specific purpose of analyzing cardiocyte functional data and extracting important functional parameters. From contractility measurements, we detect the time of onset of contraction, time to peak, contraction duration, and fast and slow recovery times. From calcium transient recording employing Fluo-3 fluorescent dye, we measure onset time, peak amplitude, fast (SERCA) and slow (NCX) exponential recovery rates, and calcium signal intensity (the integral). Averaging is used to improve signal-to-noise ratios for 10 msec sample rates. Statistical analysis of contractility and calcium transient signals show standard deviations of less than 3 in these measures. Most importantly our developments provide a way to effectively analyze functional data and extract functional parameters that before could only be retrieved manually with a considerable investment of effort and time.

Isle Royale created a unique ecological condition that allows the study of a simplified predator-prey model. We examined detailed data of moose and wolf populations for over 50 years. Agent-based models (ABM) provide a means of simulating population interactions. There exists a program, Ecobeaker, which provides a means for students to appreciate this basic predator-prey ecosystem using an ABM approach. We plan to study the system in greater detail and develop an improved ABM that better simulates the real data.
**Atomic Polarisabilities, Hyperpolarisabilities and the Factorisation of Molecular Interactions**

By Julia M. Rossi, Brandon A. Rigsbee, Kyle G. Rollin, and Michael Bromley

SAN DIEGO STATE UNIVERSITY

The properties of one and two-electron atoms and their molecules are calculated numerically using configuration interaction and perturbative methods. Firstly, we present calculations of the dynamic dipole and hyperpolarisabilities of the ground and low-lying excited states of atoms emphasising low-energy fields of interest in atomic clocks, and high-energy excitations that probe near Rydberg states. Theoretical expressions will be presented that factorise the long-range dispersion forces between two atoms into their individual scalar and tensor dipole polarisabilities at imaginary frequencies. This method yields $C_6$ dispersion coefficients in agreement with the latest theoretical values for both homo-nuclear and the hetero-nuclear interactions, e.g. Li(2s)-H(1s). The application of this methodology to di-atomic molecular symmetries involving non-$s$-wave atomic states will be emphasised.

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

By Raymond Moberly and Michael O'Sullivan

SAN DIEGO STATE UNIVERSITY

Contemporary technologists are looking for implementation strategies that will enable the realization of Low Density Parity Check (LDPC) codes in applications for wireless communication and data storage. Interest in iterative decoder design using a small number of quantization bits has been established by the published works of Zhang and Parhi and by the recent work of Planjery and Vasic. Both teams have devised designs suitable for digital logic implementation, for example in Field Programmable Gate Arrays (FPGA).

The authors have devised an approach not unlike that of Planjery and Vasic, using our previous results from finding an optimal quantization and a flexible implementation approach using an FPGA. Unlike their Binary Symmetric Channel approach, we take full advantage of the receiver sampling resolution available on a Gaussian channel; this, combined with the ability to select the quantization adaptively as the channel conditions change, allows improved gains, exceeding 0.5 dB. This research presents synthesis results showing the latency and footprint of our key computational component of the decoder design. Knowing the per-iteration computational latency and knowing how the number of iterations affects the decoding, we can evaluate trade-offs between per-iteration decoding gain and total decoding gain as we seek to optimize decoder throughput or power consumption.

**Predicting Phage Preferences: Lytic vs. Lysogenic Lifestyle from Genomes**

By Katelyn McNair, Rob Edwards, and Barbara Bailey

There are two distinct phage lifestyles: lytic and lysogenic. The lytic lifestyle has many implications for phage therapy, genomics, and microbiology, however it is often very difficult to determine whether a newly sequenced phage isolate grows lytically or lysogenically just from the genome. Using the ~200 known phage genomes, a supervised random forest classifier was built to determine which proteins of phage are important for determining lytic and lysogenic traits. A similarity vector is created for each phage by comparing each protein from a random sampling of all known phage proteins to each phage genome. Each value in the similarity vector represents the protein with the highest similarity score for that phage genome. This vector is used to train a random forest to classify phage according to their lifestyle. To test the classifier each phage is removed from the data set one at a time and treated as a single unknown. The classifier was able to successfully group 188 of the 196 phages for whom the lifestyle is known, giving my algorithm an estimated 4 error rate. The classifier also identifies the most important genes for determining lifestyle; in addition to integrases, expected to be important, the composition of the phage (capsid and tail) also determines the lifestyle. A large number of hypothetical proteins are also involved in determining whether a phage is lytic or lysogenic.

