CSESC - 2012
Computational Science & Engineering Student Conference

Welcome to the fourth annual Computational Science and Engineering Student Conference. Hosted by Purdue and organized by SIAM@Purdue, 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 to see how modeling and numerical techniques that are being applied in other disciplines.

This year's conference brings together work from several universities in both poster and oral presentations. We thank you for your participation.

Please enjoy.

siam @PURDUE

A student chapter of the
Society for Industrial and Applied Mathematics

CSESC - 2012
Computational Science & Engineering Student Conference

Schedule

12.15 – 12.40	Poster Setup	Wood Commons (CIVL)
12.40 – 12.45	Opening	CIVL 1252
12.45 – 1.15	Opening Keynote Professor Ananth Grama	CIVL 1252
1.15 – 2.15	Poster session	Wood Commons
2.15 – 2.30	Coffee break	Wood Commons
2.30 – 5.00	Student Talks	CIVL 1113, 1266, 2108
5.00 – 5.30	Closing Keynote Professor Gerhard Klimeck	CIVL 1252
5.30 – 5.45	Awards for Best Paper and Poster	CIVL 1252
5.45 – 7.30	Dinner	Adelino's

siam @PURDUE

A student chapter of the
Society for Industrial and Applied Mathematics

CSESC - 2012
Computational Science & Engineering Student Conference

Speaker Schedule

Time	Rm. 1113	Rm. 1266	Rm. 2108
2:30	Vaibhav Bhutoria	Amin Emad	Dipti Desai
2:50	Federico Antico	Xingxie Ni	Kameswararao Anupindi
3:10	Fernando Dri	Farzad Hassanzadeh	Koushik Viswanathan
3:30	Fernando Cordisco	Sunghun Jung	Biaobin Jiang
3:50	Iffat Arisa	Ali Mostafavi	Qing He
4:10	Johnathan Goodsell	Hee Jun Choi	Vu Dinh
4:30	Ariful Azad	Isaac Tetzloff	Yuanzhe Xi

siam @PURDUE

A student chapter of the
Society for Industrial and Applied Mathematics

Alphabetical list of authors and their paper abstracts:

Author	Title	Abstract
Antico, Federico	A combined experimental and theoretical study of Nickel-Titanium Shape Memory Alloy Wires adhesion to Polymeric Materials	A combined experimental/theoretical study of adhesion between a Nickel-Titanium (NiTi) shape memory alloy wire embedded in a Thermoplastic Polyolefin (TPO) matrix is presented. NiTi wire surfaces were modified to improve adhesion by functionalizing with chemical coupling agents or application of a surface microgeometry. Pull-out tests were conducted and the extent to which each treatment increased the pull-out force was quantified. Results from a nonlinear finite element analysis wherein the NiTi/TPO matrix interface is modeled with a cohesive zone model suggest that the interface behavior strongly depends on the cohesive energy during pull-out, and less on the cohesive strength. Additionally, a parametric analysis is performed to take into account how the residual stresses from manufacturing process affect the local mode mixity during debonding.
Anupindi, Kameswararao	Lattice Boltzmann Simulations of Periodic Fluid Flow Problems	Lattice Boltzmann method (LBM) offfers an alternative to the conventional simulation of fluid flows. In this approach Navier-Stokes equations are not solved rather the lattice Boltzamnn equations (LBE) are solved in a mesoscopic limit thus enabling the numerical simulation of fluid flows. In the present work, together with the general methodology of LBM, we present simulations of two-dimensional double shear layer, three-dimensional Taylor Green vortex, and applications to aeroacoustics. All the simulations are performed with the in-house LBM solver that is being developed.
Arisa, Iffat	Analyzing Properties of Asphalt Binder by Molecular Dynamics Simulation	In this study, molecular dynamics simulations are carried out to study the physical, thermodynamic, and kinetic properties of asphalt over a temperature range of 218 – 358 K. Asphalt model is taken from previous study which elemental composition is very close to SHRP AAA-1 asphalt. Asphaltene, resin, and saturate – all of these fractions have different molecular structures and they exhibit some phenomena because of temperature change. The asphalt systems are parameterized via the dreiding force field in order to determine potential energy. It gives better results than the previously used force field in literature. Simulations reveal that when temperature increases, density, heat of vaporization, and cohesive energy density decrease. Also the simulations bring out the behavior of density – temperature relationship. The slope of density-temperature curve shows a sharp change which indicates the presence of glass transition temperature. Again diffusion coefficients are investigated which revealed qualitative differences between larger (asphaltene) and smaller (saturate)

		molecules in the system.
Azad, Ariful	Meta-clustering based population matching in flow cytometry	Cell populations in a multiparametric flow cytometric sample can be characterized with finite mixture models of multivariate probability distributions. For automated registration and comparison of cell populations across samples, new algorithms are necessary to match these distributions in high-dimensional marker space. With increasing number of markers and large cohort sizes, such approaches must be both efficient and systematic. Towards this, we present flowMatch, a robust solution to the matching problem based on templates that summarize all samples from a given class, thus allowing us to study the population-level changes across different conditions and time points. We designed flowMatch as a hierarchical template-construction algorithm where each step uses a Generalized Edge Cover for optimally matching populations across samples, which are then used to create meta-clusters for a new class template. We applied the algorithm on samples obtained across different time points from healthy controls and multiple sclerosis patients treated with Copaxone and interferon beta. At each time point we created distinct templates for each of the three classes of samples and matched them across time points to follow the progression of populations defined by the corresponding meta-clusters. We detected few correlated populations across treatment arms by comparing the progression paths (converging, diverging or parallel) of the meta-clusters between the two treatment arms. To demonstrate that meta-clusters in a template preserve the common features of populations from initial samples, we applied flowMatch on 30 anti-CD3-antibody stimulated blood samples, formed templates from samples before and after stimulation, and identified a clear shift at the meta-cluster level after stimulation.
Bhutoria, Vaibhav	Direct Numerical Simulation of Compressible Homogeneous Turbulence	Reynolds Averaged Navier Stokes (RANS) solvers and turbulence models continue to be of interest. With improvements in computing power, the popularity of Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) for simulating turbulent flows has increased. Along with experiments, these simulations have become important and feasible tools in creating test results and benchmarks to establish

