CSESC 2013

Computational Science and Engineering Student Conference

Welcome to the 5th Annual Computational Science and Engineering Student Conference (CSESC 2013)! Hosted by Purdue University and organized by Purdue Student Chapter of SIAM, this interdisciplinary conference highlights the breadth of computational science and engineering research that is being done across different departments and disciplines. We gather to share our research and see how modeling and numerical techniques apply across various disciplines here at Purdue and other universities.

This year's conference brings together works from different research areas in both poster and oral presentations, from graduate and undergraduate levels. We also welcome our keynotes speakers whose individual backgrounds and experiences have had a broad range of impact that will enrich students' experience during this conference.

The CSESC is intended to provide students with an environment to share their research as well as opportunities for networking with peers. We want to make this student conference a tradition at Purdue and for this reason, we thank you for your participation and hope you would enjoy the event.

Sincerely,

siam @PURDUE

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MANN 101	Verification and Convergence of a Linearly Unstable Two Equation Problem by ***William Fullmer***
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MRGN 129	Surface-based Pseudoreceptor Modeling: Optimizing Surface Representations of Binding Sites using Experimental Protein-ligand Structure Data by ***Gregory Wilson***
MRGN 206	Quantum Computing 101 by ***Cyrus Vandrevala***
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Posters List

14.45 - 15.45 at MANN Atrium 1st
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11.00-11.30a MRGN 129

Don't Give Knives to Robots: an Old-new Era in Surgical Robotics

Juan Wachs

Assistant Professor in the School of Industrial Engineering

Purdue University

"Extracting the Fool's Stone" Hemessen (1500- 1557)
©Museo Nacional del Prado.

Robotics and automation to support and augment the surgical performance of surgeons in the operating room offer the premise of shorter, more accurate and fewer risks compare to traditional human-only surgery. In this talk, I will discuss current research in the area of surgical robotics and human robot collaboration. The talk will be focus around a current project, in which we developed the first multimodal robotic scrub nurse (Gestonurse) for the operating room (OR). Gestonurse assists the main surgeon by passing surgical instruments; this releases the surgical technician to perform other concurrent tasks. Such a robotic system has the potential to reduce miscommunication and compensate for surgical staff absences. Implications of the introduction of surgical robots, as assistants rather than autonomous agents, will have sociological and technological effects that may transform healthcare as we know it today. We will present our findings about the effects of modality training on task completion time and their meaning in terms of future applications.

About the speaker:

Dr. Juan Wachs is an Assistant Professor in the Industrial Engineering School at Purdue University. He is the director of the Intelligent Systems and Assistive Technologies Lab (ISAT) at Purdue, and he is affiliated with the Regenstrief Center for Healthcare Engineering. He completed a postdoctoral training at the Naval Postgraduate School's MOVES Institute in the area of computer vision, under a National Research Council Fellowship from the National Academies of Sciences.

Juan Wachs is a member of IEEE and the Operation Research Society of Israel (ORSIS). He has published in journals including IEEE Trans. Systems, Man, and Cybernetics, Journal of American Medical Informatics, Communications of the ACM, and the Journal of Robotic Surgery. He received his B.Ed.Tech in Electrical Education from the ORT Academic College in Jerusalem, his M.Sc and Ph.D in Industrial Engineering and Management, Information Systems and Intelligent Systems tracks, respectively, from the Ben-Gurion University of the Negev. Recently Wachs was awarded the Air Force Young Investigator Award 2012.

13.15-13.45 MRGN 129

From Microelectronics to Nanoelectronics:

Reflections on the role of CSE

Mark Lundstrom

School of Electrical and Computer Engineering

Network for Computational Nanotechnology

Purdue University

Semiconductor electronics has been on a remarkable ride, and it is far from over. Since Gordon Moore formulated his famous law in 1965, progress in semiconductor technology has continued unabated, and the result has transformed the modern world. Microelectronics has become nanoelectonics, and the transistor has become the most ubiquitous device on the planet. In this talk I will review the history of microelectronics, describe the present status of nanoelectronics, and speculate on the future of nanoelectronics. The development of this field over the past 50+ years presents a valuable case study on the role of numerical simulation in science and engineering, and I'll reflect throughout the talk on lessons learned.

About the speaker:

Marl Lundstrom is the Don and Carol Scifres Distinguished Professor of Electrical and Computer Engineering at Purdue University where his teaching and research center on the physics, technology, and simulation of electronic devices. He is a member of the U.S. National Academy of Engineering, and a fellow of the IEEE, APS, and AAAS. Lundstrom was the founding director of the NSF-funded Network for Computational Nanotechnology, which has a mission of research, education, leadership, and service to the nation's National Nanotechnology Initiative. The NCN's science gateway, nanoHUB.org, now serves a global community of 250,000 users per year. nanoHUB-U is becoming the global resource for education in nanotechnology. Lundstrom currently directs a new NSF initiative, NEEDS – Nano-Engineered Electronic Devices and Systems. NEEDS is a Purdue, Berkeley, MIT partnership directed connecting material and device technologists to circuit and system designers.

17.15-17.45 MRGN 129

Making Do With Less: An Introduction To Compressed Sensing

Kurt Bryan

Professor of Mathematics

Rose-Hulman Institute of Technology

Suppose a bag contains 100 marbles, each with mass 10 grams, except for one defective off-mass marble. Given an accurate electronic balance that can accommodate anywhere from one to 100 marbles at a time, how would you find the defective marble with the fewest number of weighings? You've probably thought about this kind of problem and know the answer. But what if there are two bad marbles, each of unknown mass? Or three or more? An efficient scheme isn't so easy to figure out now, is it? Is there a strategy that's both efficient and generalizable?

The answer is "yes," at least if the number of defective marbles is sufficiently small.

Surprisingly, the procedure involves a strong dose of randomness. It's a nice example of a new and very active topic called "compressed sensing" (CS), that spans mathematics, signal processing, statistics, and computer science. In this talk I'll explain the central ideas, which require nothing more than simple matrix algebra and elementary probability.

