**COLLOQUIUM Fall 2018**

**Francisco Ortegn Gallego**

**Director and Professor of Mathematics**

**Department of Mathematics**

**Universidad de Cdiz, Spain**

# Steel Heat Treating: Mathematical Modelling and Numerical Simulation of an Industrial Problem

**Thursday, September 6, UTC SIM Center Auditorium, 4:00–4:50 pm.**

**Abstract**. Steel is an iron and carbon alloy. Steel used for industrial purposes has a carbon content of up to about 2% in weight. Other alloying elements may be present, such as Cr and V in tool steels, or Si, Mn, Ni and Cr in stainless steels. Most of structural components in mechanical engineering are made of steel. Some of these components, such as wheels teeth, bevel gears, pinions, etc., are committed to transmit certain types of movement (rotational or longitudinal). As a result, the contact surfaces of these workpieces are particularly stressed. The goal of steel heat treating is to obtain a satisfactory hardness. Before any heat treatment, steel is a soft and ductile material. Without any heating treatment, and because of surface stresses, the teeth of the gear will soon get damaged and they will not engage properly.

In this talk, we will be interested in the mathematical description and numerical simulation of the hardening procedure of a car steering rack. This particular situation is one of the main concerns in the automotive industry. In this case, the goal is to increase the hardness of the steel along the toothed line and keeping at the same time the rest of the piece soft and ductile to reduce fatigue. In addition, we will describe a mathematical model for the heating-cooling step of a steel workpiece leading to the desired hardness. The resulting model consists of a strongly coupled nonlinear system of PDEs/ODEs. A simplified version of this model is used for the numerical simulation of the hardening industrial process of a car steering rack.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Fall 2018**

**Manuel Muoz Mrquez**

**Professor of Mathematics**

**Department of Mathematics**

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**Benchmarking with DEA. Introduction to Data Envelopment Analysis**

**Wednesday, September 12, UTC SIM Center Auditorium, 3:00–3:50 pm.**

**Abstract**. Data Envelopment Analysis, in the following DEA, is a methodology introduced by Charnes, Cooper and Rodes in 1978 to compare the efficiencies of a set of homogeneous units that produce several outputs from the same set of inputs. This methodology has become very popular in many different topics and it has been combined with many optimization techniques. For each Decision Making Unit, DMU, not only does the DEA analysis provide an efficiency score, but it also provides a peer set. The peer set can be used to guide the managers making decisions leading the DMUs to an optimal performance.

The DEA methodology is a non parametric method that estimates the frontier of technology given by the efficiency units. For each DMU, DEA considers two sets of weights, one set for inputs and one set for outputs, setting up what are called virtual input and virtual output, and it measures the efficiency through the ratio between virtual output and virtual input for each unit. The weights are selected in the most favourable way to the unit that has been evaluated.

The first part of the talk is devoted to introduce the DEA methodology, showing how it can be used to benchmark the DMUs.

Usually, the selection of the variables to be included in the analysis are made by the managers, so one can assume a correct selection. But a bad selection of the variables to include in the model could bias the results. So, the task of selecting the set of variables becomes an important task. To this topic and how one can handle that problem, is devoted the second part.

In the next section, a case study with a classical set of data is showed.

The talks ends with a section devoted to conclusions and future research.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Fall 2018**

**Joaquim Jdice**

**Instituto de Telecomunicaes**

**Portugal**

**Linear Complementarity Problems:**

**Applications, Formulations and Algorithms**

**Wednesday, September 26, EMCS Rm. ?, 3:30–4:30 pm.**

**Abstract**. The Linear Complementarity Problem (LCP) consists of finding two nonnegative vectors satisfying linear constraints and complementarity conditions between pairs of components of the same order. The LCP has found many applications in several areas of science, engineering, finance and economics. In this talk the LCP and some important extensions of this problem are first introduced together with some of their most relevant properties and applications.

A number of formulations of optimization problems are shown to be formulated as an LCP or one of its extensions. These include Linear and Quadratic Programming, Affine Variational Inequalities, Bilevel Programming, Bilinear Programming, 0-1 Integer Programming, Fixed-Charge Problems, Absolute Value Programming, Copositive Programming, Fractional Quadratic Programming, Linear and Total Least-Squares Problems, Eigenvalue Complementarity Problems, Matrix Condition Number Estimation, Clique and Independent Numbers of a Graph and Mathematical Programming with Cardinality Constraints. The most relevant algorithms for solving LCP and its extensions are briefly reviewed. The benefits and drawbacks of solving these optimization problems by using complementarity algorithms applied to their formulations are discussed. Finally, some topics for future research are presented at the end of this talk.