**Computational Modeling of Field-Assisted Sintering**

By Cristina Garcia Cardona, Eugene A. Olevsky, and Veena Tikare

SAN DIEGO STATE UNIVERSITY

A three-dimensional multi-scale model of Field-Assisted Sintering is presented. The model captures the complexity of the multiphysics phenomena involved in field-assisted sintering by coupling: electrical, thermal, stress-strain and densification components. The calculations are based on the finite-element (macroscopic scale) and kinetic Monte-Carlo (mesoscopic scale) codes. Specimen’s macroscopic behavior is described through a non-linear viscous constitutive relation. The simulation of the densification is based on local conditions, and micro-scale factors as grain growth are also taken into account. Thus not only distributions of current density, temperature and strain fields can be obtained but also a spatial density and grain size evolution can be computed. The sintering constitutive parameters such as sintering stress, bulk and shear viscosity moduli are determined through Monte-Carlo simulations of the grain-pore structure evolution. This corresponds to a true 3D, multi-scale, multiphysics modeling of sintering.
Featured Posters

**Unified Curvilinear Ocean Atmosphere Model (UCOAM)**
*By Mohammad Abouali and Jose Castillo*

Unified Curvilinear Ocean Atmosphere Model (UCOAM) is Large Eddy Simulation (LES) code solving Navier-Stoke’s Equations in ultra-high resolution curvilinear grid. UCOAM uses fully non-hydrostatic approach; hence, it is capable of performing simulations on curvilinear grids with horizontal resolution of couple of meters. UCOAM is capable of simulating both atmospheric and oceanic flows. UCOAM is part of General Curvilinear Environmental Model (GCEM).

**Towards the Parallelization of a Full, 3D, Curvilinear Coastal, Ocean, and Atmospheric Model**
*By Mary Thomas and Jose Castillo*

The General Curvilinear Environment Model (GCEM) System, is a Large Eddie Simulation (LES) CFD model. The GCEM is the only environmental model in existence today that uses a full, 3D curvilinear coordinate system, which results in increased accuracy, resolution, and reduced times to solution. Major components include the Unified Curvilinear Ocean Atmosphere Model (UCOAM), the General Curvilinear Coastal Ocean Model (GCCOM), and the General Curvilinear Atmosphere Model (GCCAM), the Distributed Coupling Tools (DCT), the Data Assimilation Unit (DAU), and the Computational Environment (CE). The CE is based on the Cyberinfrastructure Web Application Framework (CyberWeb). In this paper, we present early results of the first parallel version of the UCOAM component of the GCEM model.

**Implementing Data Assimilation Scheme in Shallow Water Equation with Curvilinear Coordinates**
*By Mariangel Garcia, Barbara Bailey, Dany De Cecchis, and Mohammad Abouali*

Various Data Assimilation (DA) schemes applied to a simplified curvilinear coordinates Shallow Water Equation (SWE) is considered in this poster. The true state and the background solution are defined in order to compare the performance of different DA schemes with different observation, frequencies, and accuracies. Two test cases are presented, one in a sine pool with close boundary condition and constant depth, and the second using a more complicated mesh. The goal is implementing Kalman Filter Techniques to study how to incorporate measured observations into a dynamical system model in order to produce accurate estimates. The proposed methods are based on discretization of the governing nonlinear equation using finite difference method in staggered mesh.