About the speaker:

Kurt Bryan (Ph.D., 1990, University of Washington) is Professor of Mathematics at the Rose-Hulman Institute of Technology. He has also held a post-doctoral position at the Institute for Computer Applications in Science and Engineering (ICASE) at NASA's Langley Research Center, worked in industry from 1984 to 1990 as a mathematician and statistician at Blount Industries, and been a visiting faculty member at Rutgers University and the U.S. Air Force Academy. His research interests lie mainly in partial differential equations, especially inverse problems related to non-destructive testing. He is particularly interested in teaching applied mathematics to undergraduates, and for the past 11 years has directed students in Rose-Hulman's summer REU program.

LECTURE ABSTRACTS

(in order of appearance)

9.30-10.00a MRGN 129

Intelligent Alarm System Management Applied to Continuous Pharmaceutical Manufacturing

Anshu Gupta

Department of chemical Engineering, Purdue University

One of the important challenges in effective real time process management is the implementation of intelligent systems that can assist human operators in making supervisory control decisions, instead of simply sounding an alarm when process variables go out of range. Operator failures to exercise the appropriate mitigation actions often have an adverse effect on product quality, process safety, occupational health and environmental impact. The economic effect of such exceptional events is immense; an estimated $20billion/year loss in petrochemical industry has been reported. The challenges and opportunities for improvements are even larger in the pharmaceutical manufacturing domain because so much of the processing involves particulate and granular systems whose characteristics tends to be more problematic than that of fluids. Early detection and diagnosis of process faults while the plant is still operating in a controllable region can help avoid abnormal event progression, production disruptions and productivity losses.

An IAS framework has been developed to deal with fault detection, diagnosis and mitigation of conditions that result from process anomalies. The framework developed uses a combination of Principal Component Analysis (PCA), Signed Digraphs (SDG) and Qualitative Trend Analysis (QTA). PCA has been used for fault detection and SDG/QTA techniques have been used for diagnosis based on faults signature. An ontological database has been created to maintain records of the signatures of a number of exceptional events typical of a dry granulation line and their associated mitigation strategies. Once a fault is diagnosed a respective mitigation strategy is displayed to an operator. The EEM framework has been applied to continuous pharmaceutical product manufacturing line consisting of feeders, blender and roller compacter; and was able to detect and diagnose various commonly occurring exceptional events, either in a given equipment or throughout the whole continuous line, such as; ‘No powder entering roll region’, ‘varying moisture and content uniformity of powder’ and ‘bridging of powder in feeder’; within few seconds of their inception and to provide mitigation advisories to the operator.

9.30-10.00a MRGN 206

Strategies for Dynamic Soft-Landing in Microelectromechanical Switches

Ankit Jain

Department of Electrical and Computer Engineering, Purdue University

Electromechanical switches offer the advantage of low power dissipation compared to their counterpart semiconductor switches. At micro- or nanoscale, they are used in wide range of application including RF-MEMS capacitive switches, ohmic switches, and NEMS relays. The structure of these switches involves two electrodes-one fixed and other movable separated by an air-gap. In the off-state, the two electrodes are separated by an air-gap and offer very high impedance whereas in the on state two electrodes comes in contact and exhibits very low impedance. During switching from off to on state, the movable electrode hits the fixed electrode with very high impact velocity and causes contact to degrade. Electromechanical contact or dielectric degradation associated with this hard landing of movable electrode is a technology-inhibiting reliability concern for micro/nano electromechanical switches. In this work, we propose two novel schemes for dynamic soft-landing that obviate the need for external feedback circuitry. Instead, the proposed resistive and capacitive braking schemes can reduce impact velocity significantly without compromising other performance characteristics like pull-in voltage and pull-in time. Resistive braking is achieved by inserting a resistance in series with the voltage source whereas capacitive braking requires patterning of the electrode or the dielectric. Our results have important implications to the design and optimization of reliability aware electrostatically actuated electromechanical switches.

10.00a – 10.30a MRGN 129

Hemoglobin Binding Dynamics: Insights from 30,000 Simulations

Grant Rotskoff

Department of Mathematics, University of Chicago

Molecular Dynamics (MD) simulation provides an unmatched resolution for the study of biological molecules, such as proteins. However, this technique is inherently limited by the tremendous computational resources needed to produce trajectories of a sufficient length to model biological timescales. In particular, the study of rare events such as transitions between adjacent free energy minima is not feasible with current technology. In order to address this limitation, we implement a highly parallel sampling method which allows us to describe a minimal free energy path for the transition between the oxygenated and deoxygenated hemoglobin structures. These data provide significant insight into the protein's oxygen binding mechanism at a resolution previously unavailable.

10.00a – 10.30a MRGN 206

Highly Dexterous Piezoelectric Micro Actuators

Aarti Chigullapalli
Department of Mechanical Engineering, Purdue University

In this work we investigate microstructures comprised of piezoelectric material that have the ability to achieve unprecedented displacement upon applied voltage. These smart microstructures lead to distinct advantages over conventional microactuators such as elimination of hermetic sealing, greater translational displacement, and greater rotational displacement by several orders. Our piezoMEMS work on the converse piezoelectric mechanism. In our design we sandwich piezo material between two metal strips and place four of them in an H- shape, such that upon application of voltage compression occurs on one side and extension occurs on the other side, forming an 'S' shape with large lateral deflection. Due to its shape we call it 'S-Drive'. By coupling pairs of S-Drives we were able to achieve large in-plane or out-of-plane deflections. We present these novel piezoelectric actuators that are able to produce extremely large translational (> 100 microns) or rotational deflections (> 10 degrees) or shear (>100 microns). We call these actuators extremely large deflection actuators (ELDA), the translation actuator is given the name elongation (ELDA1), the shear actuator is shear (ELDA2) and the actuator with rotational deflection is twistoflex. We also explore the piezoelectric effect to operate as "solid state muscles" to facilitate robust insect-like dexterity for microscale robotics and we call these "Microid". This is predicted to walk, run, and jump in various directions, continue to walk once flipped upside down on their back, traverse through harsh terrains such as sand, pick up, carry, and place relatively large loads, withstand large impacts or acceleration.

