# Computational Science and Engineering Student Conference

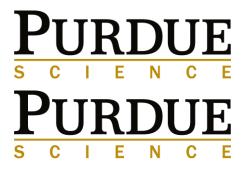


March 2014

Hosted by the Society of Industrial and Applied Mathematics at Purdue University

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MATHEMATICS



COMPUTER SCIENCE

AERONAUTICS AND ASTRONAUTICS



ELECTRICAL AND COMPUTER ENGINEERING





# Location

The location for the conference will be Gerald D. and Edna E. Mann Hall and the Burton D. Morgan Center for Entrepreneurship (Purdue's Discovery Park)







Site

Map

# Schedule

TIME	ROOM	EVENT
8:00 -9:00 AM	MANN Atrium	Breakfast and registration
9:00 - 10:20 AM	MRGN 121	Oral presentations (session #1)
9:00 - 10:20 AM	MRGN 129	Oral presentations (session #2)
10:20 - 10:40 AM	MANN Atrium	Coffee Break
10:40 - 12:00 PM	MRGN 121	Oral presentations (session #3)
10:40 - 12:00 PM	MRGN 129	Oral presentations (session #4)
12:00 - 3:00 PM	MANN Atrium	Lunch
12:00 - 3:00 PM	MANN Atrium	Poster session
3:00 - 4:00 PM	MRGN 121	Plenary speaker
4:00 - 4:30 PM	MRGN 121	Awards ceremony

# **Presentations order**

Oral presentations (Session # 1)			
Name	Title		
Pikee Priya	Modeling Microstructural Evolution during Homogenization of 6xxx and 7xxx series Aluminum Alloys		
Alex Plotkowski	Numerical Simulation of Solidification and Free Floating Grains in DC Casting of Aluminum Alloys		
Sara Rodriguez Gomez	Analysis of the modal coupling at low resonances in the Colombian Andean bandola		
Oral presentations (Session # 2)			
Name	Title		
Christopher Hagmann	Building Perfect Brackets		
Karthik Padmanabhan	Molecular analysis of glyphosate resistance in giant ragweed		
Emery Goosens	Detecting High-Order Interactions Using Single-Layer Neural Networks		

Oral presentations (Session # 3)		
Title		
Erasure coding for fault oblivious linear system solvers		
Efficient spectral Galerkin methods for electronic Schrodinger equation		
A mathematical programming approach to the optimization of switch virtual keyboards		

# **Oral presentations (Session # 4)**

Name	Title
Sayan Biswas	The Proper Orthogonal Decomposition (POD) in Turbulent Combustion
Bomi Kim	Approximate Dynamic Programming and Duality Methods in Credit Default Swap Option Valuation
Wubeshet Woldemariam	Estimating Annual Maintenance Expenditure for Infrastructure: An Artificial Neural Network Approach
Yankai Cao	Clustering-Based Interior-Point Strategies for Convex Stochastic Programs

# **Presentations**

# Numerical Simulation of Solidification and Free Floating Grains in DC Casting of Aluminum Alloys

Alex Plotkowski Materials Engineering, Purdue University aplotkow@purdue.edu

#### Abstract

Numerical methods have become a powerful tool for modeling a wide variety of materials processing applications, including the solidification of metallic alloys. One of the processes at the forefront of modeling efforts in this area is direct chill (DC) casting of aluminum alloys, a semi-continuous process that produces billets for further downstream processing. Since grain refiner is often used in this process, one of the challenges for modeling is accounting for free floating solid particles dispersed within the liquid metal. In particular, current methods for representing the attachment of these particles to the rigid interface lack detail. Strategies for modeling solid motion will be reviewed, and the method implemented at the Purdue Center for Metal Casting Research will be discussed. Focus will be on the current state of modeling particle packing in large scale castings. Current models tend to assume that particle interactions reach a critical point at some volume fraction solid value at which the solid begins to act as a rigid structure. This approach has several disadvantages including neglecting the local fluid flow. A simple velocity based model has been implemented at Purdue. These models will be compared, and avenues for future research will be identified.

