12th Annual ACSESS





Friday, April 17, 2015
12:00 pm - 5:00 pm
SDSU's Parma Payne Goodall Alumni Center

For Applied Computational Sciences and Engineering & Computational Science Curriculum Development

CSRC

San Diego State University

12:00 pm	**Registration / Buffet Lunch**	
	Ezra Bejar, Industry Projects Coordinator Computational Science Research Center San Diego State University	Moderator
1:00 pm	**Stanley Maloy, Dean** College of Sciences 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
1:30 pm	**Daniel Goldin, Chairman and CEO** Intellisis Corporation Introduction by John Newsam Chair, CSRC Advisory Board	Keynote Speaker Bridging Academia with Industry
2:30 pm	**Blitz Oral Presentations**	
3:00 pm	**Poster Presentations / Reception**	
4:00 pm	**Paul Paolini & Satchi Venkataraman** Associate Directors Computational Science Research Center San Diego State University	Poster Presentation Awards and Closing Remarks

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Welcome to the 12th Annual ACSESS Event

It is with great pleasure to welcome our local tech and biotech industries, board members and CSRC faculty, and students to our Applied Computational Science and Engineering Student Support (ACSESS) Annual Event.

ACSESS was created twelve years ago with the vision to create stronger links between academic computational scientists, industry professionals and technology officers. This year program is a reflection of the support and aspiration to foster CSRC educational and research missions; instilling graduate students interest in industry problems and pursuing careers in technology and biotechnology sectors.

We appreciate the strong faculty and student participation in our event, and our special thanks go to our CSRC board members for their continuous advice, as well as our company sponsor's for the financial commitment to our teaching and research missions.

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.

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A Nonparametric Approach in Covariate-Modulated Local False Discovery Rate for Genome-Wide Association Studies

By Rong W. Zablocki, Richard A. Levine, Andrew J. Schork, and Wesley K. Thompson
Advisor: Richard A. Levine and Wesley K. Thompson

Genome-Wide Association Studies (GWAS) have presented a new challenge to statisticians as such associations need to be detected from many genetic variants, each with individually small effects, but from relatively large sample sizes. In this scenario, Bonferroni-derived thresholds are severely underpowered. The local false discovery rate (fdr) provides and approach to detect non-null associations, but is limited in its ability to discover non-null loci due to an assumption of exchangeability between single nucleotide polymorphisms (SNPs). Different approaches to a covariate-modulated fdr (cmfdr), to incorporate important covariates into the fdr and break the exchangeability, have been proposed but themselves are restricted by parametric distributional assumptions. The current work proposes a novel nonparametric Bayesian extension to cmfdr through a two-group semi-parametric mixture model, utilizing B-splines for the nonparametric component, and develops a Markov chain Monte Carlo fitting routine. We illustrate our proposed methods on a large GWAS application. In particular, we show that our approach dramatically improves power and demonstrate that SNPs declared significant by our method replicated in much higher numbers, while maintaining the comparable replication rate relative to the usual fdr.

This research is supported National Institutes of Health funds and the Computational Science Research Center at San Diego State University.

Phenotyping Diverse Bacteria for Metabolic Network Reconstruction

By Daniel A. Cuevas, Heqaio Liu, Tucker Lopez, and Blaire Robinson
Advisor: Robert Edwards

Genome-scale metabolic reconstructions of organisms require gene presence/absence information to assert metabolic capabilities. In order to improve model accuracy and parameterize the models, assertions should be compared against experimental results. This feedback reconciliation enables the model to obtain new information about its metabolic network in order to perform more accurately, thus providing insight into organism-specific metabolic processes.

We are building models for a wide variety of bacteria and to provide high-throughput tools for bacterial metabolic reconstruction. We created a public database containing bacterial growth information populated with growth curves of a diverse set of bacteria grown in different minimal media compositions. The growth curves are used to parameterize mathematical models that allow us to identify growth, no growth, or intermediate types of growth in a high-throughput manner. The bacterial genomes were annotated using RAST platform and draft metabolic models automatically generated. We reconcile the metabolic models with the experimental growth predictions in order to improve accuracy of whole genome annotation and model construction. KBase, a DOE programming environment for systems biology, is used for FBA and reconciliation.

To date, thirty eight bacteria have been grown on up to 192 different minimal media compositions. Our recently published analysis pipeline PMAnalyzer was used to model these growth curves, and the raw and processed growth curves are available from http://edwards.sdsu.edu/dbbp. The genomes of each of these bacteria have been annotated and metabolic models constructed on the KBase platform. All reconciled FBA models have been shared on KBase. Overall, our modeling predictions are at least 85 percent accurate, but the accuracy is dependent on the coverage of the genome sequence and the accuracy of the annotations.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

Parallel Algorithms for Tomographic Maximum Likelihood Reconstruction

By Joe Hellmers
Advisor: Fridolin Weber

Muon Tomography can be used to detect high-Z materials using the naturally occurring spectrum of muons reaching the earth's surface. Currently implemented computational methods use the Point Of Closest Approach (POCA) algorithm. This algorithm is relatively simple and does not require many computational resources, but it is not as precise as other methods, and, more importantly, it can yield false images for the high-Z materials, which in real world applications would result in false positive detections. A better method is the Maximum Likelihood Reconstruction. The full 3-D algorithm can be quite accurate, but it is also quite computer random access memory and processor intensive. The goal of our research is to modify the algorithm for parallel processing, implement the algorithm on multiple processors and explore the speed of reaching reasonable solutions based on processing power applied.