10.30a – 11.00a MRGN 129

Light at the End of the Tunnel? A New Method for Identifying Ligand Tunnels in Proteins

Laura Kingsley
Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University

In proteins with buried active sites, understanding how ligands migrate through the tunnels that connect the exterior of the protein to the active site can shed light on substrate specificity and enzyme function. Many of the current methods for tunnel prediction do not explicitly incorporate the ligand or protein flexibility during tunnel prediction. A growing body of evidence suggests that protein flexibility and protein-ligand interactions may reshape tunnels and even expose new tunnels as the ligand migrates toward the active site. We have developed a novel tunnel prediction methodology, IterTunnel, which combines geometric tunnel prediction with steered molecular dynamics to incorporate protein flexibility and ligand migration into the tunnel prediction process. We applied our method to Cytochrome P450 2B6, a central target in drug design due to its role in drug metabolism. In comparison to geometric prediction alone, our method found several additional tunnels that were exposed by either a loop or helix shift. Furthermore, many of the tunnels uniquely identified by IterTunnel were found to be amongst the most energetically favorable tunnels for ligand egress in Cyp 2B6.

10.30a – 11.00a MRGN 206

Understanding the Damage Tolerance of the Radular Teeth of the Cryptochiton Stelleri

Enrique Escobar de Obaldia
Department of Civil Engineering, Purdue University

The tip of the ultrahard radular tooth of the C. Stelleri is reported as the hardest and stiffer bio mineralized material known today (E~125 Gpa and Py~ 430 μN). A rod-like structure composition, a nanoscale pattern design and sliding between the organic and mineral interfaces are some of the mechanism used to explain these unique mechanical properties. Efforts have been made with microscopic techniques (i.e. SEM, TEM and Xray diffraction) to fully understand these phenomena, despite these techniques our ability to make direct observations of the potential abrasion resistance mechanisms acting at the microscale during these tests remains a challenging task. In this presentation, we will show the 3D finite element models and the experimental results obtained from indentation of elastic and composite materials with a rod-like substructure. The model is capable of capturing the onset of cracking and damage at the interfaces.

11.30 – 12.00 MRGN 129

Low Computational Complexity Algorithm for Signal Detection in Wireless Communication System

Ali Elghariani

Department of Electrical and Computer Engineering, Purdue University

The field of mixed-integer nonlinear programming (MINLP) optimization has a wide spectrum of applications in many areas of engineering, applied mathematics, applied science. Integer Quadratic programming (IQP) problems are special cases of MINLP problems which contain quadratic objective functions and integer constrains on the variables. Recently there has been a growth interest in applying IQP in the area of communication and signal processing such as filter design, cognitive radios and network routing and scheduling.

In this research work IQP is introduced for the topic of signal detection in wireless communication systems, where the detection process represents the essential part of the receiver design. Maximum Likelihood (ML) detection algorithm, which is the optimum detection algorithm, is deemed impractical because of its prohibited computational complexity. In this work, ML problem is reformulated as IQP problem and then solved using Branch and Bound (BB) algorithm, which is a systematic search tree of the continuous solutions in which the integer variables are successively forced to take integer values.

We show first how the computations are saved when IQP with BB algorithm is used compared to ML computations and then we propose some modifications to the standard BB search tree for further computational complexity saving. The idea based on squeezing the number of nodes in the BB search tree vertically and horizontally by anticipating the most probable nodes that could lead to the optimum solution and leave the nodes that are less probable.

As an application for this proposal, we implemented the idea in spread OFDM wireless communication system. The benefit of the computational complexity saving is confirmed through Monte Carlo simulations using MATLAB software.

11.30 – 12.00 MRGN 206

Phase Field Dislocation Dynamics Model and its Connection to Molecular Dynamics

Lei Cao

Department of Mechanical Engineering, Purdue University

Experimental and theoretical studies on nanocrystalline (nc) plasticity reveal that the mechanical behavior of nc materials cannot be characterized only by the average grain size, without considering the effect of the grain distribution. To quantify uncertainties in the prediction of the inelastic response, including yield and creep, we carry out dislocation dynamics simulations with a Phase Field Dislocation Dynamics model. The dependence of the yield stress on the grain size and initial dislocation density is characterized and compared to the Hall-Petch relation. The comparison between the predicted yield stress on uniform and non-uniform grained nc Nickel indicates that grain size distribution has a more significant influence on the yield stress for smaller grains.

11.30 – 12.00 MANN 101

SemCache: Semantics-aware Caching for Efficient GPU Offloading

Nabeel AlSaber
Department of Electrical and Computer Engineering, Purdue University

Recently, Graphical Processing Unit (GPU) libraries have made it easy to improve application performance by offloading computation to the GPU. However, using such libraries introduces the complexity of handling explicit data movements between GPU and CPU memory spaces. Data movement is expensive, and hence communication costs need to be minimized. When using these libraries with complex applications with multiple levels of abstraction, it is very difficult to reason about how multiple kernel invocations interact with one another, and hence avoid redundant communication. What is needed is an automatic approach to managing CPU-GPU data movement that can dynamically optimize communication.

In this paper, we introduce SemCache, a semantics-aware GPU cache that automatically handles CPU-GPU communication and eliminates redundant communication. Its key feature is the use of library semantics to determine the appropriate caching granularity for a given offloaded library (e.g., matrices). We applied SemCache to Basic Linear Algebra Subprograms (BLAS) libraries to provide a drop-in replacement library. Since SemCache handles communications automatically, it requires no GPU experience from the programmer. Our caching technique is efficient because it only tracks matrices instead of tracking every memory access at fine granularity. Experimental results show that our system can dramatically reduce redundant communication for real-world computational science application and deliver significant performance improvements, beating GPU-based implementations like CULA and CUBLAS (NVIDIA CUDA BLAS).

12.00 – 12.30 MRGN 129

Finding Quantum Circuits for the Simulation of Quantum Chemistry

Anmer Daskin

Department of Computer Science, Purdue University

Quantum computers are based on quantum mechanical systems behaving according to the Schrodinger equation, governed by the Hamiltonian operator of the system. The time evolution operator of a quantum system is described by a unitary matrix considered as a quantum gate. The implementation of a given computation represented by a unitary matrix on a quantum computer requires to find an array of elementary quantum gates whose product implements the given computation. This decomposition is known as the quantum circuit design problem. Any computation on quantum computers can be represented by a unitary matrix which shows the time evolution of the system. Computations on quantum computers including the simulation of quantum chemistry require the decomposition of unitary matrices into some elementary quantum gates whose implementations are known.