# **Approximate Dynamic Programming and Duality Methods in Credit Default Swap Option Valuation**

Bomi Kim Industrial Engineering, Purdue University kim1248@purdue.edu

#### Abstract

We describe an effective approach to evaluate Bermudan Credit Default Swap (CDS) options (i.e., CDS options with multiple discrete exercise opportunities). While a closed form solution is available for European CDS options, one cannot compute Bermudan CDS options analytically. Therefore, simulation is required to price Bermudan CDS options. Here, Approximate Dynamic Programming (ADP) and duality methods are applied to find an estimate of Bermudan CDS option price. We propose approximations for optimal exercise policy to estimate lower and upper bounds for Bermudan CDS option price. While lower bounds of the option price are obtained from the primal ADP problem with the exercise strategy we approximate, upper bounds of the option price are computed using a martingale in the duality methods. The default intensity of the underlying reference company is modeled with the Cox, Ingersoll and Ross (CIR) process.

## **Building Perfect Brackets**

Christopher Hagmann School of Chemical Engineering, Purdue University chagmann@purdue.edu, cdhagmann.github.io

#### Abstract

The NCAA men's basketball tournament highlights data analytics to the everyday person as they look for help building their brackets. A k-Nearest Neighbors algorithm is proposed to compare new opponents to previously played teams. A distance between teams is calculated to determine the most similar teams and to weigh the value of each win or loss to the teams. The value of k is determined from previous years and applied to 2014. Results are compared to other predictions for 2014.

# **Detecting High-Order Interactions Using Single-Layer Neural Networks**

Emery Goossens Statistics, Purdue University emerygoossens@gmail.com

#### Abstract

The explosion of (deep) neural networks research in the past decade has produced powerful and flexible prediction techniques as well as the accompanying algorithmic (e.g. momentum, dropout) and computational infrastructure (GPUs) necessary to make them feasible in commercial applications. Because neural networks become analytically intractable beyond a single-hidden layer, however, it is often difficult to determine which specific inputs, as well as the interactions between these inputs, are useful in decreasing prediction error in such complex models (i.e. feature selection). We propose an exploratory data analysis technique using the square of the smooth rectified linear unit activation function to detect high-order feature interactions in a single-layer neural network using training and test data. This method has three key features that, together, are uncommon to most exploratory data techniques: 1) the ability to approximate interactions of an arbitrary order without specifying them explicitly 2) a means of identifying which features (or interaction of features) are important 3) an existing well-developed optimization framework for massive datasets. An attempt to motivate this interaction approximation procedure through its relation to classical statistical models is also given. Initial results within the context of simulated genetic data have shown some success at detecting two-, three-, and four-way interactions.

# Molecular analysis of glyphosate resistance in giant ragweed

Karthik Padmanabhan Department of Biological Sciences, Purdue University kpadmana@purdue.edu

#### Abstract

Giant ragweed is one of the most competitive annual weeds in corn and soybean production across the eastern Corn Belt in the United States. The use of glyphosate (commercial name: Roundup) and glyphosate-ready crop systems were effective in managing giant ragweed populations for several years. However, in the last decade, glyphosate-resistant giant ragweed have been reported in the eastern combelt and Canada resulting in a huge problem to farmers and requiring use of additional preemergence and postemergence for acceptable control in order to avoid yield loss. The research reported here has the goal of identifying the genes responsible for conferring glyphosate resistance. Both glyphosate-resistant and glyphosate-sensitive biotypes of giant ragweed were studied using a RNA-seq experiment. Total mRNA was extracted from leaf disks of untreated and glyphosate treated leaves over a time-course of 0 to 6 hours after herbicide application and the transcriptome of sensitive and resistant giant ragweed biotypes were compared. We have identified a list of genes that were differentially expressed between the two biotypes as the first step in eventually identifying genes responsible for the glyphosate resistance observed.