		the veracity of turbulence models. Most turbulent models have been designed for low-speed, incompressible flows. Compressibility corrections to these models become important in high Mach number flows. Specifically, these corrections manifest themselves as effects of compressibility on the dissipation rate of turbulent kinetic energy. For compressible flows two extra terms, pressure dilatation and dilatation dissipation, appear in the turbulent kinetic energy equation. Existing models model the ratio of dilatation dissipation to solenoidal dissipation as a function of the turbulent Mach number and the pressure dilatation is neglected. Recently modified compressibility corrections have been proposed based on the notion that the growth rate in compressible free shear flows level off at a turbulent Mach number, as seen in experiments and DNS. In this work, we simulate decaying isotropic turbulence and homogeneous shear flow using DNS. High fidelity of the simulations increases the computational cost. The original code was written at a time when the size of RAM was limited. For simulating flows on a larger domain serial code was modified to run on modern, parallel distributed architecture. We observe the trends of the statistical quantities and take a look at the flow features.
Choi, Hee Jun	Accelerating the convergence of Krylov Deferred Correction	Spectral deferred correction (SDC) methods for solving ordinary differential equation(ODEs) were introduced by Dutt, Greengard and Rokhlin(2000). Looking at SDC as an iterative method, krylov deferred correction(KDC) was developed by Huang, Jia, Minion(2006). KDC solves defect equation using GMRES with low order(forward or backward Euler) precondition. In this paper, we present a high order preconditioner and do some numerical comparision with KDC.
Cordisco, Fernando	Interfacial toughness on sinusoidal elastic patterned bi-material interfaces	A computational model is used to study the behavior of a crack that propagates along a sinusoidal cohesive interface between two dissimilar elastic solids under remote mode I loading. The effective toughness of the interface is computed as a function of material and geometric parameters. For sufficiently large elastic mismatch, it is found that the fracture mechanism transitions at a critical ratio of roughness amplitude to wavelength () from continuous propagation of a single crack, to a mechanism involving nucleation and coalescence of daughter cracks ahead of the main crack. This transition substantially reduces the toughening effect of the interface roughness. The results suggest some guidelines for practical design of failure resistant interfaces through appropriate choice of geometric, material, and cohesive parameters.
Desai,	A Comparative	There has been a growing concern over the enrollment by US

Dipti	Usability Study of Personalized Informational Websites	citizens into Science, Technology, Engineering and Mathematic (STEM) positions. With ever growing outsourcing, the US is on the verge of losing its global technological competitiveness. Governmental as well as non-profit organizations are in constant lookout of ideas, programs and initiatives that encourage more US citizens to consider STEM careers. One of the most common recommendations out of these councils and existing programs, is to involve such groups into STEM that have not been represented well in the overall population. Underrepresented groups need more attention, personalization, motivation and encouragement by institutions and industries for the government to practically achieve their targeted numbers in STEM (Business-Higher Education Forum, 2010). With resources highlighting the importance of internet personalization to web users, this research focuses on redeveloping Computer and Information Technology (CIT) department website for prospective students, specially the underrepresented minorities; in order to learn students' perceptions of the website, its content and usability.
Dinh, Vu	An experimental design algorithm for dynamics recovery of ODEs systems	Many problems in applied sciences are governed by a dynamical system of diff erential equations with unknown parameters, where the quantity of interest is the dynamics (time course) of some state variable of the system. The traditional approach to study such systems is designing experiments to improve the estimation of the parameters of the system. Generally, this problem of parameter identification is an ill-posed inverse problem, and in many case (when the system is lack of identifiability), unsolvable even if we have an infinite amount of data. Another issue arises in practice (especially in systems biology) is that data from experiments are usually sparse and noisy, which makes any effort to use interpolation or regression methods to identify the dynamics become invalid, no matter how well the experiments are chosen. To overcome these difficulties, in this talk, we propose a novel approach to the problem. Instead of trying to identify the parameters, we construct a probability distribution on the whole parameters space, based on how well the system controlled by a set of parameter values fits the data. Using this probabilistic framework, we sequentially design the experiment to maximize the amount of information we get about the system form each experiment. This algorithm helps detect the most important features of the dynamics (that need to be measured), then the average dynamics estimator (ADE) is employed for a complete dynamics recovery.
Dri, Fernando	On the multiscalemec	Cellulose nanocrystals (CNCs) are a promising family of environmentally friendly nanoscale reinforcing materials. They

	hanics of the hierarchical structure of cellulose nanocrystals	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.
Emad, Amin	Casual Compressive Sensing for Gene Network Inference	We propose a novel framework for studying causal inference of gene interactions using a combination of compressive sensing and Granger causality techniques. The gist of the approach is to discover sparse linear dependencies between time series of gene expressions via a Granger-type elimination method. The method is tested on the Gardner dataset for the SOS network in E. coli, for which both known and unknown causal relationships are discovered.
Goodsell, Johnathan	Micromechanical intrinsic flaw distribution model for prediction of the hole-size effect in the off-axis tensile specimen	Prediction of the hole-size effect in a composite 10 degree off-axis tensile specimen has been accomplished by means of a computationally-efficient intrinsic flaw distribution model. Unnotched specimens were tested to determine the intrinsic flaw length distribution. The flaw length distribution was used to predict the failure site and failure stress for specimens containing circular holes with diameters ranging from 1.59 mm to 12.70 mm. Predictions are shown to agree well with the experimental results for the most likely failure site and failure stress. These results suggest that the hole-size effect in off-axis tensile specimens can be effectively predicted by the developed intrinsic flaw distribution model, which is progress toward the reduction of experimental testing by means of computer simulation.
Hassanzadeh, Farzad	Novel distance measures for rank aggregation	The problem of rank aggregation arises in research areas as diverse as computer science, social sciences, management, and marketing. Rank aggregation may be succinctly described as follows: given a set of rankings, each produced by an expert, find the ranking that minimizes the sum of the distances to the original