This talk may be appropriate for all students with a strong interest in research.

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**COLLOQUIUM Fall 2018**

**Eleni Panagiotou**

**Department of Mathematics**

**University of Tennessee at Chattanooga**

## A Study of Entanglement in Physical Systems and its Relation to material properties and function

**Friday, September 28, UTC SIM Center Auditorium, 3:00–3:50 pm.**

**Abstract**. Many physical systems, such as biopolymers and polymer melts, are composed by macromolecules which cannot cross each other and attain entangled conformations. The entanglement complexity in these systems affects dramatically their mechanical properties. In this talk we will see methods by which one can measure entanglement in collections of open or closed curves in 3-space and in systems employing Periodic Boundary Conditions (PBC). We show how our results can be used in practice by performing fully three-dimensional computational simulations of polymeric chains entangled in weaves of a few distinct topologies and with varying levels of chain densities. Our topological measures of entanglement indicate the global topology is the dominant factor in characterizing mechanical properties. We also discuss the role of entanglement in proteins and how it correlates with protein folding kinetics. Our aim is to introduce a new model of protein folding kinetics that supports the prediction of a proteins folding rate from the topological and geometrical structure of its native state. Finally, we discuss how polymer architecture can affect material properties. Using Field Theoretic Simulations we show how varying the number of arms in bottlebrush polymers leads to instantaneous nematic phase transition.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Fall 2018**

**Glenn F. Webb**

**Department of Mathematics**

**Vanderbilt University**

# Spatial Spread of Epidemic Diseases in Geographical Settings: Seasonal Influenza Epidemics in Puerto Rico

**Friday, September 21, EMCS Rm. 422, :00–:50 pm.**

**Abstract**. A deterministic model is developed for the spatial spread of an epidemic disease in a geographical setting. The model is focused on outbreaks that arise from a small number of infected individuals in subregions of the geographical setting. The goal is to understand how spatial heterogeneity influences the transmission dynamics of susceptible and infected populations. The model consists of a system of partial differential equations with a diffusion term describing the spatial spread of an underlying microbial infectious agent. The model is applied to simulate the spatial spread of the 2016-2017 seasonal influenza epidemic in Puerto Rico. In this simulation, the reported case data from the Puerto Rican Department of Health are used to implement a numerical finite element scheme for the model. The model simulation explains the geographical evolution of this epidemic in Puerto Rico, consistent with the reported case data.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Fall 2018**

**Ken Millett**

**Department of Mathematics**

**University of California, Santa Barbara**

**Knotting and Entanglement in Macromolecules**

**Monday, October 22, EMCS Rm. , :00–:50 pm.**

**Abstract**. The fundamental character and consequences of knotting and entanglement in macromolecular chains, i.e. as measured by the nature of the knot type or the level of linking between one sub chain and another, disjoint, sub chain, will be described. We will see how we can recognize and quantify such structure using a new visual metric, the fingerprint, that has been created for these specific purposes by consider some concrete instances of such structures.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Fall 2018**

**Lakmali Weerasena** *

**Department of Mathematics**

**University of Tennessee at Chattanooga**

## A Piece-wise Constant Approximation Approach to Fin Optimization

**Friday, November 2, EMCS 3:00–3:50 pm.**

**Abstract**. We find the optimal form of a fin attached to a heated surface face in steady-state. A fin is a thin component attached to a larger body or structure. Fins are used to increase surface areas for heat transfer purposes. The fin performance is measured using efficiency and effectiveness. In this study, we design a fin which maximizes efficiency subject to a fixed volume. In order to evaluate the performance of the designed fin, we consider other (known) fins of the same volume. Our approach is based on a piece-wise constant approximation of the design. We develop an algorithm and conduct several numerical experiments for diverse physical parameters of a fin. Our optimization problem is similar but not identical to the problem studied by L. Hanin. We discuss the applicability of Schmidt's hypothesis for our model. The numerical results confirm that the proposed piece-wise constant approximation finds fins with good efficiency. We also study the trade-off between two performances (efficiency and effectiveness) of a fin.

