

FRIDAY SESSION 1: BIOMATHEMATICS

Don Giddens¹, **Suo Jin**¹, **John Oshinski**^{1,2}

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Georgia Institute of Technology and Emory Medical School*

Hemodynamics In Individual Subjects: Applications And Challenges In Cardiovascular Disease

The various forms of cardiovascular disease are complex in their origins and their manifestations in individual subjects. A number of “risk factors” are well known, but mechanisms at the cellular and molecular levels are not fully understood. It is now appreciated that mechanical forces can have significant effects on biological function, from the scale of organs, such as the heart and arteries, to the expression of various molecules on and within cells. For example, fluid dynamic wall shear stress (WSS) is known to affect endothelial cell function, and low and oscillating WSS is associated with atherosclerotic plaque localization. While valuable information can be gleaned from cell culture studies, it is important to view the artery as an interactive system and to study cardiovascular pathophysiology within its *in vivo* environment. A challenge is therefore to be able to describe hemodynamics in individual subjects with an appropriate degree of precision. We will discuss the potential of using computational modeling, coupled with noninvasive imaging, to yield flow field information that may prove valuable in the study of cardiovascular disease. Examples will be presented that emphasize interactions of fluid dynamic forces with tissue and that also highlight issues associated with accuracy and validation.

Hiroyoshi Toyoshiba and **Christopher J. Portier**
National Institute of Environmental Health Sciences

Two- Stage Model Of Carcinogenesis With Controlled Replication

Cancer is a disease with three distinct processes; initiation, mutation and replication. Initiation refers to the mechanisms that start the process of carcinogenesis in an organ or tissue. Initiation can result from mutations, changes in cellular biochemistry and/or alterations in tissue structure or function; in most cases, the initiating event is assumed to be a mutation. Selection of the initiated cell(s) for increased replication can occur by several processes including direct stimulation of growth factor pathways and/or selective killing of non-initiated cells. Finally, cancer is a multistage process for which it is believed several mutations are necessary to result in cancer formation. The altering processes of mutation and replication move cells and colonies of cells closer to cancer. Numerous publications have addressed this multistage nature of the cancer process[1-3].

Tissue structure can play an important role in the cancer process. Different cells within different tissues and organs play very different roles in tissue function and ultimately should play different roles in carcinogenesis. Some tissues (e.g. liver) are fairly homogenous collections of cells, all with similar functions. Other tissues (e.g. lung) are highly structured mixtures of different cell types, each with its own functional role. Finally, a third type of tissue (e.g. skin and gut lumen) are composed of mostly one type of cell but with a structure in which cells move from one area of the tissue in which they are formed (e.g. stem cell basal layer) to an area in which they serve their main purpose and eventually die (e.g. villus of gut lumen). It is this third category of tissue/organ we wish to address in this manuscript.

Multistage models of carcinogenesis are widely used in the analysis and interpretation of cancer data[4-10]. The most commonly used model is the two-stage model[11, 12]. The model hypothesizes a single pathway to carcinogenesis consisting of two stages, normal cells (stage 0) stage and initiated cells (stage 1) stage. At each stage, we have cells that can go through a linear birth-death process and also mutate to a higher stage. The two-stage model assumes that all cells act independently of all other cells and that cells have no restrictions on the number of births they can go through. From this second assumption, the expected number of cells of the usual two-stage model can exceed the physiological capacity of the animal/human system being analyzed. In organs like the gut lumen and skin, there appears to be a limit of the number of replications possible for the progeny of the stem cell populations. In this manuscript, a new mathematical model is developed where the birth-death process is limited for stem cell progeny and, even when the birth rate exceeds the death rate, the tissue will not grow out of control[13]. This new model is compared to the two-stage model using an existing analysis of colon cancer from the literature.

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FRIDAY SESSION 2: MULTISCALE/NUMERICAL ANALYSIS

Todd Arbogast

University of Texas, Austin

Two-Scale, Locally Conservative Subgrid Upscaling for Elliptic Problems

We present a two-scale framework for approximating the solution of a second order elliptic problem in divergence form. The problem is viewed as a system of two first order equations with the divergence equation representing conservation of some quantity. We explicitly decompose the solution into coarse and fine scale parts. Moreover, the differential problem splits into the coupled system (1) a coarse-scale elliptic problem in divergence form, and (2) a fine scale problem localized in space. Solving the second problem for the fine scale part of the solution in terms of the coarse part, we obtain an operator mapping the coarse scale to the fine. Substituting this operator in the coarse problem results in an upscaled problem posed entirely of the coarse scale. Numerical approximation by a subgrid upscaling technique gives a computable algorithm. Since the fine scale is localized in space, an efficient algorithm results by using an influence function (numerical Greens function) technique to solve the fine subgrid-scale problems independently of the coarse-grid approximation. Moreover, the coarse-scale problem remains locally conservative. After correcting the coarse scale solution on the subgrid-scale, we obtain a fine scale representation of the solution.

We show that the scheme is second order accurate. Numerical examples representing flow in a porous medium are presented to illustrate the effectiveness and applicability of the method.

Ohannes Karakashian
University of Tennessee

Additive Schwarz Methods For A Discontinuous Galerkin Method.

We discuss some two-level nonoverlapping and overlapping additive Schwarz methods for a discontinuous Galerkin method for solving second-order elliptic problems. The methods serve as preconditioners for the conjugate gradient method. Numerical experiments are presented.

FRIDAY SESSION 3: MATERIAL SCIENCE/FLUIDS

John Zweck
University of Maryland, Baltimore County

Reduction Of Nonlinear Effects In Optical Fiber Communication System

With the rapid growth in the global flow of information, there is increasing demand for high data-rate optical communications systems for both local metropolitan networks and long-haul continental and trans-oceanic links. The transmission of light in optical fibers is governed by the nonlinear Schrodinger equation, and its generalizations. In modern optical communications systems the pulses which represent individual bits spread out across each other as they propagate. A major goal of the system design is to recompress the pulses at the receiver without introducing too much distortion due to nonlinearity and other effects. In this talk I will discuss some of the issues involved in modeling a realistic experimental optical fiber transmission system, and discuss two methods for reducing the nonlinear effects in high data-rate, long-haul systems. I will also outline some of the mathematical challenges that we have encountered in our quest for the holy grail of optical communications, which is to compute the bit-error rate of realistic system. This research has been performed by a mathematician in collaboration with fellow members of the Photonics Laboratory at the University of Maryland Baltimore County. Our research has been partially funded by a grant from CIENA Corporation, a leading optical communications company.

Youngsuk Lee

University of Wisconsin, Madison

Large Scale Instability To Rossby Waves In The β -Plane Equation

A description is given for the unstable spectrum at large scales of the β -plane Equation linearized about Rossby waves using Floquet Theory. Techniques of continued fractions with Newton's Method are used to solve the spectral problem numerically. The results are explained in terms of resonant triadic interactions. Finally we discuss the possible relevance of the linear instability of a single mode to the generation of slow, large-scale motions in new and previous numerical calculations of β -plane flow forced randomly at small scales.