		rankings. Here, the distance function is chosen according to some predefined relevance criteria, such as similarity of ranked subjects and cut-off thresholds for the rankings. In most rank aggregation scenarios, one uses Kendall's tau distance which leads to Kemeny optimal orderings. Although Kendall's tau and many other classical distance functions, including Spearman's Footrule, are well established and well studied, they cannot take into account two important factors in rank aggregation. First, for some applications, the top of the list is more important than the bottom of the list, and hence changes to the top of the list must be compensated for by larger distances. Second, transposing elements that are similar must be less costly than transposing dissimilar elements. In this talk, we propose a distance function, termed weighted Cayley distance, based on transpositions with non-uniform costs that enables us to address the top-bottom and similarity problems. Many of the previously proposed distance functions may be viewed as a specialization of the proposed distance function. We also describe a polynomial time algorithm for computing the general form of this distance function using a variety of tools from graph theory and optimization theory. Furthermore, we study rank aggregation in a distributed context and provide convergence results, including the rate of convergence to a consensus vote.
He, Qing	An Explicit Time-Domain Finite-Element Method that is Unconditionally Stable and Physics-Based Minimal Order Reduction of Linear Networks	The root cause of the instability is quantitatively identified for the explicit time-domain finite-element method that employs a time step beyond that allowed by the stability criterion. With the identification of the root cause, an unconditionally stable explicit time-domain finite-element method is successfully created. This method is unconditionally stable in the sense that it is stable for any time step no matter how large the time step is. The proposed method retains the strength of an explicit time-domain method in being matrix free while eliminating its shortcoming in time step. Numerical experiments have demonstrated the superior performance of the proposed method in computational efficiency as well as stability compared to the conditionally stable explicit method and the unconditionally stable implicit method. The essential idea of the proposed method for achieving unconditional stability in an explicit method is also applicable to other time domain methods. In recent work, guided by electromagnetic physics, we find a minimal order model of the linear network for a prescribed accuracy to accelerate circuit simulation. It is applicable to both circuits dominated by RC effects and circuits governed by RLC or full-wave physics. For linear networks dominated by RC physics, the order of the proposed model is

		only 2 regardless of the circuit size. The proposed model preserves passivity and stability. It is frequency independent. In addition, it is constructed in linear complexity. Application to on-chip and package circuits has demonstrated the performance of the proposed physics-based minimal-order reduction.
Jiang, Biaobin	Social Balance in Genetic Interaction Networks	Social balance was found in the social network analysis by the so ciologists in 1940s that can be simply rephrased as the enemy of my enemy is my friend. In the theory of social balance, only two i n the totally four kinds of triadic relationships are balanced amon g three people: three people are all friends with each other, or two of them are friends against the third person. These relationships will become unstable if the relationships among three people beco me mutually hostile, or one hostile coexisting with two friendship s. In the long- term observation, sociologists found that unbalanced structures te nd to spontaneously change into balanced structures. Similarly, re cent studies in systems biology showed that the activities of a set of genes in living organisms are not independent: they are either p ositively or negatively related to each other. In the extreme case, i t will lead to the lethality of organisms if two extremely negativel y related genes are lost or mutated by external perturbations. Ther efore, systems biologists model these non- independent relationships among genes as a signed graph with po sitive links indicating positive interacting genes, vice versa. Furth ermore, these genetic interactions were recently found to rewire a cross different environments: lots of negatively linked gene- gene pairs are changed into positively linked under DNA damage d conditions. What kind of triadic interactions among genes keeps stable across the normal and DNA damaged conditions? Here, w e do the triadic decomposition for the yeast genetic interaction net works in the both conditions into four different triads: NNN, NNP , PPN and PPP (N=negative, P=positive). Next, we build a Marko v Chain model to describe the triadic transitions between different types of triads across the two conditions. The stationary distributi on produced by the Markov Chain model shows that two types of genetic triads, NNP and PPN, are more stable than the others, NN N and PPP. This finding in genetic interaction networks is partiall y different from the social balance: the genetic balanced structure s tend to avoid being monochromatic (NNN or PPP). The intrinsic driving force to generate these balanced structures is worth for fu rther investigation.
Jung, Sunghun	Robustness for Large Scale UAV	Large scale autonomy would mean the following: fewer operators, larger areas of coverage, and more vehicles. Rigorous optimization of decision theory based approaches to handling this

	Autonomous Operations	problem suffer from speed limits to real-time computations. In the first part, we provide solutions based on rigorous approaches, but avoid heavy real-time computation through off-line processing. For mapped regions, we convert maps into traversability graphs using trapezoidal map/voronoi type algorithms. We then find the shortest permissible paths for different vehicles using Dijkstra's algorithm and then preening the allowable paths using constraints on individual vehicles. Out third step consists in determining the minimum time taken by a given vehicle over those paths. We insert margins of safety at each level of this hierarchy by letting UAV to perform 1-D optimal control within limits of the vehicles performance so that vehicles can slow down or speed up in response to unexpected events. In the second part, We develop scalable methods by which UAVs, individually or cooperatively, can perform standard functions of search, surveillance, and ground target tracking and handoff with a minimum of human intervention, and fulfill mission requirements in real-time in highly uncertain environments. Our method relies on an offline discretization of space, followed by an offline discretization of time for the travel of different vehicles, and the offline solution of the search, surveillance, and tracking problems. These offline solutions are then used online with suitable modifications to account for environment uncertainty, UAV degradation/failure and changing mission requirements.
Mostafavi, Ali	Ex-Ante Analysis of Innovation Policies in Infrastructure System-of-Systems	This dissertation focuses on the creation and testing of a new paradigm in innovation and policy assessment in civil infrastructure system-of-systems (SoS). Many uncertain factors (e.g., economic conditions, public attitudes, political priorities, and business dynamics) affect the creation and diffusion of innovations in civil infrastructure. Policymakers who evaluate innovation policies also face known unknowns (policy outcomes whose nature is known but their probability of occurrence is not known) as well as unknown unknowns (policy outcomes whose nature and probability of occurrence are not known) due to the adaptive behaviors of the players in the system. The overarching objective of this dissertation was to create and evaluate an ex-ante analytical framework for micro-simulation of infrastructure innovation policies under uncertain conditions. The developed framework is based on the abstraction and micro-simulation of the activities and interactions of the major players in the system and its application is demonstrated for the assessment of sustainable financial innovation policies. Using the framework and data obtained from a wide range of sources ranging from historical records and case studies to interviews with subject