This research is self-supported.

A Beam Steering Linear Antenna Array with Novel Simultaneous Frequency Agility and Polarization Reconfigurablity

By Behrouz Babakhani
Advisor: Satish K. Sharma

In this abstract, a beam steering linear (1×4) antenna array with novel simultaneous frequency agility and polarization reconfigurablity is presented. This includes development of a (i) Wideband frequency agile antenna, (ii) Polarization reconfiguration control circuit and (iii) Beam forming network with digital phase shifters and low noise amplifiers (LNAs). The array radiating elements consist of a circular microstrip patch and a concentric annular ring patch around it. Four varactor diodes have been placed between the central patch and the ring patch. By varying the varactor capacitance values, the coupling between the patch and ring is varied. When the varactors are biased such a way to provide low capacitance value, the antenna shows high impedance, and therefore, the patch and the ring become decoupled. In this case, only the central patch radiates in the dominant TM11 mode giving the higher frequency coverage. However, when the varactors are biased such a way that they provide high capacitance value, the antenna shows low impedance, and therefore, the patch and the ring become fully coupled. In this case, both central patch and outer ring patch participate in the radiation mechanism operating in the dominant TM11 mode and provide lower frequency coverage. Therefore, by varying the capacitance of the varactor, the resonant frequency can be varied between 1.5GHz and 2.4GHz. The overall frequency agility range of around 46% has been achieved. This antenna has been fabricated on a Rogers RT/Duroid 5880 ($\varepsilon r = 2.2$, $\tan\delta = 0.0009$, 3mm thick) and tested for impedance matching and radiation patterns.

For polarization reconfiguration, each of the circular patches is excited using two feed points which are 90° apart from each other. By exciting only one of the ports at a time, the polarization is either linear vertical or linear horizontal. By exciting both ports with equal amplitude and ±90° phase difference between them, the polarization is either right-handed circular (RHCP) or left-handed circular polarization (LHCP). Therefore, by controlling the port excitations, the polarization response can be set as linear horizontal, linear vertical, RHCP or LHCP. An active feed network consisting of RF switches and a compact wideband branch line coupler has been designed and fabricated for realizing the polarization reconfiguration. Four polarization control feed networks have been fabricated and characterized to connect with each of the array elements.

Finally, for beam steering capability, the variable progressive phase shifts between the radiating elements is applied through a beam forming network (BFN). The beam forming network (BFN) consists of LNAs, digital attenuators and digital phase shifters (one for each element). The state of the phase shifters and attenuators is set using a microcontroller. This microcontroller is driven using a Matlab code which calculates the excitation of each element as a complex number (phase and amplitude). The measured beam steering performance results for the fabricated antenna array consisting of frequency agile radiating elements, polarization reconfiguration control circuit and the beam forming network will be presented.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

Theoretical Design of Nano-Layered, Hyperbolic Dispersion Al/SiO2 with Minimum Losses

By Priscilla Kelly, Daniel White, and Lyuba Kuznetsova
Advisor: Lyuba Kuznetsova

Motivated by a greater need for increased performance in modern-day technology, this paper will review theoretical predictions for the nano-layered metamaterial Al/SiO2, which could increase the speed of devices. It will emphasis on finding the conditions for low loses since what limits metamaterials in devices today is their losses outweigh any increase in speed for use in devices. Using the Effective Medium approximation (EMA) with non-local corrections, we have investigated three major effects and their impacts on inherent losses and hyperbolic dispersion. This paper looks at the number of layers needed to reach the Effective Medium Approximation using non-local corrections. This model predicts a variation only in the perpendicular direction as the number of layers changes; this is an important factor to consider when reducing losses. The first of the trends is to find the saturation limit of non-local corrections in Al/SiO2 layers. This will tell us when the number of layers reaches the EMA; therefore the full range of optical effects Al/SiO2 layers is capable of. The second and third effects, Al fill fraction with a fixed layer height and thickness of a single layer in a sample of 20 layers, will be investigated to minimize losses. Both of these effects determine the transition wavelength to hyperbolic dispersion, which allows for fine-tuning of this dispersion to certain applications. The paper will also discuss the repercussions these properties will have on the manufacturing techniques and future applications of Al/SiO2 devices.

This research is supported by National Science Foundation funds.

Utilizing Random Forests to Evaluate Pedagogy and Inform Personalized Learning

By Kelly Spoon, Richard Levine, and ASIR Staff
Advisor: Richard Levine

A study of ways to utilize random forests in educational data mining, focusing on evaluating pedagogical approaches and interventions. Individualized treatment effects and interaction trees are presented as methods to provide personalized feedback to students in terms of the effectiveness of an intervention for a particular student based on institutional information. These methods are illustrated using data from Stat 119, an introductory business statistics course, offered in Fall 2013, focusing on the efficacy of an additional recitation course in helping students successfully pass Stat 119.