Daniel Guo

University of North Carolina, Wilmington

**Semi-Lagrangian Finite-Element Model For Shallow-Water Equations
On The Sphere**

The finite-element and semi-Lagrangian methods are used to solve the shallow-water equations on the sphere, which were rewritten in the forms of vorticity-divergence. The new formation leads to the direct application of the semi-Lagrangian method. With the rectangular element, the local mesh refinement is conveniently to implement. This results easily to carry out the regional climate modeling from global climate modeling with little or no changes.

Stephen Schecter¹ and Dan Marchesin²

*North Carolina State University*¹, *Instituto de Matematica Pura e Aplicada*², *Brazil*

Oxidation Heat Pulses For Two-Phase Flow In Porous Media

We show that when air or oxygen is injected into a one-dimensional petroleum reservoir, and oxidation or combustion is induced, an oxidation pulse can form and propagate as a traveling wave. The lead part of the pulse is a combustion front; the trailing part of the pulse is a slow cooling process. The traveling wave is shown to exist using geometric singular perturbation theory. The small parameter is heat loss to the surrounding rock formation. We will present a simplified model that makes clear the geometry of the traveling wave. A similar analysis has been done for more realistic models.

FRIDAY SESSION 4: INDUSTRIAL MATHEMATICS/CONTROL

Gema Mercado

Georgia Institute of Technology

Temperature Fronts In Microwave Heating

A new approach to study the dynamics of the thermal and electric fields in a cylindrical dielectric medium that is undergoing microwave heating is presented. The mathematical model is standard and consists in a Maxwell's wave equation coupled to a temperature diffusion equation containing a bistable nonlinear term.

When the thermal diffusivity is sufficiently small, the leading order temperature solution of a singular perturbation analysis is used to reduce the system to a free boundary problem. This approximation accurately predicts the steady-state solutions for the temperature and electric fields in closed form. These solutions are valid for arbitrary values of the electric conductivity, and thus extend the previous (small conductivity) results found in the literature.

A time-dependent approximate profile for the electric field is constructed to obtain an ordinary differential equation for its relaxation to the steady state. This equation appears to accurately describe the time scale of the electric field's evolution even in the absence of a temperature front (with zero coupling to the temperature), and can be of wider interest than the model for microwave heating.

Laszlo Kollar

The University of Texas, Dallas

Stabilization of a Digitally Controlled Piecewise Linear System

Dynamics of the controlled pendulum is investigated assuming backlash and time delays. First, a possible model of the inverted pendulum on a cart is constructed. The upper equilibrium of the pendulum is stabilized by a piecewise constant control force which is the linear combination of the sampled values of the angle and the angular velocity of the pendulum. The control force is provided by a motor which drives one of the wheels of the cart through an elastic teeth belt. The contact between the teeth of the gear (rigid) and the belt (elastic) introduces a nonlinearity known as "backlash" and causes the oscillation of the controlled pendulum around its upper equilibrium. The processing and sampling delays in the determination of the control force tend to destabilize the controlled system as well. We obtain conditions guaranteeing that the pendulum remains in the neighborhood of the upper equilibrium. Experiments were also carried out on a computer controlled inverted pendulum-cart structure and showed good agreement with the theoretical results.

Tien-Sung Chio

Washington University in St.Louis

The Formation Generating And Regrouping Problems Of Multi-Robot Teams

The significance of multi-robot systems is increasing due to the growing need to coordinate distributed operations. It is more flexible and more fault tolerant to use several simple robots than having a single powerful robot for each separate task. An interesting topic of study in multi-robot systems is to control a team of robots. The main motivation of this research is to present the method of the formation generating and regrouping for multi-robot teams. It allows multi-robot teams to group and regroup in use of interconnecting matrices to generate the desired formation shapes accordingly to serve various needed function. In order to get the insight of formation, we investigate the condition for the formation controllability of the multi-robot teams. This condition can be expressed in terms of the interconnection parameters of the multi-robot teams. It is shown that the interconnection among robot plays a fundamental role in formation of multi-robot teams. We also investigate sufficient condition for the formation stability of multi-robot teams over a finite time interval.

Ellina Grigorieva

Texas Woman's University

Applying Optimal Control Theory to Microeconomic

In this work, a non-linear dynamical model of the process of production, storage and sales of consumer goods is investigated. Optimal control problem of profit maximization with the rate of production and the price as control variables is solved. It is analytically shown that the optimal control function is a piecewise constant function with at most two switchings. It is proved that changing the rate of production or the price more than two times over some time interval cannot yield maximum profit. Numerical Runge-Kutta simulations of nonlinear system of differential equations support our theoretical results.

FRIDAY SESSION 5: MATERIAL SCIENCE/FLUIDS

Stuart S. Antman

University of Maryland

Dissipation In Solids, Invariance, And Regularity

The availability of strong dissipative mechanisms in solids often makes their governing equations tractable. Unfortunately, some such mechanisms, inspired by gas dynamics, destroy the natural invariance of material properties under rigid motions, with the consequence that the resulting solutions might be physically unreasonable. This lecture (i) shows how to remedy the lack of invariance of standard shock-capturing schemes for the hyperbolic system governing the motion of some nonlinearly elastic bodies, (ii) describes the rich but tractable class of complications, associated with strain-gradient (capillarity-type) effects, that arise for invariant systems, (iii) discusses the regularizing effects of invariant dissipative mechanisms on solutions of the governing equations, and (iv) relates some of these effects to those that arise in geometrically exact models for incompressible bodies.

Negash G. Medhin

Clark Atlanta University

Molecular Based Model for The Dynamic Response of a Rubber Rod Under Tensile Deformations.

We develop a dynamic model for the viscoelastic response of a rubber rod under tensile deformations. We present an explicit formula for the longitudinal vibration of a rubber rod with tip mass showing the interaction between density and relaxation time on the creep behaviour. We will also include the effect of random perturbations on the dynamics.

Andrea Bertozzi

Duke University

Undercompressive Shocks in Driven Film Flow

Thin films driven by body or surface stresses are common in many technological and industrial applications. Problems of interest include spin coating, de-icing of airplane wings, and lung surfactants. Recent experiments of films driven by a thermally induced

surface tension gradient with opposing gravitational force show a transition from thin films that are unstable to fingering to thicker films with stable contact line motion. This system can be modeled by a nonlinear scalar hyperbolic conservation law with a non-convex flux. The fingering transition can be explained by a change in the underlying shock structure of the front, from compressive waves that unstable to transverse perturbations, to double shocks with a leading stable undercompressive wave. We discuss the mathematical theory behind this problem and the comparison with data from recent laboratory experiments.