		matter experts, the interdependencies of finance and transportation infrastructure were explored. These interdependencies (e.g., the effects of financial market conditions on the debt-related decisions made by state Departments of Transportation) then were used to develop a hybrid agent-based/system dynamics model for micro-simulation of sustainable financial innovation policies. Using this model and Monte-Carlo experimentation, the policy landscape of transportation infrastructure in the U.S. was simulated. The model was verified and validated as follows: (1) by using sensitivity analysis and uncertainty propagation analysis, and (2) through face validity by several subject matter experts from organizations such as the World Bank, the U.S. Department of Transportation, and the Federal Highway Administration. The results suggest that the simulated policy landscape is capable of identifying the significant factors that affect policy decisions and explore scenarios for closing the financing gap under uncertain conditions. This distinctive approach is the first of its kind to simulate the U.S. transportation infrastructure policy landscape by simulating the micro-dynamics of the system. This framework has the potential to be adopted for ex-ante simulation of the landscape of sustainable policies towards expansion of alternative energy systems, enhancing intelligent transportation systems, and improving the resilience of electric grids.
Ni, Xingxie	A Fast Eigenmode Algorithm for Simulation of Lamellar PlasmonicMeta materials	The eigenmode based methods, for example, spatial harmonic analysis (SHA) method and rigorous coupled wave analysis (RCWA) method, are among the most versatile methods for analyzing the diffraction of electromagnetic waves by periodic structures. They are non-iterative and mesh-free techniques for obtaining the exact solution of Maxwell's equations. The accuracy of the solution depends solely on the number of modes in the eigenmode expansion of the field. However, they all suffer from the basis mismatching between the actual eigenmodes inside the simulated structures and the basis, usually Fourier basis, which the solver depends on. This problem is extremely severe when simulating plasmonicmetamaterials, an artificial material designed to achieve advantageous and unusual electromagnetic properties. A very large number of modes are usually required to resolve such kind of structures due to the high-order plasmonic modes inside the structure. In this paper, we introduce a new formulation based on transfer matrices to obtain the eigenmodes of a two-dimensional structure. The eigenmodes of the structure are given by the roots (zeros) on a complex plane of a single non-linear equation. We use Lehmer-Schur algorithm, which is based

		on Argument principle, to locate zeros with a relatively good accuracy as well as a fast and reliable convergence. The algorithm is validated with finite element method (FEM) and SHA method using a metal-dielectric lamellar nanostructure. The accuracy of the eigenmodes obtained by the proposed algorithm is very high (with relative error as low as 1e-10) and is comparable with SHA method using very large number of modes. With approximately same accuracy, it is twenty times faster than SHA method. The algorithm is parallelized using Linux implementation of POSIX threads and we obtain a speedup about three with eight processors.
Tetzloff, Isaac	Using Linear Relaxations to Approximate Integer Programming Solutions for Aircraft Allocation	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; it is also a function of how airlines use new aircraft along with other existing aircraft to satisfy the passenger demand for air transportation. Previous research to measure fleet-wide impacts of new aircraft uses an integer programming approach to allocate existing and future aircraft to routes representing commercial air transportation within or to / from the United States. The allocation problem represents how the airline chooses to use the new aircraft.The allocation tool can analyze the impact of new aircraft on environmental and market fleet-level metrics, but the current integer programming formulation can take up to several hours to find an optimal solution. One way to decrease the time to compute a solution is to use the linear relaxation of the problem (allow the integer decision variables to take on continuous values) and employ various rounding schemes to create an integer solution. Preliminary studies using a linear relaxation greatly reduce the computation time of an allocation that maximizes airline profit; however, the rounding scheme used to transform the fractional solution from a a linear relaxation to the integrality requirements of aircraft allocation has a strong influence on the quality of the solution from the linear relaxation. This presentation will discuss various rounding schemes used on a linear relaxation and how the different schemes impact the solution quality.
Viswanathan, Koushik	Digital Radiography and Computed Tomography - Simulation and	X-ray imaging - comprising of X-ray radiography simulation and reconstruction of volumes from 2D CT projection samples, finds extensive application in the fields of medical imaging and non-destructive testing. Radiography simulation involves determining 2D X-ray radiographs from complete 3D information (CAD

	reconstruction techniques	description) and scanning geometry, while reconstruction involves (partial or complete) recovery of volume/ slice data from a number of 2D/1D projections. This work addresses both simulation and reconstruction. Simulating X-ray radiography imaging on CAD models amounts to evaluating the X-ray attenuation law for virtual rays passing through the 3D volume and is most often done using the ray-casting technique, employing ray-polygon intersection tests. An alternate algorithm is introduced, inspired by classical rasterization techniques used for computer graphics, and its implementation on consumer-grade graphics hardware (GPU) is discussed. On the other hand, CT reconstruction is a very well studied problem and is usually tackled using the Filtered Backprojection algorithm. The motivation behind this algorithm is explored and implementations on CPUs and GPUs are compared. Some sample images are presented and an open-source X-ray imaging package - XRaySim, is introduced.
Xi, Yuanzhe	Superfast algorithm for Toeplitz Problems	We present some superfast and stable algorithms for Toeplitz linear systems, least squares and eigenvalue problems. Based on the displacement equation, a Toeplitz matrix T is first transformed into a Cauchy-like matrix C, which has the properties of fast matrix-vector multiplication and small off-diagonal numerical ranks. By exploring these two properties, the hierarchically semiseparable (HSS) matrix approximation to C can be constructed in nearly linear complexity. Then one linear comlexity linear system solver, three linear complexity least squares solvers and one linear complexity (for each eigenvalue) eigensolver are proposed. The efficiency and stability of our algorithms are studied through various classical numerical tests on matrices varying from well-conditioned to very ill-conditioned ones. In these tests, our new methods are generally much faster and more accurate than some recent solvers.