* **with Boris P. Belinskiy, Department of Mathematics and James W. Hiestand, Department of Mechanical Engineering, University of Tennessee at Chattanooga**

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Spring 2019**

**Department of Mathematics and SimCenter**

**Min Wang**
**Kennesaw State University**
**Georgia**

## Optimal Control to a Facultative Mutualism System with Harvesting

**Friday, January 25, EMCS 422, 2:00–2:50 pm.**

**Abstract**. Mutualism (or interspecific cooperation) is the way two organisms of different species exist in a relationship in which each individual fitness benefits from the activity of the other. An organism is classified as facultative when it benefits from the interaction yet can survive on its own. The mutualistic interactions strongly influence the structure and dynamics of ecological systems and have become an important focus of research. In this talk, a general facultative mutualism model with harvesting is proposed. Instead of the long-term dynamical model behavior, a short-term optimal feedback control problem subject to the proposed model is investigated. The existence and the necessary conditions of the optimal control are proved. Numerical simulations are carried out to demonstrate the applications as well. The proposed model covers many existing facultative mutualism models as special cases. The results on the associated optimal control problem provide a generic solution to develop optimal harvesting strategies for the models in the literature. KeywordsFacultative, harvesting, mutualism, optimal control.

This talk may be appropriate for all students with a strong interest in research.

## COLLOQUIUM Spring 2019

## Department of Mathematics and SimCenter


## John Gounley
## Oak Ridge National Laboratory


## Scalable Simulations of Blood Flow

## Friday, February 1, SimCenter Auditorium (Rm. 105), 2:30–3:20 pm.


**Abstract**. Computational simulations of blood flow offer the means to study a wide range of phenomena, from cardiovascular disease to the metastatic progression of cancer. However, performing large-scale and high-resolution simulations of blood flow requires a scalable computational framework to run efficiently on high-performance computing resources. In this talk, we discuss the development of such a framework using HARVEY, a parallel hemodynamics solver. We focus on the implementation of two numerical schemes, the lattice Boltzmann and immersed boundary methods, for a distributed memory environment and assess their scalability. This work is in collaboration with Amanda Randles (Duke) and Erik Draeger (LLNL).


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**COLLOQUIUM Spring 2019**

**Department of Mathematics and SimCenter**

**K.B. Kulasekera**
**Department of Bioinformatics and Biostatistics**

**University of Louisville, Louisville, Kentucky**

# Selection of the Optimal Personalized Treatment from Multiple Treatments with Multivariate Outcome Measures

**Friday, March 1, SimCenter Auditorium (Rm. 105), 2:15–3:05 pm.**

**Abstract**. In this work we propose a novel method for individualized treatment selection when the treatment response is multivariate. For the K treatment ( $K > 2$ ) scenario we compare quantities that are suitable indexes based on outcome variables for each treatment conditional on patient specific scores constructed from collected covariate measurements. Our method covers any number of treatments and outcome variables, and it can be applied for a broad set of models. The proposed method uses a rank aggregation technique to estimate an ordering of treatments based on ranked lists of treatment performance measures such as smooth conditional means and conditional probability of a response for one treatment dominating others. The method has the flexibility to incorporate patient and clinician preferences to the optimal treatment decision on an individual case basis. A simulation study demonstrates the performance of the proposed method in finite samples. We also present data analyses using HIV and Diabetes clinical trials data to show the applicability of the proposed procedure for real data.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Spring 2019**

**Department of Mathematics and SimCenter**

**Mahboub Baccouch**
**Department of Bioinformatics and Biostatistics**

**University of Nebraska at Omaha**

**Omaha, NE 68182, USA**

# Discontinuous Galerkin methods for solving differential equations: Superconvergence, error estimation, and adaptivity

**Friday, February 22, SimCenter Auditorium (Rm. 105), 2:15–3:05 pm.**

**Abstract**. Discontinuous Galerkin (DG) finite element methods are becoming important techniques for the computational solution of many real-world problems describe by differential equations. They combine many attractive features of the finite element and the finite volume methods. These methods have been successfully applied to many important PDEs arising from a wide range of applications. DG methods are highly accurate numerical methods and have considerable advantages over the classical numerical methods available in the literature. The main advantages include: they (i) handle problems having discontinuities such as those arising in hyperbolic problems ( *e.g.* shocks), (ii) handle problems having sharp transition layers such as those arising in convection-diffusion problems, (iii) handle problems with complex geometries, (iv) suitable for long time simulation ( *e.g.*, they maintain the phase and shape of the waves accurately), (v) produce efficient parallel solution procedures, (vi) exhibit optimal convergence rate, and (vii) achieve very nice superconvergence results, which can be used to design asymptotically exact a posteriori estimates of discretization errors. Error estimators are essential to steer adaptive schemes where either the mesh is locally refined ( $h$ -refinement) or the polynomial degree is raised ( $p$ -refinement). Furthermore, DG methods can easily handle meshes with hanging nodes, elements of various types and shapes, and local spaces of different orders. Finally, DG methods provide accurate and efficient simulation of physical and engineering problems, especially in settings where the solutions exhibit poor regularity. For these reasons, they have attracted the attention of many researchers working in diverse areas, from computational fluid dynamics, solid mechanics and optimal control, to finance, biology and geology.