FRIDAY SESSION 6: INDUSTRIAL MATHEMATICS/CONTROL

Richard J. Braun

University of Delaware

A Model for Crystal Growth on a Masked Substrate

A variety of models in which the growth of a crystal depends only on its shape are currently in use; such models are geometric growth models. Some of the models currently in use will be reviewed. The review will contrast some models for epitaxial growth on substrates for the cases with and without masks. New results for a model with anisotropic surface energy, mobility and diffusion will be presented. A variety of shapes seen experimentally are reproduced by the model. Mathematically, the model uses a growth law which specifies the normal velocity of the crystal surface as a function of the direction of the normal and the curvature at each point; a marker particle method with remeshing is used to advance the surface. This work is in collaboration with Mikhail V. Khenner and Michael G. Mauk, and is supported by the NSF via grant DMS-9631287.

John A. Burns

Virginia Tech

Numerical Approximations of Dynamical Systems

In this paper we discuss some fundamental issues concerning the use of numerical schemes for approximating dynamical systems. In particular, we focus on problems having to do with the preservation of system properties under approximation. Such issues are known to be important when using numerical methods for optimization and control design. Although there is a well developed convergence theory when solutions are restricted to compact time intervals (Trotter-Kato Theorem, Lax Equivalence Theorem,

etc.), these theories do not always extend to long time behavior. For example, consider the differential equation

$$\dot{x}(t) = F(x(t)), \quad 0 < t < +\infty, \quad (1)$$

with initial data

$$x(0) = z \in Z$$

Assume that one has constructed a sequence of *approximating dynamical systems* on spaces $Z_N \subset Z$ defined by

$$\dot{x}_N(t) = F_N(x_N(t)), \quad 0 < t < +\infty, \quad (2)$$

with approximating initial data

$$x_N(0) = z \in Z_N.$$

Under suitable assumptions (consistency and stability) one might be able to construct convergence numerical schemes so that

$$x_N(t) \rightarrow x(t)$$

on compact intervals $[0, T]$. However, if for example one is interested in “computing” an invariant set for the system (1) by using the approximating system (2), then the standard convergence theory needs to be extended. Simple examples are used to illustrate this point and to raise similar issues for problems with extreme sensitivities. Finally, we close with some comments on the recent use of numerical methods to “prove” the existence of non-unique solutions to certain non-linear boundary value problems.

Robert Plemmons

Wake Forest University

Wavefront Phase Encoding for Extended Depth-of-Focus Optical Imaging

We discuss the problem of wavefront phase encoding for extended focus in optical-digital imaging systems. The depth-of-focus of an imaging system is the distance in the object space in which objects are considered to be in focus. One immediate application of this research is personal identification/verification technology. We are working on better ways to "see and identify" subjects (separated by several ft. distances) with security cameras at ATMs, transportation centers, etc. We discuss and analyze a novel approach to the problem, suggested by S. Prasad, which is based on a multiple design optimization scheme obtained by parameterizing the pupil phase using a basis of Zernike polynomials.

FRIDAY SESSION 7: BIOMATHEMATICS

Frank Kozusko¹ and Zeljko Bajzer²
Hampton University¹, Mayo Clinic Rochester²

A General Solution for Gompertz Tumor Growth Based on Cell Quiescence

Tumor cell quiescence has been proposed to develop a mathematical model of cell kinetics. Tumor cells are represented as either quiescent (Q) or proliferating (P). This model has been shown to describe Gompertz type growth under special parameter selection.

Here the model is extended to form a general solution. The normalized Gompertz function can be represented as $N(t) = \exp\{k_+[1 - \exp(-k.t)/k]\}$. The quiescent model guarantees Gompertz growth when the cell kinetic parameters and the transition rates to/from quiescent/proliferating satisfy a constraint relationship, which is a function of N , k_+ and k . When the Gompertz parameters k_+ and k are specified, the proliferating cell population is determined by the loss/death rate (μ_q) of the quiescent cells. A production ratio: $R_p = (\beta - \mu_p) / \mu_q$ is defined, where β is the proliferating cell reproduction parameter, μ_p / μ_q are the death rates of the proliferating/quiescent cells respectively. The final proliferation fraction is determined to be $PF_\infty = (P_\infty / N_\infty) = 1 / (1 + R_p)$. The general solution is shown to be consistent with the special parameter solutions.

Laura Potter

US Environmental Protection Agency

Mathematical Methods For Addressing Uncertainty And Population Variability In Biological Models

Variability is an inherent feature of most biological systems, occurring both within an individual and across populations. Deterministic and probabilistic-based methods have been developed to incorporate such intra-individual and inter-individual variability into mathematical models for biological systems. In this presentation, these methods will be outlined and applied to a toxicokinetic model for the systemic transport of trichloroethylene (TCE).

TCE is a widespread environmental contaminant and toxicant that is known to accumulate in the fat tissue of humans and animals. This accumulation and the heterogeneous physiological properties of fat tissue (e.g., widely varying fat cell size, lip distribution, and blood flow) suggest a spatially varying model for the transport of TCE within the fat. An axial dispersion-type model will be presented that specifically

accounts for the variability of TCE concentrations that occurs within the fat tissue of an individual.

In most cases, experimental measurements of toxicokinetic data such as tissue concentrations are collected from multiple individuals. Probabilistic-based parameter estimation methods have been developed that incorporate the resulting inter-individual variability into the parameter identification process. Formulations of these estimation problems for the TCE model and related theoretical and computational results will be presented. (This abstract does not reflect EPA policy)

J. Patrick Wilber

Texas A&M University

The Convexity Properties of Constitutive Models for Biological Soft Tissues

During the last three decades, the theory of nonlinear elasticity has been used extensively to model biological materials. These efforts reflect the widespread belief that crucial to understanding diseases of the human cardiovascular system and to developing effective diagnoses and treatments are good constitutive models for the mechanical response of biological soft tissues. Although these efforts have generated many different models, surprisingly little work has been done to examine the mathematical features of the various models proposed. For example, convexity, which in its various guises is central for much of modern nonlinear continuum mechanics, has not been carefully explored. In this talk we will present our recent work analyzing the mathematical properties in particular the convexity properties of a general class of constitutive models, special cases of which correspond to important models, like the Fung model, currently used in the biomechanics literature. Also, we will explain how our results are of practical importance to the experimentalist who wishes to construct models that not only fit data well but also make sense mechanically according to established results in nonlinear continuum mechanics.