Alphabetical list of authors and their poster abstracts

Author	Title	Abstract
Abdul Massih Said, Michel	Interactive Urban Ecosystem Design	We address the problem of interactive design of urban spaces by integrating plants in urban environments. We have developed an interactive simulation and procedural system for 3D urban models. Using our CUDA-based interactive system we can simulate spatial distribution of a large ecosystem embedded in a city. We have achieved a performance of 50M-70M collision tests per second allowing for 250,000 plants being simulated at 5-6 fps on a Tesla C2050
Arisa, Iffat	Predicting the Failure of Composites Using Fuzzy Systems	Composite laminates are widely used in industry due to their outstanding geometrical, mechanical and physical properties. However, predicting the failure of these composite laminates is complex and non linear as it is affected by the non uniform distribution of the fibers and there are several modes that control the composite failure. Therefore, this problem is qualified to be modeled using fuzzy systems. A modified learning from examples (MLFE) algorithm is used to build the rules and membership functions while Recursive least squares (RLS) algorithm is used to tune the system. Thirty training points developed by a finite element model are used to train the fuzzy system. The classical lamination theory (CLT) was used to evaluate the performance of the fuzzy system using six simulation points. It is shown that the fuzzy system was capable of predicting the failure of composite laminates. The analysis also shows that the error for the simulation points depends significantly on the selected training points.
Bauman n,Dougl as	Correcting for Amplification Bias in Next-Generation Sequencing Technologies	Next-generation sequencing (NGS) technologies have opened the door to a wealth of knowledge and information about biological systems, particularly in genomics and epigenomics. These tools, although useful, carry with them additional technological and statistical challenges that need to be understood and addressed. One such issue is amplification bias. Specifically, the majority of NGS technologies effectively sample small amounts of DNA or RNA that are amplified (i.e., copied) prior to sequencing. The amplification process is not perfect, and thus sequenced read counts can be extremely biased. Unfortunately, current amplification bias controlling procedures introduce a dependence of gene expression on gene length, which effectively masks the effects of short genes with high transcription rates. In this work we present a novel procedure to account for amplification bias and demonstrate its effectiveness in estimating true gene expression independent of gene length.

Dolan, Patrick	Unraveling the Complex Network of Virus-Host Interactions in Hepatitis C Virus	The (+) RNA genome of Hepatitis C virus (HCV) encodes 3 structural proteins and 7 nonstructural proteins. Using this small payload of effectors the virus alters the global behavior of the host cell in order to create an environment conducive to its own replication. Often these effects are mediated by protein-protein interactions. Therefore, we have performed a large-scale yeast two-hybrid (Y2H) screen to identify potential virus-host protein-protein interactions. Our study identified 106 unique interactions between 7 HCV and 94 human proteins. 42% of these human proteins (or the genes encoding them) have been previously implicated in HCV infection in other large-scale screens. Using a combination of biological and computational approaches, we have interrogated the complex network of protein interactions to identify the key features of the network that may provide insights into HCV infection and HCV-related disease progression. Analysis of the cellular targets of HCV proteins for enrichment of gene ontology terms, protein families and cellular pathways revealed a number of cellular processes previously implicated in HCV infection, including lipid and cholesterol metabolism and cytoskeletal proteins. This analysis identified several new potential targets including the complement system, microtubule organizing centers and cell cycle regulation. We have also used graph theoretic approaches to identify the global perturbation on the host cell's protein interaction network, which has revealed a potentially important role for cell death processes including the caspase family of proteins. Further pathway analysis suggested extensive targeting of proteins involved in the PI3K-Akt-mTOR pathway, which is an important regulator of cell survival and proliferation and has been implicated in numerous cancers. We have also compared our HCV interactome to the interactome from a parallel screen with dengue virus proteins, another member of the family Flaviviridae, to identify common interactions and common cellular functions targeted by the two viruses. Using siRNA screens to inhibit the expression of cellular proteins, we demonstrated that 4 of the 10 shared targets tested were required for the replication of both viruses. These shared interactions may reveal common features of the life cycle and evolutionary history of the family Flaviviridae.
Han, HyeJoo	Assortativity of social networks in dreams	Transitivity and assortativity are important parameters of social networks. Suppose links in a network represent friendship. Transitivity refers how likely two people are to be friends if they have another friend in common. Assortativity refers how connectivity of people is correlated with connectivity of their friends. Studies have shown that transitivity and assortativity are