In this talk, we give an overview of the main features of DG methods and their extensions such as the local DG (LDG) methods, which are natural extension of the DG methods aimed at solving higher-order equations. We first introduce the DG method for solving nonlinear ODEs and present several properties that render them so attractive such as convergence, superconvergence phenomena, a posteriori error estimation, and mesh adaptivity. Then, we extend the methods to other PDEs such as convection, convection-diffusion, wave, KdV, Euler-Bernoulli equations. Furthermore, we present a stochastic analogue of the DG and LDG methods for stochastic equations. Some open problems and future research directions will be mentioned.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Spring 2019**

**Department of Mathematics**

**Jonathan Troup**
**Department of Mathematics**

**University of Oklahoma**

# Students Development of Geometric Reasoning about the Derivative of Complex-Valued Functions

**Tuesday, February 26, EMCS 218, 3:00–3:50 pm.**

**Abstract**. In this paper, I share results of a case study describing the development of two undergraduate students geometric reasoning about the derivative of a complex-valued function with the aid of Geometers Sketchpad (GSP). My participants initially had difficulty reasoning about the derivative as a rotation and dilation. Without the aid of GSP, they could describe the rotation and dilation aspect of the derivative for linear complex-valued functions, but were unable to generalize this to non-linear complex-valued functions. Participants use of GSP, speech, and gesture assisted with discovering function behavior, generalizing how the derivative describes the rotation and dilation of an image with respect to its pre-image for non-linear complex-valued functions, and recognizing that the derivative is a local property. Key words: Amplitwist, Complex-valued function, Derivative, Dynamic Geometric Environments (DGEs), Gesture

This talk may be appropriate for all students with a strong interest in Math Education.

**COLLOQUIUM Spring 2019**

**Department of Mathematics and SimCenter**

**Ying Chen**
**Department of Mathematics**

**Purdue University**

**West Lafayette, IN**

# Efficient Numerical Methods for Multiphase Tumor Growth with Distinct Membrane Energies

**Monday, March 4, SimCenter Auditorium (Rm. 105), 3:00–3:50 pm.**

**Abstract**. This talk touches upon state-of-the-art methods for solving nonlinear partial differential equations. The underlying approach is to develop efficient energy stable schemes for phase field models. I will first give brief examples on (i) tumor growth with membrane surface energy, (ii) incompressible Cahn-Hilliard Navier-Stokes fluid systems, and (iii) materials science models incorporating strong anisotropy and Willmore regularization. Then I will focus on modeling tumor growth in complex dynamic microenvironment with membrane bending energy. The techniques have been applied to study breast cancer growth, invasion and microlocalization. These will be illustrated with simulation results. Finally, I will conclude with some future directions.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Spring 2019**

**Department of Mathematics**

**Yuan Liu**
**Department of Mathematics**

**Mississippi State University**

# High Order Structure-Preserving Numerical Methods for Convection-Diffusion-Reaction Equations

**Monday, March 22, EMCS 422, 3:00–3:50 pm.**

**Abstract**. Convection-diffusion-reaction(CDR) equation is one of the widely used mathematical models in science and engineering. It describes how one or more substances distributed under the influences of convection, diffusion and reaction processes. In this talk, we will present some recent work on high order numerical methods for solving CDR equation under two cases. (1) When there are only convection terms, the CDR equation is hyperbolic conservation laws. We will talk about the development of high order bound-preserving numerical methods. (2) When there are only diffusion and reaction terms, Krylov implicit integration factor discontinuous Galerkin methods on sparse grids are proposed to solve the equation in high dimensional cases.

This talk may be appropriate for all students with a strong interest in Mathematical research.