Cammeey E. Cole

Meredith College

Age-Structured Modeling And Optimal Control Applied To Erythropoiesis

Erythrocytes are the blood cells whose primary function is to deliver oxygen to the tissues. The control of erythropoiesis is governed by the hormone erythropoietin, which is released in the bloodstream based on a negative feedback mechanism that detects partial pressure of oxygen in the blood. This age-structured model has two major classifications of cells: precursor cells and mature cells. The precursor cells are structured by their maturity level relative to their hemoglobin content; the mature red blood cells are structured by age. The system was written in weak form and reduced from an infinite

dimensional system to a system of ordinary differential equations by employing a finite element formulation. The control of this process is governed by the hormone erythropoietin. The form of the feedback of this hormone is unknown. Although a Hill function has previously been used to represent this feedback, it has no physiological basis, so an optimal control problem was formulated in order to find the optimal form of the feedback function and to track the total number of mature cells. Numerical results for both forms of the feedback function will be presented.

Shigui Ruan

Dalhousie University, Halifax, Nova Scotia, Canada

and

Vanderbilt University, Nashville, TN, USA

Global Dynamics of a Ratio-Dependent Predator-Prey System

Recently, ratio-dependent predator-prey systems have been regarded by some researchers to be more appropriate for predator-prey interactions where predation involves serious searching processes. However, such models have set up a challenging issue regarding their dynamics near the origin since these models are not well-defined there. In this paper, the qualitative behavior of a class of ratio-dependent predator-prey system at the origin in the interior of the first quadrant is studied. It is shown that the origin is indeed a critical point of higher order. There can exist numerous kinds of topological structures in a neighborhood of the origin including the parabolic orbits, the elliptic orbits, the hyperbolic orbits, and any combination of them. These structures have important implications for the global behavior of the model. Global qualitative analysis of the model depending on all parameters is carried out, and conditions of existence and non-existence of limit cycles for the model are given. Computer simulations are presented to illustrate the obtained results.

FRIDAY SESSION 8: MULTISCALE/NUMERICAL ANALYSIS

Omar Lakkis

University of Maryland

A Posteriori Error Analysis For The Mean Curvature Motion Of Graphs

We study a Finite Element discretization of the motion by mean curvature of a surface described by a graph.

That is the equation

$$\partial_t u / \sqrt{1 + |\nabla u|^2} - \operatorname{div}(\nabla u / \sqrt{1 + |\nabla u|^2}) = f$$

on a bounded domain with Dirichlet boundary conditions and initial values.

And a posteriori analysis of the error is carried out. This provides us with local indicators, which are then exploited in order to design adaptive mesh refinement algorithms. The main purpose is to decrease the computational effort for the same error tolerance with respect to the usual global refinement.

Numerical examples are provided to compare adaptive (local) versus non-adaptive (global) mesh refinement.

In collaboration with Gerhard Dziuk and Ricardo H. Nochetto

Marc Laforest *

University at Stony Brook

A Posteriori Error Estimate For Front-Tracking For Nonlinear Systems Of Conservation Laws

In this talk, we present a posteriori error estimate in the L^1 norm for front-tracking approximate solutions to hyperbolic systems of conservation laws. This result extends the L^1 stability theory of Bressan, Liu, and Yang and depends on their L^1 equivalent functional. Our method shows that with the help of their functional we can distinguish between the numerical error and the amount of entropy produced by the underlying physical system. Front-tracking approximations are piecewise constant approximations constructed under the assumption of small total variation. As in the Glimm scheme, the nonlinearities generated during wave interaction can be controlled. The numerical error is measured by a quantity similar to the residual but computed from an exact Riemann solver. This local error estimator coincides with an estimator of Kuznetsov for scalar conservation laws.

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S.S. Ravindran

University of Alabama

Real Time Computational Algorithms For Optimal Control Of An MHD System

The flow of weakly electrically conducting fluids can be controlled by applying electromagnetic forces originating from electrodes and permanent magnets suitably placed on the surface of the body. We consider the possibility of separation control for a

two-dimensional bluff body with reduced-order modeling. Model reduction is achieved by combining proper orthogonal decomposition (POD) and Galerkin projection. POD allows one to extract the dominant modes in the observed physical phenomena and to define the smallest possible solution space. This can be exploited in a Galerkin framework to reduce a nonlinear infinite dimensional model to a small finite dimensional model. The resulting reduced order model can be solved in real time and is very attractive for control purposes.

We present numerical experiments with several spanwise magnetic field distributions. Dramatic separation delays are observed on all cases. Our methods are found to be efficient and fast, and our methods demonstrate a significant reduction in computational time.

Jue Yan

Brown University

A Local Discontinuous Galerkin Method for KdV-type Equations

We develop a local discontinuous Galerkin method for solving KdV type equations containing third derivative terms in one and two space dimensions. The method is based on the framework of the discontinuous Galerkin method for conservation laws and the local discontinuous Galerkin method for viscous equations containing second derivatives, however the guiding principle for inter-cell fluxes and nonlinear stability is new. We prove L^2 stability and a cell entropy inequality for the square entropy for a class of nonlinear PDEs of this type both in one and multiple spatial dimensions, and give an error estimate for the linear cases in the one dimensional case. The stability result holds in the limit case when the coefficients to the third derivative terms vanish, hence the method is especially suitable for problems which are "convection dominated", i.e. those with small second and third derivative terms. Numerical examples are shown to illustrate the capability of this method. The method has the usual advantage of local discontinuous Galerkin methods, namely it is extremely local and hence efficient for parallel implementations and easy for h - p adaptivity.

Luis Melara and Petr Kloucek

Rice University

The Computational Modeling Of Internal Domain Walls In Crystals

We introduce a finite element method which is piecewise continuous on the microscopic scale of the spatial resolution h that is discontinuous on the mesoscopic scale $h^\delta \in (0,1)$, with the scaling parameter δ determined by the equidistribution of the free energy. The method is designed to capture the morphology of mesoscopic needle twin structures frequently found in ferroic and coelastic crystals. The approach is based on a domain decomposition method that interpolates between the scale on order of the size of crystal

and the microscopic scale of finite element approximation h . The scale interpolation h . The scale interpolation is enabled by incorporating a frequency adaptivity. The computational results, such as the one plotted on Figure 1, exhibit geometrical structures observed in uniaxial ferromagnets and in the vicinity of the Austenite-Martensite interfaces

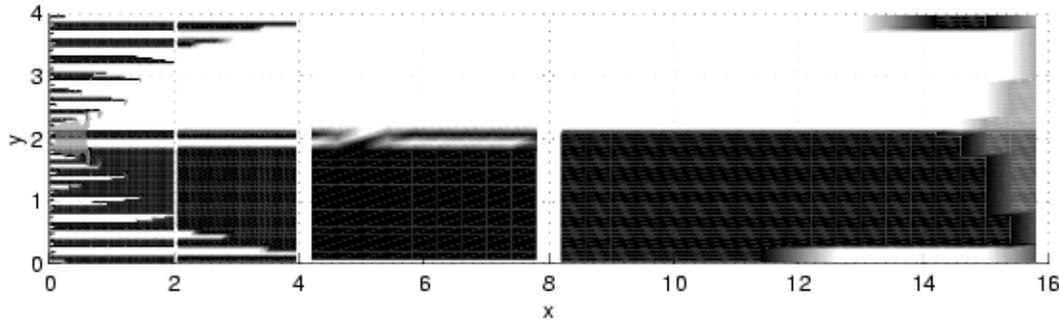


Figure 1: Splitting of a Martensitic twin. The black color represents gradient $(0,1)^T$, the white color represents the gradient $(0,-1)^T$. The picture summarizes finite element computation of the Implicit Partial Differential Equation $(u_x^2 - \varepsilon)^2 + ((u_y)^2 - 1)^2 = 0$. $(x,y) \in (0,16) \times (0,4)$. $0 < \varepsilon \ll 1$, with homogeneous boundary conditions on $(0,4) \times (0,16) \setminus \{x=16\}$. The solution simulates branching.