**Integrating CyberInfrastructure Resources and Services with the CyberWeb 2.0 Application Frameworks**
*By Carny Cheng, Jose Castillo, Smita More, Hetang Shah, and Mary Thomas*

The next generation of Cyberinfrastructure (CI) software must seamlessly couple high-end and low-end resources, networks and services, with users and applications in a manner similar to the way the Internet and Web function now. Additionally, the evolution of the current suite of emerging Web 2.0 technologies that are driving the Internet, the Web, networks and computing, is moving software development to a services oriented architecture (SOAs) approach that abstracts functionality and implementation from the interfaces needed to access the services. Complicating this problem is the fact that Web services, SOA's and cloud computing are ubiquitous computing platforms, and although CI has expanded beyond the traditional high performance computing and associated HPC applications it is not scaling. The existing CI software stack and approach to software tools and application development must be modernized to effectively utilize current technologies. In addition, software tools are needed that can both improve the way things work now, and scale with new infrastructure and tools. In this paper, we report on our efforts to develop a CI enabled framework, including the software components needed to build CI Applications. For this, we have prototyped the Cyberinfrastructure Web Application Framework (CyberWeb), using the Pylons Web Application Framework and other emerging grid, Web 2.0 and IT technologies. CyberWeb improves on standard Web application toolkit functions (e.g job execution, account management, task history, GSI authentication, etc) by hosting applications as Web services, portal Web pages, or Web 2.0 gadgets. CyberWeb interfaces to local and remote clusters, cloud resources, and supports different authentication schemes. CyberWeb supports two key tools: (1) a database (with admin Web pages) for configuring CyberWeb installations to connect CIApps, users, local services, web services, and campus clusters with remote services and resources; (2) a simple job distribution Web service framework (Jodis) that distributes application workloads across heterogeneous computing systems.

**Projected Hartree-Fock in a Shell Model Basis**
*By Joshua T. Staker*

We implement projected Hartree-Fock in a shell model basis and compare against exact numerical results from full space diagonalization. We consider the accuracy of projected Hartree-Fock for the excited state spectrum in the cases of the s — d and p — f fixed parity shells as well as cases of mixed parity in the p - sd shell. The accuracy of valence proton-neutron number configurations are also considered including even-even, odd-odd, and odd-A.
Featured Posters

**The Dengue Prevention Consortium Project: Space-Time Dynamics of the Emergence of Severe Dengue Disease in Peru. What Does the Future Hold?**

*By Karen Campbell*

In Peru, documented cases of dengue disease from 1994 through 2010 indicate an emerging space-time transmission pattern regulated by geography, weather, and human population distribution. Recent introduction and co-circulation of multiple dengue virus serotypes in Peru has been associated with an emergence and acceleration of DHF incidence which previously was sparse. In forecasting the future for Latin America, we often consider the dengue history in areas of Southeast Asia, such as Thailand, where dengue virus transmission has been hyper-endemic for decades. In Thailand, we observed large seasonal epidemics of DHF that persist in multi-year cycles throughout the entire country. Is Peru headed toward similar oscillatory dynamics with large DHF epidemics or does the Latin American transmission setting suggest something different?

In this poster, we provide an overview of The Dengue Prevention Consortium activities and ongoing work to assess the space-time dynamics of dengue virus transmission in different ecological and entomological settings. We are currently assessing the spatial structure and temporal patterns related to transmission and incidence of severe disease with respect to predictive factors observed in the environment, human population distribution, and changes in immunity-based mass-action dynamics associated with the introduction of new serotypes and strains. In Peru, we have identified important and rarely observed changes in country-wide disease patterns during transitions from one-to-two-to-three-to-four circulating serotypes.

Peru is entering a new phase of dengue virus transmission with the ongoing regional presence of all four dengue serotypes. What does the future hold regarding incidence of severe dengue disease in the Peruvian population and its impact on the public health infrastructure? In collaboration with the Peru Ministry of Health and Thailand Ministry of Public Health, we are developing a broad scale, high resolution, agent based model to simulate dengue transmission dynamics, predict risk of severe disease, and comparatively assess effectiveness of various surveillance and prevention strategies. Anticipation, quantification, and control of the threat of severe disease are public health priorities for Peru and Thailand.