**COLLOQUIUM Spring 2019**

**Department of Mathematics**

**Yanyan He**
**Department of Mathematics**

**New Mexico Tech**

# Non-probabilistic Numerical Approaches for Uncertainty Quantification

**Friday, March 29, EMCS 422, 3:00–3:50 pm.**

**Abstract**. Uncertainty is inevitable in computer-based simulations. To have a better representation of the physical system or the quantity of interest, understanding and quantifying the uncertainty in simulations are critical. In this talk, we will focus on the numerical approaches of uncertainty quantification (UQ) and briefly mention the applications of UQ in various disciplines. Specifically, we will talk about two of the main aspects of uncertainty quantification: model form UQ and parametric UQ. For model form UQ, observational data is available and physical constraints are incorporated into model correction process to enforce the important physical properties of the underlying system. The estimation of both model output and model parameters can be improved. For parametric UQ, we discuss the use of both probabilistic and non-probabilistic approaches in UQ and propose an efficient numerical strategy based on fuzzy set theory to quantify the uncertainty in model output propagated through physical systems.

This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Spring 2019**

**Department of Mathematics**

**Olgur Celikbas**

**West Virginia University**

**On the torsion of tensor products of modules**

**Monday, April 01, EMCS 422, 3:30–4:30 pm.**

**Abstract**. Tensor products are important objects used in many areas such as mathematics, physics and engineering. For example, the tensor analysis of Ricci and Levi-Civita was crucial in Einstein's work on general relativity. The term "tensor" comes from the Latin tendere, which means "to stretch", and the widespread adoption of it in physics and mathematics is mostly due to Einstein [5]. Given two nonzero finitely generated modules M and N over a commutative Noetherian local ring R, the tensor product M RN tends to have torsion, in general. Hence the assumption that M(x)R N is torsion-free in uences the structure of M and N, as well as that of R. This connection made its first appearance in Auslander's 1961 seminal paper [1]. A beautiful result Auslander proved in this paper is that, if R is a regular local ring which contains a field (e.g., R = C[[x1,...,xn]]) and M(x)R N is torsion-free, or equivalently, is a first syzygy module, then both M and N are first syzygy modules. In 1994, Huneke and Wiegand [6] obtained a natural extension of Auslander's result for the case where R is a hypersurface ring (e.g., R = C[[x1,...,xn]]=/( f ), where f is a nonzero element in the square of the maximal ideal). More precisely, Huneke and Wiegand proved that, if R is a hypersurface domain, and M(x)R N is reflexive, or equivalently, is a second syzygy module, then both M and N are second syzygy modules.
In this talk I will discuss a consequence of the aforementioned result of Huneke and Wiegand [7] concerning the depth and support of tensor products. The talk is based on the papers [2, 3, 4].

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This talk may be appropriate for all students with a strong interest in research.

**COLLOQUIUM Spring 2019**

**Department of Mathematics**

**Margaret M. Wiecek**
**School of Mathematical and Statistical Sciences**

**Clemson University**

**Monday, April 8, EMCS 422, 2:00–2:50 pm.**

**Abstract**. Decision making in the presence of uncertainty and multiple conflicting objectives is a real-life issue, especially in the fields of engineering, public policy making, business management, and many others. The conflicting goals may originate from the variety of ways to assess a system's performance such as cost, safety, and affordability, while uncertainty may result from inaccurate or unknown data, limited knowledge, or future changes in the environment. To address optimization problems that incorporate these two aspects, we focus on the integration of robust and multiobjective optimization.

Although the uncertainty may present itself in many ways due to a diversity of sources, we address the situation of objective-wise uncertainty only in the coefficients of the objective functions, which is drawn from a finite set of scenarios. Among the numerous concepts of robust solutions that have been proposed and developed, we concentrate on a strict concept referred to as highly robust efficiency in which a feasible solution is highly robust efficient provided it is efficient with respect to every realization of the uncertain data. We apply this concept to uncertain multiobjective linear programs (UMOLPs).

We develop properties of the highly robust efficient set, provide its characterization using the cone of improving directions associated with the UMOLP, derive several bound sets on the highly robust efficient set, and present a robust counterpart for a class of UMOLPs. As various results rely on the polar and strict polar of the cone of improving directions, as well as the acuteness of this cone, we derive properties and closed-form representations of the (strict) polar and also propose methods to verify the property of acuteness. Moreover, we undertake the computation of highly robust efficient solutions. We provide methods for checking whether the highly robust efficient set is empty, computing highly robust efficient points, and determining whether a given solution of interest is highly robust efficient. An application in the area of bank management is included.

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