		highly correlated in empirical networks. This study investigated transitivity, assortativity and their relationship in five social networks of characters in dreams. It also tested how well transitivity and assortativity can be predicted from comparable networks randomized by edge rewiring. Only one of the five networks is assortative like real world social networks are; the other four networks are neutral or disassortative like online social networks are. Assortativity is highly correlated with transitivity for the five dream networks. Comparable networks randomized by edge rewiring give good estimates of transitivity and assortativity for most networks, but consistently underestimate them. Consistently lower transitivity of random networks indicates that social networks in dreams are not random. Nonetheless, assortativity of a dream social network can be well predicted from transitivity of the network using linear regression for the two parameters of comparable random networks.
Hu, Bingjie	Protein pharmacophore selection using hydration-site analysis	Virtual screening using pharmacophore models is an efficient method to identify potential lead compounds for target proteins. Pharmacophore models based on protein structures are advantageous because a priori knowledge of active ligands is not required and the models are not biased by the chemical space of previously identified actives. However, in order to capture most potential interactions between all potentially binding ligands and the protein, the size of the pharmacophore model, i.e. number of pharmacophore elements, is typically quite large and therefore reduces the efficiency of pharmacophore based screening. We have developed a new method to select important pharmacophore elements using hydration-site information. The basic premise is that ligand functional groups that replace water molecules in the apo protein contribute strongly to the overall binding affinity of the ligand, due to the additional free energy gained from releasing the water molecule into the bulk solvent. We computed the free energy of water released from the binding site for each hydration site using thermodynamic analysis of molecular dynamics (MD) simulations. Pharmacophores which are co-localized with hydration sites with estimated favorable contributions to the free energy of binding are selected to generate a reduced pharmacophore model. We constructed reduced pharmacophore models for three protein systems and demonstrated good enrichment quality combined with high efficiency. The reduction in pharmacophore model size reduces the required screening time by a factor of 200-500 compared to using all protein pharmacophore elements. We also describe a training process using a small set of known actives to reliably select the optimal set

		of criteria for pharmacophore selection for each protein system.
Huang, Jiajie	Identification and classification of conserved RNA structural motifs using a graph theoretical approach	Originally known as a genetic information carrier, RNA also plays a critical role in multiple cellular processes including transcriptional and translational regulation. Known functional RNA classes include transfer RNA, ribosomal RNA, ribonuclease P RNA, small nucleolar RNA, small nuclear RNA, transfer-messenger RNA, and regulatory elements in untranslated regions of messenger RNA. However, the majority of functional RNA motifs are yet to be identified. Compared to DNA and protein, whose conserved functional motifs can be identified based on underlying sequence similarity, RNA functional motifs lack a reliable signal at the sequence level. However, RNA sequences with similar functions have conserved secondary and higher-order structures. RNA topology, the global organization of local structural elements (stems, loops, pseudoknots, etc), offers an approach for identifying unknown but conserved functional elements. In this study, we have developed a graph theoretical approach that is able to identify a set of topological features in an RNA graph; this set of features defines a unique structural fingerprint of the RNA molecule. By comparison of RNA structural fingerprints, we can identify conserved structural motifs across RNAs. Such conservation may be indicative of as-yet unknown function. Our preliminary results on four known functional RNA classes exhibited successful identification of specific conserved structural motifs in each class. Further classification using this class-specific motif information reached an accuracy of over 90%. The identification of RNA with similar structural features is a step towards structure-based prediction of RNA function.
Kingsley, Laura	The Role of Protein Flexibility in Mechanism Based Inhibition of CYP2C9 by Tienilic Acid	In silico screening is a valuable tool in the drug development process, it reduces the time required for lead identification by trimming compound libraries before they proceed to more costly experimental screening. One of the main reasons compounds fail to reach market is a poor ADMET (absorption, distribution, metabolism, excretion and toxicity) profile which results in the drug either not reaching its target or causing side-effects. The Cytochrome P450 (CYP) enzyme family plays a central role in two of these properties, metabolism and toxicity. CYP enzymes account for over 75% of the metabolic reactions in the human body and due to their prominent role in metabolism, CYP enzymes are also responsible for many drug-drug interactions that result in toxicity. Mechanism based inhibition (MBI) is one type of drug-drug interaction that occurs a compound irreversibly binds to a CYP enzyme rendering it inactive, and delaying further

		metabolism of both the mechanism based inhibitor and other circulating drugs until additional CYP enzymes can be synthesized. In silico identification/prediction of MBIs has remained a challenging task partially due to the complexity of CYP enzymes, here we use CYP2C9 as a model system to investigate how protein flexibility influences MBI by Tienilic Acid (TA). Mutation of residue 365 in CYP 2C9 to either Ala or Gly prevents TA from acting as an MBI toward the enzyme and we propose that this protective effect could be due to increased flexibility within the CYP2C9 active site.
Li, Yan	Assessing Colonoscopy Screening Strategies Using A Partially Observable Markov Chain Model	Colorectal cancer (CRC) is notoriously hard to combat for its high incidence and mortality rates. However, with improved screening technology and intelligent screening strategy, CRC is more likely to be detected and cured at early stage. Among the available tests, colonoscopy is commonly used as it has been shown to be effective in reducing CRC incidence and mortality. We develop a partially observable Markov chain (POMC) model to assess the cost-effectiveness of the current recommended colonoscopy screening guideline. We incorporate detailed precancerous adenoma states in our model and describe state transitions with incomplete adenoma detection and removal. We investigate the effects of varying screening frequency, initial screening age, and screening compliance rate, on the cost-effectiveness of the current guideline. Numerical experiments and sensitivity analyses are performed to evaluate the current guideline and its variations. Given the fact that our model incorporates great detail on precancerous disease progression and colorectal adenoma removal, it is expected to be helpful in policy making for observation-based colonoscopy screening.
Nielsen, Tanner	Applied Hybrid RANS-LES Simulations	Hybrid RANS-LES is a fairly new modeling approach that reduces the computational expense of high Reynolds number, wall-bounded flows. The flow is modeled by RANS (Reynolds Average Navier-Stokes) near the walls, which requires less grid resolution, and then switches to LES away from the walls in order to capture the large-scale unsteady structures of the flow. This utilizes the strengths of each respective model and allows more realistic simulations of high Reynolds number wall-bounded flows. An additional consideration for accurate modeling of high Reynolds number flows is the inlet condition. In order to capture the large-scale unsteady features of a flow using LES, turbulent inlet conditions must be provided. Recycling/rescaling is one technique used to maintain and sustain a turbulent inlet. Simulation results obtained from VULCAN, a NASA research code, will be presented. Results will include: hybrid RANS-LES