SATURDAY SESSION 9: BIOMATHEMATICS

Hans Othmer

University of Minnesota

Mathematical And Computational Challenges Posed By Models Of Biological Systems

Complex, tightly coupled networks of interacting components arise at every level of biological organization, ranging from gene control networks to ecological networks. A major challenge in understanding hierarchies of such networks is to understand how simple, reproducible responses arise from these complex networks, how robust they are to inevitable fluctuations in components, and how one can embed microscopic-level

information into population-level models. We will describe some of the mathematical and computational approaches being developed for this purpose, using several model systems from cell biology and physiology.

Glenn Webb

Vanderbilt University

The Steady State Of A Tumor Cord Cell Population

The equilibrium equation of a proliferating tumor cord cell population is analyzed. The population is structured by age and by radial distance from the interior blood vessel, which the cord surrounds. The population densities satisfy nonlinear partial differential equations for proliferating and quiescent classes of tumor cells. Sufficient conditions are given on the fraction of cells, which enter proliferation to assure the existence of a unique steady state.

SATURDAY SESSION 10: MULTISCALE/NUMERICAL ANALYSIS

Christopher L. Cox

Clemson University

Opportunities For Applied Mathematicians In Modeling Of Polymer Processes

The talk will begin with a brief overview of polymeric fiber spinning and film casting processes. Then governing equations used to model certain flows associated with these processes will be presented. Numerical techniques for approximating the solution of these equations will be discussed, including a Matlab solution of a one-dimensional problem and finite element solutions of higher dimensional problems. A description of an object-oriented modeling package, being developed by CAEFF students and faculty members, will be given.

Susanne C. Brenner
University of South Carolina

Stress Intensity Factors And Singular Solutions

It is well known that the regularity of the solution of an elliptic boundary value problem is adversely affected by the presence of reentrant corners, cracks or jumps of coefficients across interfaces. The consequent lack of regularity is responsible for the poor performance of standard finite element methods. Remedies developed over the years include local refinement and the p (or hp) version of the finite element method.

In this talk we present an alternative approach where the optimal convergence of the P_1 finite element method on quasi-uniform grids can be recovered even for problems with reentrant corners, cracks or interfaces. This is achieved by combining the singular function representation of the solution, the extraction formulas for the stress intensity factors and the full multigrid methodology.

SATURDAY SESSION 11: MATERIAL SCIENCE/FLUIDS

Sue Minkoff
University of Maryland

Coupled Fluid Flow, Geometrical Deformation, and Seismic Modeling

Over the lifetime of an oil field, reservoir geology can change substantially causing economic disasters such as well failures as well as platform collapses and the loss of human life. In some parts of the world, accurate numerical modeling of fluid production from these fields requires coupled flow and mechanical deformation modeling. We present an algorithm for staggered-in-time, 2-way coupling of flow and geomechanics. Modifications to the geomechanics code allow changes in pore pressure to be included in the total stress calculation. The geomechanics code produces volumetric strain-induced porosity and permeability updates for the flow simulator. Time-lapse seismic modeling involves taking oil field “snapshots” periodically during field production. In numerical feasibility studies for time-lapse seismic imaging, output pressures and saturations from reservoir simulation are used to update seismic velocities and density in the reservoir interval. This analysis assumes the rocks surrounding the reservoir are not changing with time (only the fluids change). However, in these weak-formation reservoirs, the reservoir geology will alter substantially during production due to subsidence. We present numerical examples which illustrate the impact coupled flow and mechanical deformation modeling has on predictive seismic modeling.

Karl Glasner
Duke University

The Long Time Dynamics Of Spinodal Dewetting In Thin Fluid Films

Many thin fluid films are subject to instabilities caused by a competition of short and long range forces. In the short term, the fluid breaks into droplets connected by an ultra-thin film. Droplet arrays will then coarsen over a long timescale. In the context of a one-dimensional lubrication model, this slow dynamics can be analyzed to yield a set of evolution equations for the droplet masses and positions. From these, information about the coarsening rates of large arrays of droplets can be obtained.

Yalchin Efendiev
Texas A&M University

Dynamics of heterogeneous aerosol coagulation

The study of aerosol dynamics is often limited to homogeneous aerosol particles. However, it is becoming increasingly apparent that multi-component aerosol particles are of both industrial importance and an area in need of significant research activity. I will talk about our recent studies in modeling and computation of heterogeneous aerosol coagulation.

Michael Shearer
North Carolina State University

Thin Flow Near A Dynamic Contact Line

A fourth order nonlinear pde describes the flow of a thin liquid film up an inclined surface, under the opposing forces of gravity and shear stress. The Navier slip condition allows a small amount of slip between the liquid and the solid surface near the contact line; it is designed to remove the stress singularity that occurs under the usual no-slip condition. I present analytic and numerical results for the ODE satisfied by traveling wave solutions representing the contact line dynamics. This talk is based on joint work with Andrea Bertozzi and Robbie Buckingham

SATURDAY SESSION 12: INDUSTRIAL MATHEMATICS AND CONTROL

Qin Sheng

University of Dayton

An Application Of The Exponential Splitting In Crystallinity Gradient Simulations Of Injected Semi-Crystalline Polymers

Injection molding of semi-crystalline polymers is one of the most important yet complicated fabrication processes that combines polymer rheology, heat transfer, and crystallization kinetics. Traditionally, simulations of this process are approximated by 2-dimensional (2D) mathematical models based on the Hele-Shaw flow theory. Simulation models are often important, or even crucial, for understanding the detailed crystallization structure, for designing the optimal control of the quality of the products and for achieving higher productivity in the industry. In this talk, we will consider a 3D mathematical model of the semi-crystalline polymer flow and the distribution of crystallinity in an injection molding process. A second order parallel splitting algorithm is employed to achieve the necessary accuracy and efficiency in computations. Calculated values of flow-wise (flow-thickness plane) and width-wise (width-thickness plane) crystallinity distributions are then compared with experimental results (syndiotactic polystyrene (244,000 Mol. Wt.) is used). The structure-oriented simulation method developed is not only capable of describing moldability parameters, but is also able to predict the characteristics of ultimate properties of the final products

David Szurley

Optimal Control For Polymer Processing

An overview of the polymer fiber spinning process will be given. One-dimensional governing equations for melt spinning with flow-induced crystallization will be presented along with a solution method. We will show how optimization can be used to improve upon polymer quality, and results (numerical results by simple algorithms) will be presented. Optimization based upon sensitivities applied to the thin filament equations will be discussed, and preliminary results will be shown.