# A computer-aided diagnosis system to identify regions of pathologic change in temporal subtraction images of the chest

Katherine Lee Computer Science, Purdue University katherineclee@purdue.edu

#### Abstract

Radiologists often compare sequential radiographs side-by-side in order to identify regions of change and evaluate the clinical significance of such regions. Some changes in pathology, however, may be overlooked or misinterpreted. For this reason, temporal subtraction (TS) images provide an important tool for enhanced visualization. Not all areas of  $\hat{a} \in \hat{c}$  change  $\hat{a} \in \cdot$  demonstrated on a TS image, however, are caused by pathology. The purpose of this study was to develop an automated computer-aided diagnosis (CAD) system to locate regions of change or false regions of change caused by misregistration artifacts. The dataset used in this study contained 120 images, on which an experienced radiologist outlined 74 regions of true pathologic change that were used as the gold standard. Through gray-level thresholding and initial false-positive reduction, an initial set of candidates was extracted and input to a classifier. A five-fold cross-validation method was employed to create training and testing groups. Both false-candidate

regions as well as the gold-standard regions were used as training data. Of the three classifiers tested (support vector machine, logistic regression, and linear discriminant analysis), the logistic regression classifier performed the best with a sensitivity of 96% and specificity of 84%; receiver operating characteristic (ROC) analysis resulted in an area under the ROC curve of 0.94. These results show promise in the performance of the CAD system to detect regions of pathologic changes in TS images of the chest. (This work was done in conjunction with Charles Ho (Rice University) and Samuel G. Armato III PhD. (University of Chicago).

# Modeling Microstructural Evolution during Homogenization of 6xxx and 7xxx series Aluminum Alloys

Pikee Priya Materials Engineering, Purdue University ppriya@purdue.edu

#### Abstract

Homogenization of as-cast ingots is essential before extrusion of aluminum alloys, reducing microsegregation, dissolving low melting temperature phases, spheroidizing precipitates, and facilitating dispersoid precipitation. These changes reduce flow stress, minimize recrystallization, and enhance surface finish during extrusion. A numerical study of homogenization in 6xxx series (Al-Si-Mg-Fe-Mn) and 7xxx series (Al-Zn-Cu-Mg) alloys is done. A Finite Volume-Cellular Automaton model is developed to simulate the phase transformations and the morphological changes occurring during homogenization at the SDAS (µm) length scale. The thermodynamic and kinetic data required by the model are obtained from commercial softwares (Thermo-Calc and DICTRA respectively). A 1D Finite Difference model is also developed to simulate microstructural changes during cooling after homogenization, at the dispersoid (nm) length scale. Dissolution of Mg2Si precipitates, transformation of β-AlFeSI to α-Al(FeMn)Si (6xxx series) and transformation of n (MgZn2) to S-phase (Al2CuMg) (7xxx series) is predicted. The transformations in 6xxx are governed by diffusion and are driven by the difference between the local interface composition and the equilibrium values found as a function of temperature and curvature. The transformations for 7xxx are a lot more sluggish and are interface-controlled. Homogenization is simulated at different temperatures and different compositions to study the phase transformation kinetics and microstructural evolution. The results from the study are compared to experimental observations.

# Analysis of the modal coupling at low resonances in the Colombian Andean bandola

Sara Rodríguez Gómez Civil Engineering, Universidad EAFIT srh89s@gmail.com

#### Abstract

We present the Colombian Andean bandola, a "drop shaped" Colombian stringed instrument, in the context of musical acoustics. Musical acoustics has emerged as a branch that studies the sound produced for musical purposes. In this field, the acoustics of stringed instruments like guitar and violin has been extensively treated. As a result, the modal analysis made at low resonances has provided a model for the instrument behavior along its range of pitch

# The Proper Orthogonal Decomposition (POD) in Turbulent Combustion

Sayan Biswas School of Aeronautics and Astronautics Engineering, Purdue University biswas5@purdue.edu