This research is supported by CSU Chancellor's Office (Promising Course Redesign) funds and the Computational Science Research Center at San Diego State University.

Regularization of Singular Sources for PSIC Computations of Particle-Laden Flows with Shocks

By Jean Piero Suarez and Gustaaf Jacobs
Advisor: Gustaaf Jacobs

We propose a high-order regularization technique with optimal scaling for time-dependent singular Dirac-delta sources in the numerical solution of hyperbolic conservation laws arising in the simulation of particle-laden flows with shocks with the particle-source-in-cell (PSIC) method. In one dimension, the regularization is based on a class of compactly-supported piecewise polynomials that approximates the Dirac-delta distribution with the desired order of accuracy away from the singularity. The overall accuracy is controlled by the number of vanishing moments and smoothness of the piecewise polynomials plus the support length (optimal scaling). We have developed a theoretical criterion for the optimal scaling that leads to optimal order of convergence in the numerical solution of a linear (advection) and a nonlinear (Burgers) scalar hyperbolic conservation law with a singular source, as well as the nonlinear Euler equations with singular sources, a system of hyperbolic conservation laws governing compressible fluid dynamics with shocks and particles. A Chebyshev collocation method (spectral) discretizes the spatial derivatives in the scalar equation tests. A multi-domain high-order high-resolution hybrid spectral-WENO method discretizes the Euler equations. We aim to enhance the accuracy of the PSIC method by using the proposed regularization technique with optimal scaling.

This research is supported by Department of Defense Air Force Office of Scientific Research funds, National Science Foundation funds, and the Computational Science Research Center at San Diego State University.

Parallellization of evoQSAR Modeling Framework and Graphical User Interface Design using PyQt for Drug Design

By Eric Su, Gene M. Ko, Rajni Garg, Sunil Kumar, and Mary Thomas
Advisor: Sunil Kumar

Computational models can be very time consuming to develop due to the complex nature of the problem and lack of simple analytical solutions. This work focuses on improving an existing toolkit 'evoQSAR' for quantitative structure-activity relationship (QSAR) analysis. We first introduce the concept of parallelization into evoQSAR, and then develop a user friendly graphical user interface (GUI). Parallelization helps to decrease computation time by increasing efficiency through the division of independent tasks, normally ran sequentially, in parallel. A user friendly GUI will open the functionalities of evoQSAR to a greater audience, including chemists, other pharmaceutical companies, and fellow researchers. The parallelization will be implemented using the Python Multiprocessing Library, and the PyQt framework will be used for GUI developments.

This research is self-supported.

Operator Evolution for Ab Initio Nuclear Theory

By Micah Schuster
Advisor: Calvin Johnson

The past two decades have seen a revolution in ab initio calculations of nuclear properties. One key element has been the development of a rigorous effective interaction theory, applying unitary transformations to soften the nuclear Hamiltonian and hence accelerate the convergence as a function of the model space size. For consistency, however, one ought to apply the same transformation to other operators when calculating properties other than spectra. In this work we use the similarity renormalization group (SRG) to soften the Hamiltonian and, for the first time, compute the matter radius of 3H, 4He, and 6Li.

This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory (LLNL) under Contract DE-AC52-07NA27344. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award Numbers DE-FG02-96ER40985 and DE-FC02-07ER41457 and the Computational Science Research Center at San Diego State University.

How Many MLCs Should Impersonate SLCs to Optimize SSD Performance?

By Wen Pan, Wei Wang, Deng Zhou
Advisor: Tao Xie

Since an MLC (multi-level cell) can be used in an SLC (single-level cell) mode, an MLC-based flash SSD typically uses a fixed small portion (called log partition) in the SLC mode to accommodate hot data so that its overall performance can be improved. In this paper, we show that a fixed capacity of a log partition without considering workload characteristics can lead to an unexpected overall performance degradation. Contrary to intuition, we notice that blindly enlarging the capacity of a log partition would also result in worse performance due to the increased garbage collection cost in a data partition, which serves cold data. How many MLCs should impersonate SLCs under a particular workload to achieve an optimized performance is still an open question. To answer this question, we first measure write costs on each partition and their impact on the overall performance of an SSD. Next, a hardware-validated write cost model is built. Based on the model, we demonstrate that for each workload there always exists an optimal partitioning scheme. Further, to verify the effectiveness of our workload-aware dynamic partitioning strategy, we implement an FTL (flash translation layer) called BROMS (Best Ratio Of MLC to SLC), which adaptively adjusts the capacities of two partitions according to the workload characteristics. Experimental results from a hardware platform show that BROMS outperforms a fixed partitioning scheme by up to 86%.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