		simulations of a non-reacting scramjet combustion chamber (sonic jet injection into a supersonic cross-flow), turbulent inlet generation using the recycling/rescaling technique of a high Reynolds number flat plate simulation, and two-dimensional reacting cavity flow of hydrogen injection into supersonic cross-flow (also a scramjet combustion chamber simulation).
Rahman, Reazur	Finding conserved topology in RNA Structures	RNA molecules play an intricate role in many cellular processes, but unlike protein and DNA, our ability to predict and compare RNA structure is limited. Divergent RNA molecules with similar functions, are likely to have similar structure but might have no detectable resemblance in sequence. So, a sequence homology based approach for prediction and comparison is not very reliable. Moreover, only a fraction of biologically relevant stems are predicted by RNA structure prediction methods based on Minimum Free Energy (MFE) approaches, due to restrictions of the algorithms and inaccuracies in energy parameters. At the cost of some overprediction, the set of MFE predicted stems can be extended to include pseudoknots and suboptimal stems. To identify structurally similar RNAs, we need a tool that can find conserved stem topologies in a set of RNA structures, without relying on the primary sequence. We propose a comparative graph theoretical framework to learn these biologically critical structures. We convert RNA structures to a graph representation (XIOS RNA graph) that includes pseudoknots and mutually exclusive structures, thereby representing ensembles of RNA structures in a single graph. We develop "XIOS Match", a RNA structure matching tool, by using a maximal subgraph isomorphism algorithm, and use it to identify the greatest topological match for a set of RNA structures. We apply our tool to different types of RNA, including ensembles of near MFE structures, and demonstrate that conserved motifs discovered for various RNA species are likely to have functional and structural significance.
Sen, Arpita	Endocytosis and cell division	We have recently reported a novel cellular signaling mechanism by which epsin, a protein involved in cellular uptake and viability, is also involved in regulating cell division. Deregulated epsin function disrupts cell proliferation and leads to abnormalities in cell division, a hallmark of cancer and other developmental diseases. This role of epsin is conserved from yeast to humans. Our research requires the analysis of large amounts of microscope images to identify factors that affect epsin mediated abnormalities, and we have been successful in identifying some of them. Specifically, we have been able to determine the exact regions in epsin that is necessary to interfere with cell division. To analyze these images we used a quantitative approach where we counted

		the number of cells that were unsuccessful in completing cell division as a percentage of the total sample size. We also devised a method to estimate the severity of this cell division defect based on the concept of circularity. Briefly, circularity is a measure of polarized extension and can be defined as follows: Circularity = Area of a cell / Area of a circle of the same perimeter = 4 pi * Area of a cell / Square of Perimeter. Preliminary analysis of images suggests that severity and circularity are inversely proportional to each other. This robust quantitative approach will enable us to obtain much more information from the images than what visual inspection of the data would provide.
So, Joey Chung Yin	Skill Acquisition, Transfer, and Retention on Simulated Heavy Construction Equipment	Objective: We examined whether part-task training produces better learning and retention than whole-task training of a trench-and-load task performed on a hydraulic excavator simulator. Background: For complex perceptual-motor tasks that involve several components and require spatial awareness of the environment, part-task training will be effective if the benefit of being able to focus attention on each component outweighs the costs of integrating the components. We predicted that such would be the case for learning to operate an excavator. Method: A part-task training group practiced separate Carrier-Positioning, Trenching, and Truck-Loading modules, whereas a whole-task training group practiced the Trench-and-Load module, which combines elements from the other modules. The latter module, using different scenarios, was performed by both groups immediately after training and following a 2-week retention interval. Results: 1. Learning curves fit to performance of the whole-task group across the initial training, immediate test, and retention test sessions, using the least-squares method, showed two power function components. 2. Production rate on the trench-and-load task was better overall on the retention test than on the immediate test. 3. The part-task group showed improvement on the retention test compared to the immediate test, whereas the whole-task group did not. 4. Functions for production rate showed that an initial deficit for the part-task group was eliminated by the end of the immediate test, with that group showing higher productivity rates than the whole-task group on the retention test. Conclusion: Part-task training on the excavator simulator results in better skill retention than whole-task training. The benefit of part-task training is likely to be found for other tasks requiring control of implements in various environments. Application: Part-task training can result in better retention of complex perceptual-motor skills involving several components, even when immediate transfer to the whole task does not show better performance than

		whole-task training.
Tehrani, Faraz	Semi-Analytical Solution for Analysis of Pile Groups Using Calculus of Variations	Pile foundations are structural elements commonly used in construction industry that transfer the load from the superstructure to the underneath bearing soil. It is very common to use group of piles in building a foundation system due to the higher capacity of pile groups compared to single pile. Although this type of foundation has been vastly used for many years, there are still challenges to analyze pile groups and the sounding soil, efficiently. Nowadays numerical methods such as finite element method (FEM) are very common tools to analyze these types of problems. However, FEM is highly computationally expensive and demands remarkable computing resources. Through the past decades many researchers have attempted to address this issue by developing analytical semi-analytic methods, nonetheless there is still no method that truly takes both piles and surrounding soil into account similar to what FEM does. The objective of this cutting edge research is to find a novel method to analyze a three dimensional problem of soil-pile group interaction within a continuum medium, in a more efficient way compared to FEM. Calculus of variations coupled with the principle of minimization of total potential energy generates two types of coupled differential equations namely a system of coupled ordinary differential equations and a system of coupled elliptic partial differential equations. The ODE system is solved analytically using eigenvalue method, whereas the coupled PDE system is solved numerically via 2D finite difference scheme. The discretized form of the PDE system will result in a large sparse system of linear equations that need to be solved efficiently. Krylov subspace methods and specifically generalized minimal residual method (GMRES) is used to obtain a solution for the PDE system of equations.
Thompson, Jared	A method for predicting jet noise scattered by a solid planar surface	Formulations exist which allow the prediction of noise from a CFD simulation provided that acoustic data is available on a data surface surrounding the region of generative behavior. Such simulations offer many advantages, but efficiently adding simulated reflections from finite planes (such as those present on the deck of an aircraft carrier) may be challenging. The time domain equivalent source method has been used in connection with a formulation for the pressure gradient to predict scattering off of closed surfaces. A variation of this method, which provides significant advantages for planar surfaces is discussed.
Vanek, Juraj	Interactive hydraulic erosion	Terrain modeling is an important task in digital content creation and physics-based approaches have the potential to simplify it by introducing a higher level of realism. However, most of the