Abbas Alhakim
University of Delaware

**On The Design And Performance Of A Test For Randomness Based
On The Statistics Of Long Runs Of Similar (Binary) Digits**

With the continually increasing computational technologies, newer and wider applications of random number generators (RNG) evolve-- in such fields as simulation and Monte Carlo techniques. This increases the need for designing new stringent tests that are capable to assess the quality of RNG's. Starting with a random binary sequence, we consider the corresponding sequence of "runs" of similar outcomes. We obtain formulas for some limiting joint distribution of the long runs and their occupation times. We show that these formulas provide stringent tests that are able to detect flaws in many of the generators that are in commercial use.

John Pelesko
Georgia Institute of Technology

Mathematical Modeling Of Microsystems

The field of Microelectromechanical systems (MEMS) has undergone a startling revolution in recent years. It is now possible to produce functioning motors that can only be seen with the aid of a microscope, gears smaller than a grain of pollen, and needles so tiny they deliver an injection without stimulating the nerve cells. While experimental work in this field has progressed rapidly mathematical modeling and analysis has lagged far behind. This presents a wonderful opportunity for the applied mathematician. In this talk we show how the construction and analysis of even simple models can shed light on phenomena and provide design guidelines for MEMS designers. Further, we discuss the relationship between micron sized electrostatic devices and macro-scale high voltage experiments. We indicate how understanding these experiments can shed light on phenomena observed in the micro-world.

Peter Mucha

Georgia Institute of Technology

Fluctuations, Side Walls And Stratification In Dilute Sedimentation

Sedimenting suspensions of monodisperse rigid spherical particles in a state of creeping flow are considered in the dilute limit, where only low-order particle–particle interactions are kept to simplify the dynamical equations. In this limit, $\tilde{O}(N)$ codes can easily simulate more than 10^5 particles and can be used to address the fundamental question of whether or not the velocity variance, ΔV^2 , scales with system size. We obtain quantitative ΔV^2 estimates for cells with side walls which agree well both with simulations and with dilute experiments. As the relative interparticle interaction strength increases, larger velocity fluctuations induce larger hydrodynamically-induced diffusivities, leading to small vertical stratifications of the particle density by the spreading of the sediment front. Such stratification cuts off the fluctuation at a scale below the system size. We present a theory for the persistent velocity fluctuations in such stratified environments, and compare with simulations and experiments demonstrating that stratification effects are responsible both for steady–state deviations from system-size scaling and for persistently –decaying fluctuations that have been observed in recent experiments.

This talk presents work done in collaboration with M.P. Brenner and B.I Shraiman

Bo Li

University of Maryland

Island Dynamics in Epitaxial Growth of Thin Films

This work is concerned with the analysis and improvement of island dynamics models that have been recently developed for the epitaxial growth of crystal thin films. We first examine the linear stability for two island dynamics models, namely the irreversible aggregation model and the attachment-detachment model. We then derive from the step-edge kinetics the boundary velocity and the Gibbs-Thomson relation, and propose a new set of boundary conditions to replace that in the irreversible aggregation model. This is a joint work with Russel Caflisch.

David Schaeffer
Duke University

**Ill-Posed Partial Differential Equations In Granular Flows: Discreteness And
Nonlinearity**

In this lecture I will discuss a discrete-space/continuous-time approximation of the continuum equations of a model that describes antiplane shearing of granular material; more precisely, I will discuss a 1D problem extracted from the model. Like many equations for the dynamics of granular flow, these equations are linearly ill-posed. Despite the linear ill-posedness of the PDE, the solution to this (nonlinear) finite-difference equation remains *bounded for all time in the max norm*. This boundedness demonstrates a striking interaction between discreteness and nonlinearity.

The model can be cast as a single, second-order equation for the (scalar) velocity w , which has $w(x,t) \equiv 0$ is an equilibrium solution. A typical solution with initial conditions $w(x,0)$ close to the equilibrium solution quickly develops grid oscillations that saturate when their slope is $\mathcal{O}(1)$; following saturation, the solution undergoes a long transient that we may describe as *coarsening*, during which its profile has many small jumps that gradually coalesce into one large discontinuity. The discontinuity, which is stable and persists indefinitely, may be regarded as a shear band. Much of this behavior---in particular, the size of the jump at the shear band---can be predicted analytically, but the location of the shear band depends *extremely* sensitively on the initial conditions.

A striking conclusion of this paper is the scaling law for the number of jumps $K(t)$ remaining at a given time t :

$$K(t) \sim \left(\frac{N}{t} \right)^{1/3}$$

where $N = \delta^{-1}$ is the total number of grid points.

Although I will not discuss this in the lecture, similar problems with ill-posedness, discreteness, and coarsening arise in many areas, including image processing, microstructure models of fracture, phase transitions in crystals, and population models.

SATURDAY SESSION 14: INDUSTRIAL MATHEMATICS/CONTROL

L. Pamela Cook
University of Delaware

Unambiguous Polymer Characterization Via At-Line Capillary Viscometry

The goal of this work (joint with E. Nwankwo of DuPont Corp., G.Schleiniger and B. Wood of U. Del.) is to extend the applicability of flow referenced capillary viscometry (FDRCV) to real-time at-line measurement of polymer diffusivities thus leading to unambiguous real time at-line polymer characterization. This will result in significant savings for industry. Experimentally, a plug of dilute polymer is introduced into a fully developed (constant volumetric flow rate) flow of a solvent in a capillary. Measurements of pressure are taken downstream resulting in a polymer mixture profile. The plateau of the profile has, in the past, been linked to the intrinsic viscosity of the polymer. In this work we link the profile leading and trailing edge shapes to the polymer diffusivity leading to a much improved characterization of the polymer. The fluid/constitutive equations describing the process are those of a two fluid mixture with one fluid being a dilute viscoelastic mixture, the other a Newtonian solvent. The non-dimensional equations are analyzed both numerically and asymptotically for their dependence on the dilution parameter and especially for their dependence on the Peclet number, the product of the Reynolds number and the Schmidt (inverse diffusivity) number. The results extend the work of Taylor on dispersion to a polymer mixture thus to fluids of highly differing viscosities and elasticities.