In this small talk, I ask-and answer-questions concerning the quantum circuit design problem: How hard is it to find quantum circuits? What are the possible methods and applications of some of those methods to the simulation of quantum chemistry and quantum computing?

12.00 – 12.30 MRGN 206

Computational Multiscale Modeling of the Hierarchical Structure of Cellulose Nanocrystals

Fernando Dri
Department of Civil Engineering, Purdue University

Cellulose nanocrystals (CNCs) are a promising family of environmentally friendly nanoscale reinforcing materials. They have been shown to exhibit remarkable mechanical properties and high order of functionality through a well designed hierarchical structure ranging from the atomic level to the micron scale. We propose a multiscale framework to analyze the thermomechanical properties of CNCs, employing quantum mechanics (QM), atomistic- and continuum-based models to describe and predict thermal and mechanical behavior of CNCs. In this talk we will present i) a summary of the current state of the art in CNC modeling, (ii) some of our progress on ab-initio studies to characterize the elastic properties and thermal expansion coefficient using Density Functional Theory (DFT), (iii) molecular dynamics (MD) simulations of the individual and collective behavior of cellulose chains and (iv) the development of continuum/discrete theories to represent the mechanical behavior of CNCs. Finally, we will end our presentation with a discussion on how this multiscale approach can be used to connect theory with experiments (X-Ray diffraction and AFM nanoidentation) in the pursuit of practical applications of CNCs.

12.00 – 12.30 MANN 101

The Challenge of Meeting 2050 CO2 Emission Goals

Isaac Tetzloff

Department of Aeronautics and Astronautics, Purdue University

Many efforts to mitigate the environmental impact of aviation -- like NASA's Subsonic Fixed Wing (SFW) Project -- place high importance on reducing fuel burn, nitrous oxide (NOx) emissions, and noise of future aircraft. However, the environmental and economic impact of a new aircraft is not solely a function of the aircraft's performance, but also how airlines use new aircraft along with other existing aircraft to satisfy the passenger demand for air transportation. An optimization problem finds the optimal allocation of existing and future aircraft to routes representing commercial air transportation within or to / from the United States to measure various fleet-level metrics. Examining fleet-level environmental metrics helps assess how aircraft meeting NASA's SFW goals could impact fleet-level environmental goals established by the International Air Transport Association (IATA). Results indicate that goals set forth by IATA for 2050 CO2 emissions appear attainable with an aircraft allocation to minimize fuel burn and future aircraft that meet the NASA N+2 and N+3 SFW fuel consumption goals.

13.45 – 14.15 MRGN 129

Population Balance Model Based Multi-objective Optimization of a Continuous Plug-Flow Antisolvent Crystallizer

Bradley Ridder

Department of Chemical Engineering, Purdue University

Crystallization is a major separation unit operation in fine chemical and pharmaceutical manufacture. Over 90% of drugs are small organic molecules crystallized from solution. Predominantly, industrial crystallization is done batch-wise, despite clear evidence of the economic advantages of continuous manufacturing. In this work, we discuss our progress to date on the steady-state optimization of a continuous segmented antisolvent plug-flow crystallizer (PFC) for the production of flufenamic acid, an anti-inflammatory drug. The crystal size distribution (CSD) is a critical parameter in the manufacture of pharmaceuticals, since it strongly impacts further downstream processing, as well as the dissolution kinetics of the drug within the human body. In the modeled PFC, an unseeded intake stream flows into the first baffled tube, where it mixes perfectly with the first input side stream of antisolvent. Crystallization occurs, and this mixture is then fed into the next tube section with a new antisolvent stream. This process continues recursively until the exit is reached, yielding the final CSD. By altering the antisolvent flow rates in the various sections, the supersaturation can be controlled along the length of the crystallizer. Nucleation and growth kinetics of the crystallization process are strongly dependent on the supersaturation, and this gives us a method for manipulating final CSD. The process is modeled using steady-state population balance model (PBM), and the differential equations are solved using a high-resolution finite volume scheme. A multi-objective optimization (MOO) framework is used to investigate the optimal antisolvent profile. Our chosen objectives are maximizing the weight-mean size (L43) and minimizing the coefficient of variation (CV). MOO is performed on single-segment PFC as well as a multiple-segment configuration.

13.45 – 14.15 MRGN 206

Avoiding Self-interaction and Static-correlation Errors with Partition Density Functional Theory

Jonathan Nafziger
Department of Physics, Purdue University

Density-functional embedding methods provide promising strategies for bridging length-scales in electronic-structure calculations. However, the applicability of these methods is limited by the errors incurred in by available exchange-correlation functionals. Two of the most significant and pervasive of these are the self-interaction and static-correlation errors. By writing the delocalization error of approximate exchange-correlation functionals as the difference between the self-interaction error of isolated fragments and of sharply-defined `fragments-in-molecules' in the framework of Partition Density Functional Theory (PDFT), we show how this error can be avoided without renouncing to simple local and semi-local functionals. We also show how a similar strategy allows one to avoid the static-correlation errors that plague density-functional calculations of bond-stretching processes. Our overlap-weighted-approximation (OWA) is illustrated with calculations on the two paradigm systems, stretched H2+ and stretched H2. Using the Local Density Approximation, we find in both cases our scheme leads to dissociation-energy errors of less than 3%.