Impact of Deformation on Non-Rotating Neutron Stars

By Omair Zubairi and Fridolin Weber
Advisor: Fridolin Weber

Conventional models of compact objects such as neutron stars assume they are perfect spheres. However, due to high magnetic fields, certain classes of neutron stars such as magnetars and neutron stars containing color-superconducting quark matter cores are expected to be deformed (non-spherical). In this work, we seek to examine the stellar structure of such objects in the framework of general relativity. We derive the stellar structures equations of non-spherical neutron stars and calculate stellar properties such as masses and radii and investigate any changes from standard spherical models.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

SubFlow, an Open-Source Tool for Modeling Carbon Dioxide Sequestration

By Johnny Corbino
Advisor: Christopher Paolini and Jose Castillo

The capture of carbon dioxide for its subsequent storage in brine saturated reservoirs or depleted oil fields has become a significant part of the US energy policy. In this work, we focus on the design and development of a novel application for modeling the sequestration process. SubFlow is written in C++ and uses a relational database to store simulation data. It provides 3D real-time visualization and parallel execution. Mimetic discrete operators are used in the reactive-mass transport PDE. Gear's method is employed to solve the inherited mechanism modeling geochemical kinetics.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

Dark Soliton Nucleation in Nonlinear Media

By Carlos Prieto and Ricardo Carretero
Advisor: Ricardo Carretero

We study the nucleation of topological waves in a 1D quantum superfluid with nonlocal interactions. The study is inspired by the quantum fluid properties of Bose-Einstein condensate (BEC) gases. Bose-Einstein condensation emerges as a quantum phase transition for an ensemble of boson particles at ultra cold temperatures. The evolution of BECs at low temperature can accurately be modeled, at the mean-field level, by the celebrated nonlinear Schrödinger (NLS) equation.

Experimental progress has been made to create BECs with particles with a strong dipolar moment such as in chromium. The dipole-dipole interaction adds a nonlocal term to the NLS equation in the form of a convolution. Computational work is done in C taking advantage of the CUDA-able GPU cards to accelerate the numerical integration of the GP equation.

On the other hand, previous work has focused on vortex nucleation in non-dipolar condensates by dragging impurities at supercritical speeds in the condensate. In 1D, a critical velocity can be found analytically above which dark (grey) solitons are emitted from the moving impurity. However, the case pertaining the supercritical velocity for vortex nucleation in dipolar condensates has not been considered so far. We present analytical and numerical results for the nucleation of dark solitons in 1D BECs with dipolar terms.

This research is supported by the Department of Mathematics and Statistics at San Diego State University and the Computational Science Research Center at San Diego State University.

The Crystalline Quark-Hadron Mixed Phase of Neutron Stars

By William Spinella
Advisor: Fridolin Weber

A neutron star is the superdense remnant of a collapsed star. The existence of neutron stars provides us with an opportunity to study matter at densities much higher than any terrestrial experiment can achieve. As a result of the high densities we expect neutron stars to contain exotic matter in their cores in the form of hyperons and quark matter. In our work we model neutron star matter and find that hyperons and quark matter are likely to exist in the cores of neutron stars. In particular, we find that quark matter should exist in a mixed phase with hadronic matter, and that the structure of this mixed phase could potentially have an observable effect on the speed with which a neutron star cools.

This research is supported by National Science Foundation funds, the Department of Physics at San Diego State University, and the Computational Science Research Center at San Diego State University.

Rheology and Structure of Associating Polymers

By Mark Wilson and Arlette Baljon
Advisor: Arlette Baljon

We report on the microstructural changes in a triblock copolymer network that arise in response to an oscillatory shear deformation. A hybrid molecular dynamics, Monte Carlo simulation is utilized to model associating polymers as a course-grained, bead-spring system. The end beads of the polymer chains represent functionalized groups and can form junctions with other end beads. At low temperatures the system forms a transient network by aggregating end beads. Aggregates act as nodes and chains act as links within this network. We perform bulk rheology experiments on the system and explore topological variations throughout the observed viscoelastic regime. The stress response of the system has been obtained as a function of the oscillatory frequency and amplitude in both the linear and nonlinear regimes. The approach of strain-rate frequency superposition gives indications that the rheological response is consistent over a range of strain rates. These frequency dependent properties are then correlated with observed changes in the topological network structure. The low frequency crossover of the moduli (G^'=G^'') marks an onset of restructuring within the polymer network wherein aggregates break apart, resulting in an increased density of free chains. As the system tends toward dissipative flow in lower frequencies and larger amplitudes, a more substantial restructuring is observed. The network tends to break and form larger structural elements along with increasing the multiplicity of chains bridging between two aggregates.

This research is supported by National Science Foundation funds, Dept of Defense DURIP funds, and the Computational Science Research Center at San Diego State University.

Comparison of Ensemble Filters for Data Assimilation

By Colette Smirniotis and Barbara Bailey
Advisor: Barbara Bailey

Data assimilation (DA) is the process of combining observations with the output from physics-based numerical models and is used for the purpose of updating and improving forecasts. DA problems are most common in atmospheric and ocean data applications. There has been an increase in the amount of available real time observed ocean and atmospheric data as well as advances in deterministic ocean and atmospheric models, which makes Monte Carlo statistical methods ready for advancing the field of DA. Two commonly used algorithms are the ensemble Kalman filter (EnKF) and the ensemble adjustment Kalman filter (EAKF). This project uses an advection model to compare the performance of the EnKF and the EAKF under different conditions, including varied ensemble size and observation density.