#### Abstract

Turbulence is a subject of boundless scientific and technological importance, and yet one of the least understood till date. Combustion adds more compliancy to turbulence, be in mathematical modelling or in experiments. A better mathematical model to capture all aspects of turbulent combustion needs well understanding of process itself. An approach to solve such complicated phenomena is to divide it into many simpler or lower dimensional processes. Proper Orthogonal Decomposition (POD), which finds applications in computationally processing large amounts of high-dimensional turbulent combustion data with the aim of obtaining low-dimensional descriptions that capture much of the phenomena of interest. Geometric interpretations of the POD method are presented in two utmost important transient limit phenomena in turbulent combustion-ignition and extinction. One shows low-rank approximations of ignition of H2/air lean mixture by a turbulent hot jet and the other demonstrates different POD modes of flame extinction process in a bluff body stabilized afterburner.

# Estimating Annual Maintenance Expenditure for Infrastructure: An Artificial Neural Network Approach

Wubeshet Woldemariam Civil Engineering, Purdue University wwoldema@purdue.edu

#### Abstract

For purposes of long-term planning and budgeting, infrastructure user cost allocation, and financial need forecasts, infrastructure agencies seek knowledge of the annual expenditure levels for `maintaining their assets. Often, this information is expressed in dollars per unit dimension of the infrastructure and is estimated using observed data from historical records. This paper presents an artificial neural network (ANN) approach for purposes of estimating annual expenditures on infrastructure maintenance, and demonstrates the application of the approach using a case study involving rural interstate highway pavements. The results of this exploratory study demonstrate that not only is it feasible to use ANN to derive reliable predictions of annual maintenance expenditures (AMEX) at aggregate level but also it is possible to identify the influential factors of such expenditures and to quantify the sensitivity of AMEX to such factors.

# A mathematical programming approach to the optimization of switch virtual keyboards

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#### Abstract

In special circumstances people interact with a virtual keyboard by triggering a binary switch to guide a moving cursor to target items. Such switch keyboards are commonly used by locked-in patients with severely restricted motor capabilities. Typing with such systems enable patients to interact with colleagues, but it is horribly slow and error prone. We show how to optimize the design of such systems in a way that minimizes the average entry time while satisfying an acceptable error threshold. Our optimization approach assigns characters to positions on the keyboard, identifies an optimal cursor speed, and considers a variety of cursor paths. We show how to estimate the necessary information for the optimization model and demonstrate that the resulting optimized keyboards are quite different from existing keyboard designs.

### **Clustering-Based Interior-Point Strategies for Convex Stochastic Programs**

Yankai Cao Chemical Engineering, Purdue cao142@purdue.edu

#### Abstract

Clustering-Based Interior-Point Strategies for Convex Stochastic Programs Yankai Cao, Carl Laird, Victor Zavala We present a clustering-based interior-point strategy for two-stage stochastic programs. This problem class arises in stochastic optimal control, robust design, and parameter estimation and has the property that an arrowhead block representation of the KKT system can be obtained. Each block corresponds to a scenario, which is typically obtained by sampling a probability distribution. The key idea is to perform adaptive clustering of scenarios inside the solver based on their influence on the problem. This results in a much smaller compressed KKT system and the compressed KKT system is used as a pre-conditioner for the full space KKT system. We derive spectral and error properties for the preconditioner. We also describe the features of our implementation in C++, demonstrate that scenario compression rates of up to 87% are possible, and that speedups of an order of magnitude are achievable. Finally, we demonstrate that the parallelization can push the performance further.

### Erasure coding for fault oblivious linear system solvers

Yao Zhu Computer Science, Purdue University yaozhu@purdue.edu, https://sites.google.com/site/yaozhusite/

#### Abstract

Dealing with hardware and software faults is an important problem as parallel and distributed systems scale to millions of processing cores and wide area networks. Traditional methods for dealing with faults include checkpoint-restart, active replicas, and deterministic replay. Each of these techniques has associated resource overheads and constraints. In this paper, we propose an alternate approach to dealing with faults, based on input augmentation. This approach, which is an algorithmic analog of erasure coded storage, applies a minimally modified algorithm on the augmented input to produce an augmented output. The execution of such an algorithm proceeds completely oblivious to faults in the system. In the event of one or more faults, the real solution is recovered using a rapid reconstruction method from the augmented output. We demonstrate this approach on the problem of solving sparse linear systems using a conjugate gradient solver. We present input augmentation and output recovery techniques. Through detailed experiments, we show that our approach can be made oblivious to a large number of faults with low computational overhead. Specifically, we demonstrate cases where a single fault can be corrected with less than 10% overhead in time, and even in extreme cases (fault rates of 20%), our approach is able to compute a solution with reasonable overhead. These results represent a significant improvement over the state of the art.