13.45 – 14.15 MANN 101

Stability, Verification and Convergence of a Linearly Unstable Two Equation Problem

William Fullmer

Department of Nuclear Engineering, Purdue University

The one-dimensional two-fluid model has been a subject of controversy and disagreement in the nuclear engineering and technology community for decades. While the model forms the foundation of nuclear reactor safety analysis codes, the basic model is conditionally ill-posed. The inclusion of higher order terms, whether physical, e.g. surface tension, or unphysical, e.g. artificial viscosity, can render the model well-posed. However this method of regularization retains the linearly unstable property of the originally ill-posed model at low wavenumbers, i.e. it is non-hyperbolic. This class of problems was described by Kreiss and Ystrom as "parabolic problems which are ill-posed in the zero dissipation limit." Their second nonlinear example problem will be used as a 'toy' model in the present analysis. The two-fluid model has four field equations, six if energy is included, typically needs additional closure and requires special solution techniques. The two-equation example model above is simple, general, and retains the linear stability properties of the more complicated two-fluid model, which will be shown. Kreiss and Ystrom showed that the model can be quite stable once nonlinear shock-type structures form in the solution. However, the positive growth rate makes the problem sensitive to smooth initial conditions, which, in turn, makes code verification and solution convergence challenging. It is shown with the method of manufactured solutions that verification is possible if an appropriate dimension is chosen in accordance with the linear theory. Additionally, the convergence of a particular solution will be re-assessed based on these findings.

14.15 – 14.45 MRGN 129

Surface-based Pseudoreceptor Modeling: Optimizing Surface Representations of Binding Sites using Experimental Protein-ligand Structure Data

Gregory Wilson

Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University

Pseudoreceptor methods are extensions of QSAR methods wherein a representation of the protein binding site is generated that can be used for computational structure-based drug design approaches. Surface-based pseudoreceptors represent the binding site as a surface surrounding a ligand set, with complimentary steric and physicochemical properties mapped to the surface. This surface is typically based on the solvent-accessible surface of a representative ligand or set of ligands. In this paper, we studied how well such a representation reproduces the known binding sites of experimental protein-ligand complex structures. For this purpose, we constructed the iso-surfaces at different iso-levels of ligand occupancy using a set of co-crystallized ligands for three different protein systems. Those iso-surfaces are compared to the molecular protein surfaces of co-crystalized protein-ligand complexes from the three different protein systems. From our analysis, we find that a single iso-surface is unable to fully replicate the variations in protein surfaces due to both protein flexibility and ligand diversity. Based on our analysis we recommend the use of a small number of iso-level surfaces to account for both diverse and conserved ligand features.

14.15 – 14.45 MRGN 206

Quantum Computing 101

Cyrus Vandrevala
Department of Physics, Purdue University

The rise of computational science has enabled us to solve complex numerical problems and simulate physical systems. Even though this field has shaped the way we do science, people have noticed that certain problems cannot be efficiently modeled on current computer systems; the number of operations needed to solve these problems is exponentially related to the size of the input parameters. These problems are said to have an exponential time complexity.

In the early 1980s, Richard Feynman thought of using quantum mechanical systems to efficiently simulate problems that have an exponential complexity. In quantum mechanical systems, the computational space increases exponentially with the size of the system. This enables exponential parallelism when doing calculations. A functional quantum computer could lead to exponentially faster algorithms than possible on a classical device. The tricky part about these systems is that accessing the results collapses the quantum state and requires new non-traditional programming techniques. Even so, this young area of research has experienced huge growth.

I will introduce some of the basic principles of quantum mechanics and explain how they can be used to create the building blocks of a quantum computer. Then, I will describe the structure of a basic quantum algorithm.

14.15 – 14.45 MANN 101

Order 2 Defect Correction

Heejun Choi
Department of Mathematics, Purdue University

We present a solver for ordinary differential equation which is based on spectral deferred correction (SDC). We use different kind of corrector whereas Euler's methods are applied as a corrector in SDC. Our corrector is a high order method in the sense that order of accuracy increases by 2 at each correction while 1 in SDC. If the underlying problem is constant coefficient problem, the method is same as collocation method. Hence it is A-stable. The distribution of quadrature points can be arbitrary hence Gauss type points can be also used.

15.45 – 16.15 MRGN 129

DFT Study of Structures and Activity of Mono- and Bi-functional Electrocatalysts in Alkaline Environments

Zhenhua Zeng

Department of Chemical Engineering, Purdue University

Fuel cells and electrolysers have great potential to meet our future energy needs. While there is increasing interest in the development of efficient fuel cell electrocatalysts for alkaline environments, these cells have traditionally suffered from lower activity than acid-based systems. Recently, however, it has been shown that bi-functional Ni-(hydr)oxide/Pt (111) electrocatalysts manifest activities that approach those of acidic fuel cells. In spite of the promising properties of these and related systems, the atomic-scale details underlying their operation remain largely unknown, and the present study focuses on using atomistic computational techniques to elucidate these atomic-scale phenomena.

In this talk, we describe a combined thermodynamic and Density Functional Theory (DFT) analysis of oxidation/reduction of transition metal (hydr)oxides deposited on precious metal electrocatalyst surfaces. We show how this formalism can be used to develop Pourbaix diagrams and surface phase diagrams of thin (1-2 ML) Ni (hydr)oxide films/islands deposited on close-packed Pt substrates. We then extend these models to describe three-phase boundaries between the films, the Pt substrate, and the surrounding electrolyte, and we study the hydrogen evolution reaction in alkaline media at these interfaces. In the hydrogen evolution region, a partially hydrated-Ni/Pt edge is found to be the most likely candidate for the active phase, and kinetic analysis confirms that H2O dissociation is promoted at these interfaces in comparison to mono-functional Pt catalysts. We close with a discussion of the potential for further improvement of this and related bi-functional electrocatalysts in alkaline environments.

15.45 – 16.15 MRGN 206

Spectral-Galerkin Method based on Muntz Polynomials

Yingwei Wang

Department of Mathematics, Purdue University

Imposed the mixed Dirichlet-Neumann boundary conditions, the solutions of Laplacian equations behave like $O(r^{1/2})$ near the singular points, which affects adversely the accuracy and convergence of standard numerical methods. In this talk, I will propose the spectral-Galerkin method based on Muntz polynomials, in order to recover the exponential rate of convergence in the problems with singularity. Several numerical experiments and further applications will be also presented.

15.45 – 16.15 MANN 101

Adaptive Finite Element Methods for Maxwell Equations

Shuhao Cao

Department of Mathematics, Purdue University

We solve the H(curl) problem related to Maxwell equation using the Nédélec elements, which are the correct basis to model electromagnetic waves. We present a recovery-type a posteriori error estimator to bound the finite element approximation error. A local error indicator is also constructed to perform adaptive mesh refinement. Some interesting numerical examples are shown including multiple intersecting material interfaces and nonconvex domain like Fichera cube.