This research is supported by Department of Mathematics and Statistics at San Diego State University and the Computational Science Research Center at San Diego State University.

Particle Time-Series Decomposition and the Identification of Behavior

By Vincent Berardi, Ricardo Carretero, Melbourne Hovell, and John Bellettiere
Advisor: Ricardo Carretero

Project Fresh Air is a multiple baseline clinical trial that aims to reduce secondhand smoke exposure in households via the installation of air particle monitors. The monitors are equipped with aversive visual and audio feedback that engages when air particle concentrations exceed a threshold. Measurements of indoor air concentration are collected every ten seconds over the course several months, resulting in approximately one million observations per monitor. This study focus on intervals with elevated particle concentrations, ie peaks, and identifies discriminative characteristics via proper orthogonal decomposition (POD). The classification of peaks is organically achieved via a weighted k-means algorithm performed on the POD projection coefficients. The resulting clusters are then associated with real-world activities by correlating them with information provided by study participants. Additionally, physical parameters are extracted from each peak and cluster-specific parameter distributions are compared. The POD/clustering procedure is then performed on synthetic peaks generated from these distributions allowing the effectiveness of the POD at discriminating physical parameters to be engaged.

This research is supported by National Institutes of Health funds and the Computational Science Research Center at San Diego State University.

Roziglitazone Alters Contractility Behavior in Neonatal Cardiocytes

By Esteban Vazquez-Hidalgo, Elesha Bartolotta, and Megan Malone
Advisor: Paul Paolini

Rosiglitazone is a peroxisome proliferator-activated receptor-γ (PPAR-γ) agonist with both beneficial and adverse effects on cardiac function. Previous work investigated the effects of rosiglitazone on genome-wide gene expression over 48 hours on neonatal rat ventricular cardiomyocytes in order to identify the drug's impact on cell signaling pathways.

We examined cardiocytes subjected to the drug at 0, ½, 1, 2, 4, 8, 12, 18, 24, 36 and 48 hours of exposure compared to cardiocytes under only DMSO (carrier) exposure. Results from microarray experiments determined cardiocytes exposed to rosiglitazone stress exhibited a differential gene expression profile compared to control experiments. Over 3,000 genes of the 22,518 genes studied had statistically significant expression level changes with p-values < 0.5, and 310 had p-values < 0.0001.

Cardiovascular system development, extracellular matrix, and immune response were represented prominently among the significantly modified gene ontology terms in the data set. Enrichment of transcripts involved in cardiac muscle cell differentiation and extracellular matrix provides a panel of biomarkers for further assessment of adverse cardiac outcomes in humans.

However, there is a lack of research investigating the effects of rosiglitazone on the contractile function or neonatal cardiocytes. Enzymatically isolated cardiocytes were plated and videos of contracting cardiocytes at each time point were analyzed to extract contraction time-to-peak, 50%, and 90% relaxation times for control, DMSO, and DMSO-rosiglitazone testing groups.

This research is supported by National Science Foundation funds, California Metabolic funds, and the Computational Science Research Center at San Diego State University.

Who is There and What Are they Doing? Using FOCUS and SUPER-FOCUS for an Agile Taxonomic and Functional Analysis of Metagenomic (Big) Data

By Genivaldo Silva, Bas E. Dutilh, and Robert A. Edwards
Advisor: Robert Edwards

Microbes are more abundant than any other cellular organism, and it is important to understand which organisms are present, what they are doing, and how they are doing it. In many environments a majority of the microbial community members cannot be cultured, and metagenomics is a powerful tool to directly probe uncultured genomes and understand the diversity of microbial communities by using only their DNA. Analyzing the taxonomic and functional profile present in a microbial community from unannotated shotgun sequencing reads is one of the goals in metagenomics for its valuable applications in biological research. Currently available tools do not scale well with increasing data volumes, which is important because both the number and lengths of the reads produced by sequencing platforms keep increasing.

We have developed two tools to address this problem: FOCUS, Find Organisms by Composition USage, an ultra fast model which uses k-mer abundance and non-negative least squares to profile any metagenome dataset in seconds and SUPER-FOCUS, SUbsystems Profile by databasE Reduction using FOCUS, an agile homology-based approach using a reduced SEED database to report the subsystems present in metagenomic samples and profile their abundances.