# Efficient spectral Galerkin methods for electronic Schrodinger equation

Yingwei Wang Mathematices, Purdue University wywshtj@gmail.com, http://www.math.purdue.edu/~wang838/

#### Abstract

Two efficient spectral Galerkin methods, based on Legendre and Laguerre polynomials respectively, are derived for direct discretization of the electronic Schrodinger equation in one spatial dimension. In order to treat the singularity in nucleus-electron Coulomb potential and the high-dimensionality of multi-electron wave function, two sets of underlying basis functions consisting of orthogonal polynomials in subdomains and joint functions in the global domain are used with sparse grid spectral methods based on hyperbolic cross approximations. With the help of Slater determinant, the basis functions are constructed to obey the antisymmetry relations of the fermionic wavefunctions. Numerical tests show the efficiency and accuracy of the proposed methods.

# **Poster session**

# Nexperiment: Model-based Design of Experiments Platform for Reducing Dynamical Uncertainty

Aditya Sai Biomedical Engineering, Purdue University asai@purdue.edu

#### Abstract

Nexperiment, is a novel graphical user interface (GUI) aimed at providing users a platform to apply experiment design methodologies to determine optimal designs that reduce dynamical uncertainty of model dynamics. In addition to an optimized input experiment design, Nexperiment offers sequential and parallel experiment design options, conventional Fisher Information Matrix (FIM) based experiment design, global & amp; local sensitivity analyses, data consistent dynamics identification and model simulation. It does so by providing an easy-to-use, plug-and-play interface that extracts and records essential details about the model supplied by the user. The results presented by the GUI are concise and easily implementable by experimentalists. Nexperiment provides a vital resource to those in the systems biology community by allowing them to analyze their own models for informative measurements that will support model development and refinement.

### Trelliscope: Looking at large data with trellis displays

Barret Schloerke Statistics, Purdue University bschloe@purdue.edu, http://tessera.io/docs-trelliscope/

#### Abstract

Trelliscope provides a way to flexibly visualize large, complex data in great detail from within the R statistical programming environment. Trelliscope is a component in the Tessera environment. For those familiar with Trellis Display, faceting in ggplot, or the notion of small multiples, Trelliscope provides a scalable way to break a set of data into pieces, apply a plot method to each piece, and then arrange those plots in a grid and interactively sort, filter, and query panels of the display based on metrics of interest. With Trelliscope, we are able to create multipanel displays on data with a very large number of subsets and view them in an interactive and meaningful way.

## **Meaning-Based Machine Learning**

Courtney Falk Computer and Information Technology, Purdue University falkc@purdue.edu

#### Abstract

Meaning-based machine learning is a research program to establish the efficacy of training machine learning tools on meaningful input data in order to achieve meaningful results as output. The approach outlined here builds on the theory of Ontological Semantics Technology (OST) as its basis for meaningful data. Potential features are described and discussed. And future directions such as experimental designs are laid out.

# Woodification: User-Controlled Cambial Growth Modeling

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#### Abstract

We present a botanical simulation of secondary (cambial) tree growth coupled to a physical cracking simulation of its bark. Whereas level set growth would use a fixed resolution voxel grid, our system extends the deformable simplicial complex (DSC), supporting new biological growth functions robustly on any surface polygonal mesh with adaptive subdivision, collision detection and topological control. We extend the DSC with temporally coherent texturing, and surface cracking with a user-controllable biological model coupled to the stresses introduced by the cambial growth model.