Gregory A. Kriegsmann
New Jersey Institute of Technology

Microwave Heating Of Materials: A Mathematical And Physical Overview

The use of microwaves to heat and dry materials is rapidly gaining acceptance in industry and, to some extent, in the field of biomedical engineering. The working engineering theories are based upon heuristically averaged, linear equations which adequately explain some processes, such as microwave cooking of foodstuffs, but not others. These include such phenomenon as thermal runaway and hot spot formations which have important ramifications in both biomedical and industrial applications. They are caused by the temperature dependencies of the electrical and thermal properties of the irradiated material, which make the basic underlying mathematical description to be highly nonlinear.

We shall describe a general microwave heating experiment and present several simplified models, which have been used by researchers in this field. The strengths and shortcomings of these models will be discussed and open questions, of both mathematical and computational natures, will be presented.

H. Thomas Banks

North Carolina State University

Uncertainty In Modeling And Inverse Problem Methodology

In this lecture we will discuss a number of ways in which uncertainty arises in classes of inverse problems. Examples from biology and materials will be used to motivate a framework in which parameters to be estimated are treated as random variables. Detailed results from a project on modeling uncertainty in production delays in HIV pathways will be given to illustrate the ideas.

SATURDAY SESSION 15: MATERIAL SCIENCE /FLUIDS

Zhenbu Zhang

Tulane University

Generation And Metastability Of Patterns For A Class Of Nonlinear Evolution Equations

Of concern are the properties of solutions of one space dimensional evolution equation

$$u_t(x, t) = A[u(\cdot, t)](x), \quad x \in \mathbf{R}, \quad t > 0 \quad (1)$$

where A is a nonlinear operator which is independent of the time t , maps functions of space variable \cdot to functions of x . Examples of this include some important models such as Allen-Cahn equation, Neural network model and Ising model etc.. We show that under certain assumptions on A , the solution of the rescaled version of (1)

$$u_t(x, t) = A[u(\varepsilon \cdot, t)]\left(\frac{x}{\varepsilon}\right), \quad \varepsilon \text{ small} \quad (2)$$

will develop a “transition layer structure”, i.e. a pattern, at a predictable time and that this pattern will last a very long time but will be eventually destroyed.

Vasilios Alexiades¹, Nouredine Hannoun², Tsun-Zee Mai²
*University of Tennessee & ORNL*¹, *University of Alabama, Tuscaloosa*²

Choosing Solvers for Melt Flow Computations

The choice of linear systems solvers in CFD is crucial, both for the success and the computational efficiency of the simulation. This is even more so for simulation of melting processes, in which the continuity, momentum, and energy equations are strongly and nonlinearly coupled to the moving solid-liquid interface.

We describe our numerical experiments comparing combinations of solvers for the large, sparse, banded linear systems arising from an implicit finite volume discretization of the PDEs for energy, velocities, pressure, pressure correction, and streamlines.

Guido Thoemmes

University of Darmstadt, Germany

Diffusion Approximations To The RHT Equations In Glass Cooling

The Simplified-P_N approximations to the radiative heat transfer equations in glass for the optically thick, diffusive regime are presented. The approximations are derived by applying an asymptotic analysis to the original system. The necessary boundary conditions can be obtained from variational arguments. Numerical studies for problems appearing in the simulation of RHT problems in glass cooling confirm the efficiency of the approach. Moreover, we indicate how these approximations can be applied in order to accelerate an iterative solver for the full RHT equations or to control the cooling process.

Daniel Reynolds , Petr Kloucek

Rice University

A Mesoscale Model For The Phase Transformation Kinetics Of Shape Memory Alloys, With Application To Vibration Damping

We present a new computational approach to control damping of vibrations in shape memory alloy rods. The method is based on a model of shape memory alloys using constitutive properties relating their micro and macro-scales, governing equations for heat and momentum, and a controlling process formed using a measure of the mechanical energy.

This talk focuses on a new method of forming the relation between the micro and macro-scales in shape memory alloys. These alloys develop a striated crystal microstructure, formed through the alternation of phases having symmetry related atomic lattices. Mathematically, the deformation gradients of these phases are constrained to values from

a finite set. The macroscopic response of the material thus depends on the spatial composition of these deformation gradients.

The bridge between these micro and macro-scopic scales is given via the Young measure, which provides a macro-scopic measure of the composition deformation gradients, and may be calculated through the non-local relaxation of non-attainable differential inclusions.

In this talk we will discuss the relevance of Young measure within the model of vibration damping. We will then discuss the non-local relaxation using a new subgrid projection method, and provide one-dimensional computational evidence of its benefit.

Noureddine Hannoun¹, Vasilios Alexiades², Tsun Zee Mai¹
University of Alabama¹, University of Tennessee & ORNL²

Melting of Gallium and Tin: The End of a Controversy

Melting of Gallium in a rectangular cavity heated from the wall has extensively used for assessing numerical methods for phase change problems including convection in the melt. There is a controversy about the structure of the flow of the melt. Most previously published results report one cell, while few other works found a multicellular roll structure. Experiments seem to agree with one cell findings. We present a thorough comparison between results for several schemes and grid sizes, for problem very similar, melting of tin. Our results show that a multicellular flow structure is the correct answer to the numerical experiments, and that other arguments are needed to explain the disagreement between the experimental results and numerical computations.

SATURDAY SESSION 16: MULTISCALE /NUMERICAL ANALYSIS

Jennifer Ryan
Brown University

Accuracy Enhancement of the Discontinuous Galerkin Method through Post-Processing for Multi-Domains.

Results are presented that show the accuracy of the Discontinuous Galerkin approximation to the scalar wave equation for multi-domains with different mesh sizes is increased when we apply a post-processor. This improvement in accuracy takes place away from domain interfaces.

Jae-Hong Pyo
University of Maryland

A Finite Element Gauge Uzawa Method For The Evolution Navier-Stokes Equation

The Navier-Stokes equations of incompressible fluids are still a computational challenge. The numerical difficulty arises from the incompressibility constraint, which requires a compatibility condition (discrete inf-sup) between the finite element spaces for velocity and pressure. Several projection methods have been introduced for time discretization to circumvent the incompressibility constraint, but suffer from boundary layers. They are either numerical or due to non-physical boundary conditions on pressure.

We introduce a first order Gauge-Uzawa method for time discretization coupled with a stable finite element method for space discretization. The method is unconditionally stable, consists of $d+1$ Poisson solves per time step, and does not exhibit pronounced boundary layer effects. We prove error estimates for both velocity and pressure under realistic regularity conditions via a variational approach, and illustrate the performance with several numerical experiments. This work is jointly with R. H. Nochetto.