The tools were tested with over 100 real metagenomes, and the results shows that our approaches accurately predict the taxa and subsystems present in microbial communities, and FOCUS and SUPER-FOCUS are respectively over 30,000 and 1,000 times faster than other tools.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

Reducing MLC Flash Memory Retention Errors Through Programming Initial Step Only

By Wei Wang, Deng Zhou, and Wen Pan
Advisor: Tao Xie

Retention error has been recognized as the most dominant error in MLC (multi-level cell) flash. In this paper, we propose a new approach called PISO (Programming Initial Step Only) to reduce its number. Unlike a normal programming operation, a PISO operation only carries out the first programming-and-verifying step on a programmed cell. As a result, a number of electrons are injected into the cell to compensate its charge loss over time without disturbing its existing data. Further, we build a model to understand the relationship between the number of PISOs and the number of reduced errors. Experimental results from 1y-nm MLC chips show that PISO can efficiently reduce the number of retention errors with a minimal overhead. On average, applying 10 PISO operations each month on a one-year-old MLC chip that has experienced 4K P/E cycles can reduce its retention errors by 21.5% after 3 months.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

Block-Level I/O Characteristics of Smartphone Applications and Their Implications for eMMC Design

By Deng Zhou, Wei Wang, and Wen Pan
Advisor: Tao Xie

A vast majority of smartphones use eMMC (embedded multimedia card) devices as their storage subsystems. Recent studies reveal that storage subsystem is a significant contributor to the performance of smartphone applications. Nevertheless, smartphone applications' block-level I/O characteristics and their implications on eMMC design are still poorly understood. In this research, we collect and analyze block- level I/O traces from 18 common applications (e.g., Email and Twitter) on a Nexus 5 smartphone. We observe some I/O characteristics from which several implications for eMMC design are derived. For example, we find that in 15 out of the 18 traces majority requests (44.9%-57.4%) are small single-page (4KB) requests. The implication is that small requests should be served rapidly so that the overall performance of an eMMC device can be boosted. Next, we conduct a case study to demonstrate how to apply implications to optimize eMMC design. Inspired by two implications, we propose a hybrid-page-size (HPS) eMMC. Experimental results show that the HPS scheme can reduce mean response time by up to 79.9% while improving space utilization up to 47.4%.

This research is supported by National Science Foundation funds and the Computational Science Research Center at San Diego State University.

General Curvilinear Ocean Model Application: Complete Three-Dimensional Modeling of San Diego Bay Hydrodynamics

By Randolph Bucciarelli, Mariangel Garcia, and Jose Castillo
Advisor: Jose Castillo

The General Curvilinear Ocean Model (GCOM) is unique in its ability to solve non-hydrostatic momentum equations utilizing completely three-dimensional curvilinear grids. GCOM is designed to work at super-high resolutions (tens of meters) on problems resolving strong current forces acting on complex bathymetry near the coastline. These problems include turbulence from flow through channels and curved boundaries, river and estuary flows, and how bottom surface rugosity affects current flow. The model has shown successful results in idealized simulations, this presentation details model application in studying the hydrodynamics of San Diego Bay, California. The entrance channel to San Diego Bay is unique in its use as a conduit for naval submarines, this lends itself well to application for the GCOM fully three-dimensional curvilinear approach. Specifically, estimates of tidal flow, temperature, salinity, and current velocity at small scales within the bay are nested with Regional Ocean Model System output.

This research is self-supported.

Simulation of Rock Fractures Induced in Geologic CO2 Sequestration

By Jonathan Matthews, Christopher Paolini, and Jose Castillo
Advisor: Christopher Paolini and Jose Castillo

CO2 sequestration in underground aquifers shows significant potential in reducing greenhouse gas emissions. However, rock fractures formed as a result of injection may release toxic species into the water table and CO2 into the atmosphere. A poroelastic model to compute the internal rock stresses induced by the injection of CO2-rich water has been developed. A finite element model is used to calculate the fluid pressure, mean stress, and strain induced by injection of CO2 into a geologic sandstone formation. Principal stresses are derived from the overburden pressure and mean stress, and then used to calculate a breakdown pressure. Fracture nucleation is initiated at locations where injectivity results in the pore pressure exceeding a breakdown pressure defined by a breakdown pressure model. Two such models were examined in this work, the Hubbert and Willis criterion and the Haimson and Fairhurst criterion. Implications resulting from changes in reservoir permeability and porosity are discussed, as well as optimal injection pressures that maximize mass transfer of CO2 to the reservoir while minimizing fracture initiation.

This research is supported by Department of Energy funds and the Computational Science Research Center at San Diego State University.

Mimetic Finite Differences to Simulate CO2 Subsurface Mass Transport

By Eduardo Sanchez, Christopher Paolini, and Jose Castillo
Advisor: Christopher Paolini and Jose Castillo

We explore the use of mimetic finite differences as an alternative numerical method to solve the partial differential equations that model the mass transport and concentration profiles of geologically sequestered carbon dioxide. We study the mathematical foundations and the underlying algorithms to construct higher-order one-dimensional mimetic operators, and we extend this knowledge to enable systematic derivations of their higher-dimensional counterparts. This work is then used as the theoretical foundation for the Mimetic Methods Toolkit (MTK); a C++ API implementing mimetic discretization and quadrature schemes on logically-rectangular grids. We discuss the API's design, structure, and usage philosophy. The resulting method can be used to compute the concentrations of multiple solutes in distributed-memory computers. Our applications focus on the simulation of long-term geologic sequestration of carbon dioxide.