	simulation on the GPU	existing simulations are hindered by a low level of user control, because they fail on large-scale phenomena, or because they are focused only on the modeling of limited effects. We introduce a new interactive, intuitive, and accessible physics-based framework for digital terrain editing. A terrain, composed of layers of materials, is edited with interactive modeling tools built upon different physics-based erosion and deposition algorithms. First, two hydraulic erosion algorithms for running water are coupled. Areas where the motion is slow become more eroded by the dissolution erosion, whereas in the areas with faster motion, the force-based erosion prevails. Second, when the water under-erodes certain areas, slippage takes effect and the river banks fall into the water. The user has a great level of control over the process and receives immediate feedback since the GPU-based erosion simulation runs at least at 20 frames per second on off-the-shelf computers equipped with modern graphics card.
Wilson, Gregory	Moving towards a realistic representation in surface-based pseudoreceptor modelling: an analysis of binding pockets	Surface-based pseudoreceptor methods are expansions of 3D-QSAR techniques placing physico-chemical information onto a 3D surface surrounding a set of aligned compounds that bind into the same binding site of a common protein target. With this mapping pseudoreceptor methods attempt to create models of the target protein binding site around the ligand ensemble. The surface points of the pseudoreceptor model are typically independent descriptors and property mapping onto the surface points is prone to overfitting. In this manuscript, we developed surface descriptors based on 2D Gaussian functions that can model the physico-chemical properties of binding sites of proteins. Binding pocket surfaces of a large set of experimentally determined protein-ligand complex structures are analysed and 2D Gaussian functions are used to fit the surface properties. The fitted property values differ from the original values on average by 15-25%, and on average six Gaussian functions are necessary to model each surface property. These descriptors allow for a realistic representation of the binding site and will limit the number of descriptors used throughout the QSAR optimization phase.
Xu, Mengang	Significant Enhancement of Docking Sensitivity Using Implicit Ligand Sampling	We have developed a novel methodology, named 'Ligand model' concept (Limoc)1 to explore the receptor flexibility during docking simulation. In the ligand-model concept, short molecular-dynamics (MD) simulations are performed with a virtual ligand, represented by a collection of functional groups that binds to the protein and dynamically changes its shape and properties during the simulation. The ligand model essentially represents a large ensemble of different chemical species binding to the same target protein. Limoc yields significant improvements in predicting

		native-like binding poses and quantifying binding affinities compared to static docking and ensemble docking simulations into protein structures generated from an apo MD simulation. We utilized Limoc to generate an ensemble of holo-like protein structures in combination with the relaxed complex scheme (RCS) to perform virtual screening. We developed different schemes2 to reduce the size of the ensemble of protein structures to increase efficiency and enrichment quality. Utilizing experimental knowledge about a small set of actives for a target protein allows the reduction of the ensemble size to a minimum of three protein structures increasing enrichment quality and efficiency simultaneously.
Yeh, Shu-Hao	Excitation and Entanglement Dynamics of Light Harvesting Complex II B850 Ring	The electronic excitation and the entanglement dynamics between the chromophores of photosynthetic harvesting complex II (LHCII) B850 ring have been studied and analyzed theoretically. Since the coupling energy between the adjacent chromophore electronic excitation is comparable to the bath organization energy, the modified scaled hierarchical equation of motion (HEOM) approach is implemented to treat the whole system in an intermediate coupling regime. Comparing our results to the well-studied Fenna-Matthews-Olson (FMO) protein, we found that quantum coherence of electronic excitation between chromophores also exist in this system at the same temperature level (77K), which also suggests that the excitation energy transfer coherently through the B850 ring instead of incoherent hopping. The calculation of bipartite entanglement between chromophore electronic excitation shows the existence of a long-lived entanglement in this system, illustrates that this kind of quantum effect could survive even in such a noisy environment.

CSESC - 2012
Computational Science & Engineering Student Conference

Poster Judges

Professor Nan Kong

Professor Assefaw Gebremedhin

Professor Faisal Saied

Professor Markus Lill

siam @PURDUE

A student chapter of the
Society for Industrial and Applied Mathematics

Volunteers

Aaron Goldner

Adarsh Visi Elango

Cyrus Vandersvala

Darion Grant

Megan Swift

Isaac Tetzloff

Jiajie Huang

Juan Esquivel

Kameswaranau Anupindi

Laura Kingsley

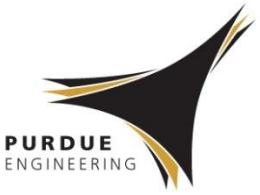
Like Yan

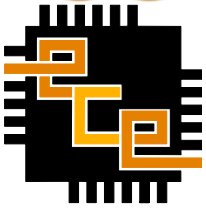
Natasha Bosanac

Takashi Kanno

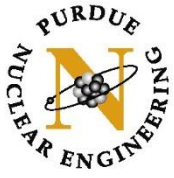
CSESC - 2012
Computational Science & Engineering Student Conference

We kindly thank our sponsors who have made this conference possible:





Center for Science of Information
A National Science Foundation
Science & Technology Center



A student chapter of the
Society for Industrial and Applied Mathematics

CSESC - 2012
Computational Science & Engineering Student Conference

Organizing Committee

CSESC 2012 is being organized by

siam @PURDUE

Jacob Haderlie(President)

Iffat Arisa (Vice President)

James (Jim) Hengenius(Treasurer)

Federico Antico (Secretary)

David Restrepo(Webmaster)

Jyoti Mathur (advisor)