### **Proceduralization of Buildings at City Scale**

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#### Abstract

We present a framework for the conversion of existing 3D unstructured urban models into a compact procedural representation that enables model synthesis, querying, and simplification of large urban areas. During the de-instancing phase, a dissimilarity-based clustering is performed to obtain a set of building components and component types. During the proceduralization phase, the components are arranged into a context-free grammar, which can be directly edited or interactively manipulated. We applied our approach to convert several large city models, with up to 19,000 building components spanning over 180 km<sup>2</sup>, into procedural models of a few thousand terminals, non-terminals, and 50-100 rules.

# Simulation Analysis, Monitoring, and Control of Operations

Joseph Louis Civil Engineering, Purdue University jlouis@purdue.edu

#### Abstract

Although the automation of construction tasks has been an active research topic since the 1970s, few robots are found on the worksite today and the fundamental construction process has remained unchanged since pre-industrial times. However, the planning and design stages of construction have benefited greatly from advances made in simulation and modeling technologies. In this research, a mechanism for leveraging information-rich simulation models to automate construction operations is developed that uses Discrete Event Simulation (DES) models of operations to drive the process in the real world using autonomous robots. The following specific research questions will be addressed to enable operation automation: (1) What modifications are required to enable DES models, traditionally used only to analyze operations, to serve as control mechanisms to orchestrate autonomous equipment thereby enabling operation automation? (2) How can the DES models, modified for control, be verified and validated before their use in the real world? (3) How can the modified DES models be used to automate any construction operation, regardless of scale and complexity? The state of the art in construction simulation, visualization, and automation serves as the foundation to answer the questions that pave the path towards the overarching goal of monitoring and controlling construction automation. The proposed methodology, while presented in the construction context, has important implications for the automation of any industry characterized by a less-structured and high-uncertainty environment, wherein tasks are subject to complex interaction between disparate resources, such as agriculture. Apart from the benefits of automation described above, the proposed research has immediate applicability for the monitoring and control of conventional construction sites, i.e. without the presence of robots. A demonstration of the framework's feasibility was performed using model robots of construction equipment and robot simulators. A discussion of the results and ongoing research work are presented in the poster.

## Identifying pathogens from fish tissues using next-generation sequencing

Kensey Thurner Forestry and Natural Resources, Purdue University kthurner@purdue.edu

#### Abstract

Invasive, aquatic species pose threats to the balance of local ecosystems by competing with native species and interfering with native habitats. Their population sizes, however, may be partly controlled by native and exotic pathogens. Traditional methods for pathogen screening (e.g. polymerase chain reaction) are cumbersome due to the large number of fish pathogens that need to be screened. We used next-generation sequencing to identify pathogen DNA present in invasive silver carp (Hypophthalmichthys molitrix) and bighead carp (H. nobilis), thereby allowing us to screen these fishes for all pathogens (dependent on availability in the NCBI database) using computational methods.

# Numerical Analysis of the Ultra-Purification of Gallium for Use in AlGaAs/GaAs Heterostructures

Kyungjean Min Materials Science and Engineering, Purdue University kjmin@purdue.edu

#### Abstract

The mobility of two-dimensional electron gas in AlGaAs/GaAs heterostructures can be increased by purification of gallium. The total impurity concentration of gallium should be reduced below 1 ppb to achieve a mobility greater than 200 million cm2/Vs. Currently, gallium is being purified by zone refining in the School of Materials Engineering at Purdue University. Zone refining is a purification technique that utilizes the solubility differences of impurities in the liquid and solid phases. The extent of purification is governed by distribution coefficient (k) which relates the amount of solute (the impurity) ejected into to the liquid at the solidification front. The process is accomplished by traversing a narrow liquid zone along the length of the Ga ingot which results (when k<1) in a continued increase of solute in the liquid and a corresponding purification of the solid. The degree of purification is a function of the distribution coefficients of the elements, the number of zone passes along the ingot, and the processing conditions such as the size and shape of the liquid zone. The distribution coefficients are often unknown and are estimated from chemical thermodynamic calculations. Furthermore, there are no analytical solutions to describe the composition of the purified ingot for multiple zone passes. The problem is further complicated by the different and varying partitioning behavior of the multiple impurity elements. In this work, processing conditions to achieve the ultra-purification of Ga with a starting purity of 99.99999% (7N) are found. Using Spimâ€<sup>™</sup>s model, a finite difference algorithm, concentrations of Ge, Fe and Zn in gallium are numerically analyzed for both single pass and multi pass zone refining. From the simulations, the size and shape of the liquid zone and the optimized number of passes are found to attain a 1 ppb total impurity concentration.