Wei Cai
University of North Carolina, Charlotte

Fast Solver for Electromagnetic Scattering in Layered Media

In this talk we will discuss fast solvers for integral equations of electromagnetic scattering in multilayered media. Computation of scattering in layered media has application in VLSI design, geophysical exploration and remote sensing. We will first review some existing fast solver for layered media and then present a new fast solver based on a window based acceleration scheme for the dyadic Green's function for layered media and the two dimensional fast multipole methods.

Abdelhamid Badran
Colorado State University

Identification of Coefficients in Differential Equation

This talk will describe a new method for identification of unknown coefficients in differential equations. The method applies a version of the Backus- Gilbert method to the identification of coefficients which are functions of the independent variables in the problem. The method will be illustrated for identifying an unknown coefficient in some differential equation and the results of some numerical experiments will be presented.

Semyon Tsynkov¹, G. Fibich², B. Ilan²
North Carolina State University¹ Tel Aviv University²

Computation of Nonlinear Backscattering Using a High-Order Numerical Method

The nonlinear Schrodinger equation (NLS) is the standard model for propagation of intense laser beams in Kerr media. The NLS is derived from the nonlinear Helmholtz equation (NLH) by employing the paraxial approximation and neglecting the backscattered waves. In this study we use a fourth-order finite-difference method supplemented by special two-way artificial boundary conditions (ABCs) to solve the NLH as a true boundary value problem. Our numerical methodology allows for a direct comparison of the NLH and NLS models and, apparently for the first time, for an accurate quantitative assessment of the backscattered signal.

SUNDAY SESSION 17: BIOMATHEMATICS

Julie S. Kimbell
CIIT Centers for Health Research

Computational Fluid Dynamics and Particle Transport in the Nasal Passages

The nasal passages represent the portal of entry for particulate matter (PM) and contain considerable capacity for deposition, uptake, and metabolism associated with deposited particles. In addition, deposition and clearance in the head can vary with nasal anatomical structure, providing various degrees of protection for the lower respiratory tract. Regional deposition estimates are needed to improve our ability to extrapolate animal response data to humans for assessment of inhaled particulate risks. Computation fluid dynamics (CFD) models of the rat, primate, and human nasal passages were used to conduct PM deposition simulations in rats, primates and humans for particle sizes between 0.5 and 10 μm . Effects of mesh refinement, a process in which the number and positions of crosshairs or nodes are adjusted in each computer mesh, and airflow rate on nasal deposition efficiency were studied. Simulation results were compared with experimental data. Differences between predictions at different mesh densities generally decreased with increasing levels of mesh refinement. These results suggested ultimate convergence to a unique value and indicated a need for predictions at one more level of mesh refinement to estimate that value. Simulated nasal deposition efficiencies in the rat generally agreed with experimental estimates. In the human, simulations predicted that fine and coarse particle deposition efficiencies were quite sensitive to the airflow rate and increased with increasing flow rate. Simulations of respiratory airflow and regional PM deposition in the respiratory tracts of rats, primates, and humans will allow us to estimate

dose to specific sites in animals and calculate exposures that produce similar doses in humans. These results could be used to reduce uncertainty in extrapolating animal results to humans for human health risk assessment.

Shannon Wynne

North Carolina State University

**Modeling and Computation of Propagating Waves from
Coronary Stenoses**

Acoustic noises are produced from a coronary stenosis. Current research exploits the shear wave fields in body tissue for detection purposes. Our investigation focuses on the propagation of shear waves through the chest cavity. In our initial effort, we consider one-dimensional and two-dimensional, homogeneous viscoelastic models, and present several computationally efficient constitutive relations based on an internal variable formulation. Results from the one-dimensional models match well with simulated data; results from the two-dimensional model match well with experimental data.

Michael C. Mackey

McGill University

**Understanding Periodic Hematological Disease: Insights from Mathematics
Translate to the Bedside"**

There are a number of interesting periodic hematological diseases [Haurie et al. *Blood* (1998), 92, 2629-2640] and some are understood through mathematical modeling [M.C. Mackey. "Mathematical models of hematopoietic cell replication and control", pp. 149-178 in **The Art of Mathematical Modeling: Case Studies in Ecology, Physiology and Biofluids** (H.G. Othmer, F.R. Adler, M.A. Lewis, and J.C. Dallon eds.) Prentice Hall (1997)]. A number of these diseases are most certainly due to a Hopf bifurcation in the dynamics of peripheral control, triggered by alteration of cellular death rates, e.g. periodic auto-immune anemia and cyclical thrombocytopenia. Others, like cyclical neutropenia, are due to a bifurcation in stem cell dynamics arising from elevated levels of apoptosis. This talk will give an overview of the status of mathematical modeling of these diseases, and the role that this modeling is playing in shaping treatment strategies. For papers related to these topics, go to http://www.cnd.mcgill.ca/bios/mackey/mackey_newpubl.html

SUNDAY SESSION 18: MULTISCALE/NUMERICAL ANALYSIS

Michael Minion

University of North Carolina

Higher Order Semi-Implicit Methods For Initial Boundary Value Pdes

A new class of semi-implicit numerical methods for partial differential equations with both stiff and non-stiff terms is presented. The methods are based on a semi-implicit version of the method of spectral deferred corrections for ordinary differential equations combined with a method of line approach. The accuracy and stability of the new ODE methods will be discussed as well as issues that arise when applying the method to PDEs with time varying boundary conditions. In particular, a loss of accuracy similar to that which occurs with Runge-Kutta methods will be discussed, and a general strategy for avoiding the loss of accuracy will be presented.

Ricardo Nochetto

University of Maryland

An Adaptive Uzawa FEM For Stokes: Convergence Without The Inf-Sup Condition

We introduce and study an adaptive finite element method for the Stokes system based on an Uzawa outer iteration to update the pressure and an elliptic adaptive inner iteration for velocity. We show linear convergence in terms of the outer iteration counter for the pairs of spaces consisting of continuous finite elements of degree k for velocity whereas for pressure the elements can be either discontinuous of degree $k-1$ or continuous of degree $k-1$ and k . The popular Taylor-Hood family is the sole example of stable elements included in the theory, which in turn relies on the stability of the continuous problem and thus makes no use of the discrete inf-sup condition. We discuss the realization and complexity of the elliptic adaptive inner solver, and provide consistent computational evidence that the resulting meshes are quasi-optimal. This is joint work with E. Baensch and P. Morin.

Zhilin Li

North Carolina State University

New Formulation And Fast Poisson Solvers For Interface Problems In Polar Coordinates

In this talk, numerical methods are proposed for some interface problems in polar or Cartesian coordinates. The new methods are based on a formulation that transforms the interface problem with a non-smooth or discontinuous solution to a problem with a smooth solution. The new formulation leads to a simple second order finite difference scheme for the PDE and a new interpolation scheme for the normal derivative of the solution. In conjunction with the fast immersed interface method, a fast Poisson solver has been developed for the interface problems with piecewise constant but discontinuous coefficient using the new formulation in polar coordinate system.