**Automating FEMVib an Ab Initio Multi-Dimensional Solver For Probing Vibrational Dynamics in Polyatomic Molecules and Free Radicals**

*By Peter Zajac*

Accurate prediction of the vibrational spectra in polyatomic molecules and free radicals depends on obtaining high quality solutions to the vibrational Schrodinger equation. A novel ab-initio solver package, FEMVib, was developed within the finite element method (FEM) framework. A mixed programming paradigm that combines C, Fortran, Python and Perl is employed to take advantage of existing numerical libraries. FEMVib has been tested to resolve the eigenvalues and wavefunctions of hundreds of vibrational energy states to high accuracy and precision.

Intermediate steps in the analysis involve an accurate and general method for point-wise evaluation of the Potential Energy Surface and G-Matrix elements as well as data sorting algorithms and grid extensions. All of these intermediate steps are crucial for accurate prediction of vibrational eigenstates and combined provide the user with an automated and robust Ab-Initio Vibrational Solver Package.

**Mathematical Modeling of Cystic Fibrosis**

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

Cystic fibrosis (CF) is the most common autosomal recessive disease in Caucasians associated with early mortality with a reported incidence of 1 in 3200 live births. Host inflammatory responses result in airway mucus plugging, airway wall edema and eventually destruction of airway wall support structure. Despite very aggressive treatment, the median age of survival is approximately 38 years. There have been a number of studies on mathematical modeling of respiratory inflammation but none of those focused exclusively on Cystic Fibrosis. This work is a first attempt to integrate CF patients’ forced expiratory volume in one second (FEV1) data into a dynamic model of the disease. The goal of our research is to use mathematical and statistical modeling techniques to better understand and control Cystic Fibrosis by capturing the complexity of interactions underlying disease activity. We used spirometric data from University of California San Diego Adult Cystic Fibrosis Center to adjust our model's constants to mimic the average CF lung's infection as a function of age. The model uses the known fractal structure of bronchioles in the lung. In this research, we simulate the lung function of CF patients by presenting a physiological model that will approximate the long term behavior of infection in CF lungs.
**Operon Analysis Using an Updated Annotation of the Ciona intestinalis Genome Reveals a Possible Role of Operons in Transcription and RNA Processing**

By Jerry Chen and Robert Zeller

In this report, we have completed a whole genome annotation of the model organism *Ciona intestinalis* using gene ontology (GO). We have also used the whole genome annotation to find statistically overrepresented annotations found within operon genes. From this analysis, we found that a large percentage of operon genes are involved in RNA transcription and processing, suggesting a role of operons in fast and efficient manufacturing of these proteins.

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**Applying the Distributed Coupling Toolkit in a Complex Domain**

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

Mesh generation could be a hard problem, specially within the domains with very complex shape. In addition, it is widely known that certain numerical problems are related with meshes with poor quality. One strategy to bypass the mesh generation problem in a very complex domain is to decompose or separate the problem domain into different blocks. Weak coupling approach could be used, where different domain region could be meshed independently. Then a two-way coupling is used to solve numerically the problem in the entire domain. In this work, the Distributed Coupling Toolkit is used to couple different and independent meshes solving the Shallow Water Equation in General Curvilinear Coordinate.

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**Vortex Ring Dynamics in the Nonlinear Schrödinger Equation**

By Ronald M. Caplan and Ricardo Carretero

Being the normal form for nonlinear propagation of envelope waves, the nonlinear Schrödinger equation (NLSE) is an ubiquitous equation with diverse applications including light propagation through nonlinear optical media and mean-field dynamics in Bose-Einstein condensates.

One of the most interesting families of solutions to the NLSE are those which exhibit topological charge. In two dimensions, these coherent structures correspond to vortices while, in the more challenging three-dimensional case, they correspond to vortex rings.

Vortex rings are ring-shaped structures which, due to their vorticity, form a toroidal area whose center ring has zero-density, with increasing density away from the center which converges to a constant-density background.

The dynamics and interactions of vortex rings in the NLSE are studied with a focus on multi-vortex ring interactions. Due to the inherent lack of a close form solution for vortex rings and the dimensionality where they live, efficient numerical methods (including compact high order numerical schemes implemented on NVIDIA graphic processing units) are developed in order to perform extensive studies of collision scenarios.
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