This research is supported by the Computational Science Research Center at San Diego State University.

Proposing the San Quintin Bay Hydrodynamic Forecast System Through Data Assimilation Scheme

By Mariangel Garcia, Isabel Ramirez, Martin Verlaan, and Jose Castillo
Advisor: Barbara Bailey and Jose Castillo

Uncertainties in the hydrodynamics model parameters have been accurately estimated through automated calibration and validation process in previous studies . However , uncertainties propagated over time are still largely unknown, and have yet to be tested in San Quintin Bay. For our research, we implemented a Delft3D Model to study the hydrodynamics of San Quintin Bay, in which Data Assimilation (DA) techniques have played an important role. The mathematical methods of DA describe algorithms for combining the observations of a dynamical system (a computational model that describes its evolution), with other relevant information. The aim of this study is to find the optimal ensemble size for the EnsKF to evaluate the long-term predictive capability of the Delft3D Model by using water level, current, and temperature measurements from different locations within the bay. OpenDA is considered an effective tool for delivering real-time forecasting via the introduction of the Ensemble Kalman Filter algorithm; therefore, the automatic procedure is expected to result in an improved model forecast.

This research is supported by the Computational Science Research Center at San Diego State University.

Microbial Growth Characteristic Database Design and Implementation

By David Fu, Blaire Robinson
Advisor: Robert Edwards

Microbes are crucial to the environment as they fulfill important roles in the carbon and nitrogen cycles, to human health and disease, and in biotechnology through food processing and genetic engineering. Microbes include bacteria, fungi, archaea, protozoa and algae. They live in every part of the biosphere, from hot springs to deep oceans, from the earth's crust to outer space. Their growth conditions also vary dramatically. However, there is currently no tool or database that provides information about microbial growth characteristics and guides on choosing proper growth conditions. Currently all of that data is in books.

The design of Microbial Growth Characteristic Database (MGCD) is based on the premise that different microorganisms will grow differently under the same conditions. The database is made up of a collection of microorganisms and their growth characteristics. Initial data sets will be imported from a literature review, including textbooks, research publications and other readily available sources. The implementation of the MGCD follows the Model-View-controller (MVC) strategy, the major user interface development architecture. The model is the database, its data and the logic. It can be accessed through an API. The view is the user interface, which contains the user input and the data presenting layer. The controller takes the user input, submits it to the API and gets the results and sends them to user interface. Each of these three modules has its own implementation, and modification of one module won't affect the other modules as long as the interface doesn't change.

Currently the main function of each part of the MVC has been implemented. Once more detailed implementation and a better user interface is complete, it will be pushed to testing and placed online.

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Stress Estimation in Integrally Based Rotors Under Multi-Mode Excitations

By AmudhaVarshini Kamaraj and Vaibhav Yadav
Advisor: Satchi Venkataraman

Traditional turbine blades have dovetail attachments which are sites of fretting fatigue failures due to the frictional sliding of the blades during vibration. Newer Integrally Bladed Rotors (IBR) eliminate the root attachment by manufacturing the rotor disk and blades as a unitized structure. IBRs eliminate sites of fretting fatigue failure; however, they also eliminate natural damping effects provided by dovetail attachments. The absence of natural damping leads to large forced-response vibration amplitudes and premature high-cycle fatigue failure. Thus, the accurate prediction of peak vibration stresses of IBRs in operating conditions is vital in estimating its fatigue life.

Conventional methods to estimate stresses due to the forced-response of IBRs rely on vibration strain measurement techniques that measure surface strains using strain gauges. These measurement techniques have various limitations and are not suitable for use when several natural modes are excited simultaneously. The accurate prediction of the blade peak stress due to multi-mode excitation cannot be established using strain measurement techniques alone and require prior knowledge of stress distribution associated with each vibratory mode. This stress distribution can be obtained using commercial Finite Element Software. This poster presents the work in progress on Rotordynamic analysis of a turbine blade under forced vibration.

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Pattern Formation in Granular Systems

By Kevin Joiner, Ricardo Carretero, and Satchi Venkataraman
Advisor: Jose Castillo

Pattern formation is of interest when studying biological, chemical and physical systems. In particular, granular materials lend themselves as an excellent physical medium for which one can study pattern formation in the context of two dimensional surface waves. Despite their substantial importance to many industrial processes and natural sciences, little is known about the macroscopic dynamics of granular materials. A kind of pattern phenomenon called oscillons is a type of localized solitary wave found on the surface of fluidized granular beds. Interestingly, oscillons are a large scale phenomena resulting from small scale interactions and have attractive and repulsive properties which resemble that of fundamental particles. Two oscillons with the same phase will repel while out of phase oscillons will attract. Therefore, the purpose of this project is to investigate the formation and behavior of oscillons in granular media in order to advance our understanding of granular dynamics and the emergence of macroscopic phenomenon via microscopic interactions.