16.15 – 16.45 MRGN 129

Fragment-based Density-functional Theory

Daniel Jensen
Department of Physics, Purdue University

Computational chemistry is a very demanding field in terms of developing new theories and applying them to the development of efficient computer programs for modeling chemical systems. The difficulty stems mainly from the large number of interactions between the electrons in a given system. These interactions are often subtle and difficult to approximate. Density functional theory (DFT) is an increasingly popular method for solving this problem because it focuses on the electron density of a given system instead of the complex many-body wave function. However, even with the speed and storage advantages of DFT over wave-function-based calculations, there is a need for improving the accuracy and applicability of traditional DFT methods to permit the study of larger and more complex systems.

Partition Density-functional Theory (PDFT) and Partition Time-dependent Density-functional Theory (PTDDFT) are extensions of DFT that allow one to partition the external potential(s), (i.e. potentials due to the nuclei and applied electric fields), into an arbitrary number of fragment potentials in a formally exact manner. Both theories are inherently parallel methods that take advantage of parallel computing in a novel and unique way. They are also helpful tools in analyzing and improving approximations used within DFT. We present recent applications of PDFT and PTDDFT to modeling chemical systems and explain how they are helping improve both chemical theory and computation.

16.15 – 16.45 MRGN 206

Superfast Structured Algorithm for Sparse Matrix Inversion

Xiao Liu

Department of Mathematics, Purdue University

Matrix computation primarily focuses on solving linear system and eigenvalue problems. In recent years, computing certain elements of the inverse becomes a bottleneck for many scientific models. Based on the rank-structured multifrontal method and previous work on computing the diagonal of the inverse, we propose a structured algorithm for computing any arbitrary entry of the inverse of a large sparse matrix. By exploiting the low-rank structures in the factorization and the inversion for certain discretized matrices in 2D and 3D, the computational cost and memory requirement for computing each block is much lower than the sparse inversion method with local dense matrices. As a direct method, it also works for ill-conditioned and indefinite matrices. Our algorithm can be applied to many disciplines, including matrix pre-conditioners in seismic imaging, the approximation of Green's function in physics and material science, the uncertainty quantification in computational finance and so on. This is a joint work with Prof. Jianlin Xia, Prof. Maarten De Hoop and Yuanzhe Xi.

16.15 – 16.45 MANN 101

Computational Screening of Crystal Morphologies from Crystal Structure

Meenesh Singh

Department of Chemical Engineering, Purdue University

Crystal morphology is a critical determinant of the physical properties of crystalline materials. Face-specific growth rates can be used to compute dynamic and steady-state morphologies of crystals growing in a specific environment. The synthesis of crystals with desired morphologies requires a framework to guide the selection of environmental conditions. The framework developed here utilizes combinatorics to generate a graph of different morphologies connected by edges describing morphology transformations. These edges collectively form a polyhedral cone containing domains of different morphologies in a crystal-state space. The face-specific growth rates of crystals allow the identification of accessible regions within the polyhedral cone using a generalized single-crystal model. Here we introduce Morphology Domain as a fundamental property of crystals which can be used to screen crystallization conditions for the controlled synthesis of desired crystal morphologies that is both facile and readily usable. A user-friendly tool, MorphologyDomain, is presented that facilitates diverse applications

16.45 – 17.15 MRGN 129

Mechanism and Kinetics Study of Manganese Catalysts for On-Demand Production of Chlorine Dioxide

Silei Xiong

Department of Chemical Engineering, Purdue University

Two manganese complexes are used in the catalytic formation of chlorine dioxide from chlorite under room temperature at pH = 5. The catalysts afford up to 1,000 turnovers per hour and remain highly active in subsequent additions of chlorite. Chlorine dioxide reaches a maximum concentration after 1 hour. Detailed kinetic modeling based on experimental measurements is applied to study the mechanism of the homogeneous catalytic reaction systems.

16.45 – 17.15 MRGN 206

Robust Explicit Nonlinear Model Predictive Control with Integral Sliding Mode

Vu Dinh

Department of Mathematics, Purdue University

A robust control strategy for stabilizing nonlinear systems in the presence of additive bounded disturbances is proposed. The proposed control architecture is a combination of explicit nonlinear model predictive control (EMPC) and integral sliding mode control (ISMC). Feasibility analysis of a finite-horizon optimal control problem involved in deriving the EMPC control action is performed over the entire state space polytope. A sparse sampling-based boundary detection algorithm is employed to compute an approximating polynomial bounding the feasible region. A sparse-grid based interpolation scheme with Chebyshev-Gauss-Lobatto nodes is used to design the stabilizing EMPC. Robustification of the designed EMPC is provided by the ISMC. Numerical studies are provided to illustrate the efficacy and performance of the proposed control strategy for the stabilization of an uncertain nonlinear dynamical system with plant-model mismatch.

POSTER ABSTRACTS

An efficient approach of Hessian Computation in Automatic Differentiation---Pushing Edges

Mu Wang
Department of Computer Science, Purdue University

Differentiation (AD) is a set of techniques for analytically evaluating the derivatives of a function specified by a computer program. A basic underlying concept used by AD algorithms is the computational graph of a function, a directed acyclic graph (DAG) where vertices represent variables and edges represent data dependencies. Such a DAG is sufficient to work with for AD algorithms for Jacobian computation, but not for Hessian computation, since the graph does not capture nonlinear interactions between variables. In 2012 Gower and Mello introduced a symmetry-exploiting graph model for Hessian computation in which the computational graph of the function is augmented with additional edges representing nonlinear interactions. Using the model, they outlined an approach called edge_pushing for Hessian computation. However there was no correct and efficient implementation of the approach so far. We extend the theory of the edge-pushing algorithm, efficiently implement the algorithm within the AD tool ADOL-C and provide preliminary experimental results comparing the edge-pushing algorithm with an established method for computing sparse Hessians via graph coloring.