# Assessment of Protein Side-Chain Conformation Prediction Methods in Different Residue Environments

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#### Abstract

Three-dimensional protein structures provide crucial information for understanding the atomic details of the vital biological tasks proteins perform, including catalysis and signaling. However, less than 0.1% of protein sequences have an experimentally solved structure. Furthermore, membrane proteins and large protein complexes are biologically important but challenging for experimental protein structure determination methods. Computational protein structure prediction is a growing alternative. Accurate prediction of protein side-chains is crucial for practical applications of protein structure models that need atomic- detailed resolution such as protein and ligand design. Of the existing software programs, few were trained or tested with protein complexes or membrane proteins. Testing side-chain prediction accuracy on these broadly relevant classes of proteins is necessary to validate the use of current methods.

### **Gradient Flow of Chevron Structures in Liquid Crystal Cells**

Lidia Mrad Department of Mathematics, Purdue University lmrad@purdue.edu

#### Abstract

In a thin cell, a chiral smectic liquid crystal (SmC\*) phase develops when molecules form layers perpendicular to the cell substrates. This perfect bookshelf structure, however, only rarely occurs. In practice, the layers tend to fold in the middle of the cell forming a chevron structure. Moreover, the SmC\* helical structure is suppressed in the thin cell which allows for two stable states. We study the molecular reorientation dynamics between these stable states in the chevron structure under the influence of an applied electric field. Our model is based on the Chen-Lubensky energy involving the molecular director and a general complex-valued layer order parameter. We use a discretized-in-time gradient flow method that requires an iterative minimization procedure to establish the existence of a solution to this time-dependent problem.

# k-Means Clustering for Data Collections on a GPU

Marek Fiser CGT, Purdue mfiser@purdue.edu, hpcg.purdue.edu

#### Abstract

We consider accelerating the simultaneous clustering of thousands of data samples using two variants of the k-means algorithm on a GPU. We use CUDA streams to perform the computations concurrently and asynchronously so that data transfer and computation can be overlapped on different streams. We employ parallelism within a block of threads on the GPU to cluster each sample in parallel, thus avoiding costly synchronization between the CPU and GPU at each iteration of the k-means clustering algorithm. The implementations were evaluated on Flow Cytometry data from Acute Myeloid Leukemia samples, where the clustering is a first step in identifying immunophenotypes to register cell populations across samples and to classify the samples. We compute 55,000 clusterings of 3,000 samples in 3.5 minutes on an NVIDIA Tesla K40 processor, whereas a serial implementation takes more than 12 hours (speedup of 200).

# Study of Transport in electronic devices with stochastic Monte Carlo method: Modeling and simulation along with submicron gate (Lg=0.1um)

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#### Abstract

In this paper we have developed a numerical simulation model to describe the electrical properties of GaInP MESFET with submicron gate (Lg =  $0.5 \text{ Å}\mu\text{m}$ ). This model takes into account the three-dimensional (3D) distribution of the load in the short channel and the law effect of mobility as a function of electric field. Simulation software based on a stochastic method such as Monte Carlo has been established. The results are discussed and compared with those of the experiment. The result suggests experimentally that, in a very small gate length in our devices (smaller than 40 nm), short-channel tunneling explains the degradation of transistor performance, which was previously enhanced by velocity overshoot.

Keywords: Monte Carlo simulation, transient electron transport, MESFET device.