We have developed an Event Driven (ED) algorithm which simulates an ensemble of interacting rigid hard spheres with no intrinsic material elasticity. In the simulation, time advances from collision to collision with, analytically exact, ballistic motion between collisions. The ED algorithm advances through collisions by using equations which map the velocities and angular velocities of each particle before and after the collision. The types of collisions considered are particle-particle, particle-wall and particle-floor.

Computer experiments using granular dynamics algorithms may be used to reliably predict oscillon behavior under various spatio-temporal conditions. We have been able to replicate well documented simulations of granular beds subjected to vertical vibrations. When a granular bed is excited via forcing from a flat (spatially uniform) floor the appearance of oscillon waves depends only on the forcing frequency and forcing amplitude. One approach we intend to employ to investigate the spatio-temporal behavior of oscillons is to couple the model of a fluidized granular bed to that of a spatially non-uniform membrane. Utilizing a curved membrane instead of a flat floor to force the granular bed may allow spatially variable forcing amplitudes to serve as a “controller” of oscillon emergence and behavior.

This research is self-supported.

Introduction of Controlled Delamination in Carbon-Epoxy Composite Laminate Specimen for Bolted Joint Tests

By Nicola Giorgi and Jeff Erickson
Advisor: Satchi Venkataraman

Bolted joints in composites are a region of interest to aerospace structural engineers trying to improve damage tolerance and durability. The fastener hole sites on composite wing skin on aircraft removed from service have been shown to present delamination damage. Life extension of aircraft with composite skins requires understanding how this delamination grows over the extended service life and at what stage or size it becomes critical damage. To understand this we are embarking on a research project to test thick composites laminates with chamfered drilled holes under bearing and bypass loads at fastener hole sites with embedded delamination. This requires producing test specimens with embedded delamination of know size at these sites. At present time there are no established standards for creating such damage. The goal of this project is to design different methods to create delamination at fastener hole sites, to identify the control parameters (load, geometry or process parameters) for each method and perform a series of experiments in which the control parameters are varied and the delamination created in the composite is measured and characterized. The goal is to identify the most controllable method for creating delamination damage and the optimum control parameters to obtain it as desired. This paper presents modeling of delamination growth at drilled holes under indentation loads. These simulations and experiments can also serve the needs for validation and verification of computational models for predicting delamination under combined shear and compression in composite materials

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Post-Buckling Analysis and Optimization of Frame-Stiffened Stitched Composite Panels

By Gabriela Sanz-Douglass
Advisor: Satchi Venkataraman

New aircraft configurations such as the Blended Wing Body (BWB) — are being explored to investigate the potential to attain higher fuel efficiencies and reduce the environmental impact of civil air transport. BWB aircraft smoothly merges the wing structures and fuselage creating a lack of a distinct separating line. The flattened and airfoil shaped BWB craft provides efficient high-lift wings and a wide airfoil-shaped body contributes to lift generation, which increases lift over drag ratio and results in improved fuel efficiency and range.

Large bending stresses arise in pressurization of noncircular fuselages. Until recently BWB planes could not be realized because conventional structural designs of durable and damage tolerant non-circular fuselages are too heavy and inefficient. NASA, the Air Force Research Laboratory, and the Boeing Company have collaborated in the development of a new low-cost, light-weight composite structural concept to enable BWB design; a new concept called PRSEUS, Pultruded Rod Stitched Efficient Unitized Structure, which uses fiber-reinforced stitched composites. In the PRSEUS concept skins, frames, stringers and tear straps are stitched together during assembly in the dry fiber form then are infused with the polymer and cured in an out-of-autoclave process. The translaminar reinforcement through stitching significantly improves the strength and durability of the layered composite materials by suppressing delamination under bending loads and stiffener or frame debonding failure modes due to bending or buckling.

Traditional aircraft composite stiffened panels are designed to avoid buckling of the skin at service loads, to avoid initiation and growth of delamination damages. In stitched composites, the stitching provides reinforcement against delamination; therefore, the structure can be designed for operation in a post buckled state with local skin buckling. This paper presents the non-linear postbuckling analysis and optimization of the PRESEUS concept. The effect of varying the frame sizing on the non-linear response of the panel under compression loading is investigated using finite element non-linear analyses. A surrogate model based optimization methodology for optimum design of the frame with constraints on local buckling load, ultimate panel collapse load and maximum allowable constraints are presented.

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Vortex Rings in Quantum Fluids

By Jake Talley and Ricardo Carretero
Advisor: Ricardo Carretero

One of the most widespread and interesting models for studying the emergence, dynamics and interactions of coherent structures is the nonlinear Schrodinger equation (NLSE). The NLSE is regularly used in the context of quantum fluids, including Bose-Einstein condensates, where it allows the prediction and description of nonlinear waves such as solitons and vortices. In three dimensions, more complex structures can be investigated, such as vortex rings, which are the subject of our investigations. Specifically, we numerically investigate the leapfrogging behavior of coaxial rings with equal charge and compare it with the dynamics from the ensuing reduced equations of motion from a fluid model derived using the Biot-Savart law with a goal of establishing criteria for its existence and stability.

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