Quantification of Structural Frame-Infill Wall Interaction for Rapid Seismic Vulnerability Assessment of Reinforced Concrete Buildings

Rabab Al Louzi
Department of Civil Engineering, Purdue University

The behavior of RC structural frames with infill walls is characterized by the interaction between the frame and the masonry wall. This interaction depends on the relative stiffness and strength of the RC frame to those of the infill wall, and the intensity of the ground shaking. The main goal of this project is to quantify the effect of structural frame-infill wall interaction (SFIWI) on strength and displacement capacity of reinforced concrete (RC) buildings subject to earthquake ground shaking. The critical contribution is the explicit consideration of the ground shaking level as well as the RC frame and infill wall properties to quantify the impact of SFIWI on overall building performance. Results from high-fidelity computational models, with calibrated structural and infill element models, will be used to provide a seismic vulnerability index that could be used in more accurate rapid seismic vulnerability assessment of RC buildings. Preliminary finite element analyses of RC frames with infill walls under lateral loading have been carried out in Abaqus/Explicit. A selection of RC frame and infill wall models have been developed. The models are calibrated based on monotonic lateral loading experiments performed by Mehrabi et al. (1994). These calibrated RC frame models and infill wall models (consisting of hollow or solid concrete bricks and concrete mortar joints) are being evaluated for fidelity using response data from cyclic tests also made by Mehrabi et al. (1996). The final fidelity checks will be made using data from dynamic tests of infilled RC frames carried out on laboratory shaketables (e.g. Hashemi and Mosalam 2006; Stavridis 2009). Field data from Haiti and Turkey, two places with richest RC frame with infill walls field data, will be used to study the performance of the computational models with uncertain material data.

Timescale Creator

Nag Varun Chunduru
Department of Computer and Information Technology, Purdue University

TimeScale Creator, a free JAVA package (www.tscreator.org) developed in conjunction with the Subcommission on Stratigraphic Information (stratigraphy.science.purdue.edu) of the International Commission on Stratigraphy and the Geologic TimeScale Foundation includes:

(1) On-screen exploration of any portion of the geologic time scale from internal datasets (ca. 20,000 biologic, geomagnetic, sea-level, stable isotope, igneous provinces, bolide impacts, images of reconstructions and fossils, and other events).
(2) Loading additional specialized regional stratigraphy datapacks of lithologies and fossil zonations compiled jointly with geological surveys (Canada, New Zealand, Britain, Belgium, China, Russia, etc.) or insertion of self-constructed datasets.
(3) Search functions, including an "in context" auto-display feature for selected geologic formations or datums.
(4) Geographic interfaces and displays of regional stratigraphy.
(5) Cross-plotting of outcrops/wells (meters) against the extensive global/regional time scales (myr) and depth-to-age conversion after user-selected control points.
(6) Display of geologic transects.
(7) On-screen "hot-curser-points" attached to datums/formations with windows and URL links to provide in-depth details.
(8) A web interface tsclite and tscWeb for online usage. User can generate bookmark and share charts.
(9) An evolution tree creator to generate and display evolution in vertebrates, humans etc.
(10) A wealth of chart-modification features and output in SVG-PDF or other formats for publication.

The software development and extensive datasets are the products of Purdue students in computer engineering and in earth sciences during the past five years. The databases and visualization package are envisioned as a convenient reference tool, chart-production assistant, and a window into the geologic history of our planet for both educational and professional users.

Sketching 3D Animations using CUDA

Juraj Vanek
Department of Computer Graphics Technology, Purdue University

Quick creation of 3D character animations is an important task in game design, simulations, education, training, and more. We present a framework for creating 3D animations using a simple sketching interface coupled with a large, unannotated motion database that is used to find the appropriate motion sequences corresponding to the input sketches. Sketches can be enhanced by motion and rotation curves that improve matching in the context of the existing animation sequences. Our framework uses animated sequences as the basic building blocks of the final animated scenes, and allows for various operations with them such as trimming, resampling, or connecting by use of blending and interpolation. A database of significant and unique poses, together with a two-pass search running on the GPU, allows for interactive matching even for large amounts of poses in template database. The system provides intuitive interfaces, an immediate feedback, and poses very small requirements on the user.

High Frequency Trading

Mengyao Wang
Department of Mathematics, Purdue University

Traders need to make predictions quickly. High Frequency Trading (HFT) provides an efficient way to trade securities on a rapid basis with computer algorithms.

Evaluation of the Numerical Dispersion in Spectral Finite Element Method with the Theory of Phononic Crystals

Nicolas Guarin
Department of Civil Engineering, Purdue University

The performance of the classical and spectral finite element method in the simulation of elastodynamic problems is evaluated using as quality measure their ability to capture the dispersive behaviour of the material. Four different materials are studied: a homogeneous non-dispersive material, a bilayer material, and composite materials consisting of a aluminum matrix and brass inclusions or voids. To find the dispersion properties, spatial periodicity is assumed so the analysis is conducted using Floquet-Bloch principles. The effects in the dispersion properties of arbitrarily lumping the mass matrices resulting from the classical finite element method are also investigated, since that is a common practice when the problem is solved with explicit time marching schemes. At high frequencies the predictions with the spectral technique exactly match the analytical dispersion curves, while the classical method does not. This occurs even at the same computational requirements. At low frequencies however, the results from both techniques coincide with the analytically determined curves. Surprisingly, at low frequencies even the results obtained with the artificial diagonal mass matrix from the classical technique exactly match the analytic dispersion curves.

Atomistic Simulation of Tunneling Field Effect Transistor

Zhengping Jiang
Department of Electrical and Computer Engineering, Purdue University

For decades, scaling of the Si-based MOSFET has enabled an exponentially increasing level of integration, packaging density and clock speed. Today heat dissipation issues prevent any performance improvement through increasing clock frequency, because supply voltage has reached the scaling limit of MOSFET technology and cannot be lowered below about 1 V without performance degradation. This fundamental power consumption issue has spurred the exploration of alternative switching mechanisms.