## Band gaps in a phase changing cellular material

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#### Abstract

In some materials, phase transformations occur by a process that resembles multistable mechanisms switching between stable configurations. This kind of transformations can also provide the mechanisms through which some biological materials obtain remarkable properties such as combinations of strength and toughness, superelasticity and shock energy dissipation, among others. We extend the notion of phase transformations to periodic cellular materials by introducing unit cells that have multiple stable configurations. Then, we present a cellular material that exhibits phase transformation and is characterized by a long serrated loading and unloading plateaus. Furthermore, the periodicity in a cellular material provides another phenomenon to study: the presence of band gaps and wave filtering. We study the dynamic behavior and wave propagation characteristics of this material. Harmonic and Bloch-periodicity analyses are performed using the finite element method and the frequency response for different cell arrangements and the dispersion relations are obtained, respectively. We are interested in potential application of this material in energy attenuation devices.

### **Shock Capturing Schemes**

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#### Abstract

The ENO scheme is a high order accurate finite difference scheme which works for piecewise smooth solutions containing discontinuities. The locally smoothest stencil is chosen, based on an adaptive procedure for each grid point, hence avoiding interpolation across discontinuities. The WENO scheme, on the other hand, considers all the local stencils, but weighs them according to their smoothness. In this case, the stencil containing the discontinuity is weighted with zero to avoid interpolation across discontinuities. There are a few choices for the WENO scheme as well. However, these schemes are found to be over-dissipative in regions away from the shock. Therefore, a Hybrid Scheme is used which has a basal compact space discretization scheme, and uses a shock detector to transition smoothly between the dissipative WENO and the non-dissipative high order compact scheme.

# **Multiple Response Factor Screening Testing Procedure**

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#### Abstract

This paper considers the factor screening problem with multiple responses for simulation experiments. The objective is to identify important factors with controlled Family-Wise Error Rate. We assume a multiple- response first-order linear model, the responses follow a multivariate normal distribution, and estimated effect coefficients also follow multivariate normal distribution. Two likelihood ratio based procedures, Sum Intersection Procedure (SUMIP) and Sort Intersection Procedure (SORTIP), are proposed and verified. Numerical studies are provided to demonstrate the validity and efficiency of our proposed procedures.

# **CFD-I** Modeling of UV Disinfection Reactors with Statistic Evaluation of System Variables

Yousra Ahmed Civil/Environmental Engineering, Purdue University yahmed@purdue.edu

#### Abstract

Ultraviolet (UV) irradiation is an effective disinfection method used in water treatment to inactivate waterborne microbial pathogens and/or indicator organisms. UV disinfection does not involve chemicals, producing few by-products compared to chemical methods. The current work aims to apply combinations of computational fluid dynamics and irradiance field models (aka, CFD-I models) to determine the performance of UV disinfection systems in wastewater treatment plants. The input parameters of the systems are measured using standardized experimental methods and on-site measuring devices Variability and uncertainty in the input parameters will be included via applying stochastic methods and uncertainty analysis techniques to obtain more efficient and more reliable UV system design than current design approaches. The simulations are carried out on a waste water UV disinfection reactor. The reactor consists of 7 channels with 384 LOW PRESSURE UV lamps in each channel. In the present work Ansys Fluent software is used for the CFD modelling to obtain the flow field of the water and the motion of particles in the UV reactor. Most of the UV reactors are characterized by high Reynolds number and turbulent flow, hence turbulence flow modeling is necessary. CFD simulation is employed also to determine the particle tracks using the particle tracking capabilities of Fluent. Another essential attribute of the UV reactors is the fluence rate (intensity field). Fluence rate distributions are determined using Photopia software, which is based on the ray tracing technique. The hypothesis of this work is that CFD-I models (which are deterministic, by nature) can be applied to simulate process performance, including variability, by allowing

appropriate variations in input variables. If this hypothesis is demonstrated to be correct, it may allow for UV system designs to be implemented that are more efficient and more reliable than current design approaches.