Tunneling Field Effect Transistors (TFETs) have been investigated intensively because of its ability to reduce the 60meV/dec subthreshold swing (SS) which limits power scaling. When a TFET is scaled down to nanometer size, quantum effects will dominate carrier dynamics and classical transport models assuming a continuous medium will eventually fail to predict device performance. Quantum transport at realistic dimensions meaning simulation domains involving thousands or even millions of atoms cannot be performed at the ab initio level due to the prohibitive computational burden. Approaches such as the empirical tight binding (ETB) method are required provided that they can embody the physics into proper parameterization. In this work, coherent transport is employed to investigate the ideal device performance. 10 orbitals (sp3s* with spin-orbit coupling) are included at each atom to accurately capture the material properties. The non-equilibrium Green's function (NEGF) method is used to study ballistic transport with the NanoElectronics MOdeling Tools (NEMO5). Performances of TFETs with different geometry configurations in their scaling limits are evaluated and compared with results from continuous models or experimental measurements. Results serve well as guidelines for device optimizations and fabrications. Computational burden imposed by devices with over 20,000 atoms are distributed to over 700 CPUs by parallelization with MPI protocol.

Exploring the Impact of an Additional Three-Body Interaction in the Restricted Three-Body Problem

Natasha Bosanac
Department of Aeronautical and Astronautical Engineering, Purdue University

Consider a binary star system (e.g., pulsar-white dwarf, pulsar-pulsar) with a significantly smaller companion, such as an exoplanet, in orbit about the binary. These systems have been observed by astronomers far beyond the reaches of the solar system. Given the absence of experimental data gathered within the vicinity of the binary, it is possible that the gravitational field near a binary star system might not be accurately modeled using only pairwise gravitational forces. In this investigation, the presence of an additional three-body gravitational interaction is considered. Many-body forces are not an entirely new concept; in fact, the importance of three-body interactions in accurately modeling force fields on the atomic scale is well established in the discipline of nuclear physics. On a much larger scale, the motion of a small body orbiting a binary star system serves as a new and interesting application. In this interdisciplinary research, computational and visualization tools are employed to study the effect of this additional contribution on possible orbits of the exoplanet. When weighted appropriately, the three-body interaction is found to significantly alter the form and existence of periodic and quasi-periodic orbits. Physically, this means that exoplanets could follow orbits that cannot be accurately recovered using traditional inverse-square gravitational forces.

Multiobservable Laser Control of Molecular Dynamics

Andy Koswara
Department of Chemical Engineering, Purdue University

In 1983 a novel study on the controllability of a quantum mechanical system coupled with an external field reveals that *coherent* steering of quantum system to a desired state is possible. Since then a new field of study known as *Molecular Quantum Control* (QC) has rapidly developed at the intersection of four established fields, namely Quantum Mechanics, Ultrafast Laser Physics, Bilinear Control Theory, and Engineering Optimization. Early theoretical and experimental applications of QC were studied on the control of photodissociation reactions. Here, the control method was employed in the perturbative regime where only two parameters of the control field are manipulated, namely the field's center frequency and its associated phase. More advanced control techniques have since been developed which manipulates higher number of field parameters. This allows for improved control of the interference between multiple quantum pathways within a quantum system to reach a target state. In this work, we demonstrate an advanced control method for laboratory QC which maximizes multiple superpositions of quantum states in an ensemble of QC systems. This is achieved by formulating the control problem as a multiobjective optimization problem and incorporating multiobjective genetic algorithm to obtain the Pareto set of QC solutions. We use atomic Rb as a test-bed for our method and implement our algorithm in a feedback control loop.

A Resource Allocation Approach to Patient-Centeredness in Primary Care

Ravindran Rajesvaran
Department of Statistics and Actuarial Science, Purdue University

Patient-centered care, one of the Institute of Medicine's six aims for 21st century healthcare, is "respectful of and responsive to individual patient preferences, needs and values, and ensuring that patient values guide all clinical decisions". A major obstacle to delivering patient centered care is the disconnect or 'gap' between patient wants and needs, which should be taken into account by any assessment of patient-centeredness. This research developed a new assessment of patient-centeredness from a resource allocation perspective and sought to determine whether it taps into any of the bases of existing measures of patient-centeredness, its relationships with patient-physician characteristics and whether better health outcomes are associated with a more patient-centered visit. Ternary plots, which were included in patient post visit surveys as well as physician pre- & post-visit surveys administered at a primary care clinic and resident training center, were created to capture perceptions of wants, needs and medical care received/delivered among three major dimensions of primary care: Health Education & Prevention, Diagnosis & Treatment as well as Follow-up, Monitoring & Management. A variety of gap-based measures of patient-centeredness were computed by taking the norm distance between different resource allocations. Analysis of variance tests were performed between these gap-based measures and patient-physician characteristics. Additionally, correlation coefficients were computed between the gap-based measures and existing measures of patient-centeredness. The results obtained indicate that the gap-based measures are significantly correlated with existing measures of patient-centeredness and characteristics of the patient-physician pair reveal significant differences in the level of patient-centeredness of visits. The new assessments appear to be an easy method for assessing resource-allocations of patients' needs, wants, and the care delivered and can be helpful in identifying characteristics of patient-physician pairs which are 'risk factors' to lack of patient-centeredness. Future work includes developing hierarchical models and extending data collection by retrospective chart review to add health outcomes such as medication adherence and future utilization.

Asymptotic Joint Normality of Counts of Uncorrelated Motifs in Recursive Trees

Mohan Gopaladesikan
Department of Statistics, Purdue University

We study the fringe of random recursive trees, by analyzing the joint distribution of the counts of uncorrelated motifs. Our approach allows for finite and countably infinite collections. To be able to deal with the collection when it is infinitely countable, we use measure-theoretic themes. Each member of a collection of motifs occurs a certain number of times on the fringe. We show that these numbers, under appropriate normalization, have a limiting joint multivariate normal distribution. We give a complete characterization of the asymptotic covariance matrix. The methods of proof include contraction in a metric space of distribution functions to a fixed-point solution (limit distribution). We discuss two examples: the finite collection of all possible motifs of size four, and the infinite collection of rooted stars. We conclude with remarks to compare fringe-analysis with matching motifs everywhere in the tree.

We would like to acknowledge our poster judges and volunteers who have greatly assisted us in hosting this conference:

Poster Judges

Prof. Ananth Grama
Professor of Computer Science & Director of Computational Science and Engineering Program, Purdue University

Prof. Mark Daniel Ward
Assistant Professor in Statistics, Purdue University

Volunteers

Aaron Goldner (*EAS*)

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