Classification of Shapes using Complex Elliptical Shape Distribution

In this presentation, we discuss classification procedures in a shape analysis context. We derive discriminant rules in shape space, while considering shape distributions as members of the complex elliptical family of shape distributions for the data. In particular, we consider the complex Watson distribution as a special case and develop MAP (Maximum A Posteriori Estimates) of parameters involved and calculate misclassification probabilities using Monte Carlo methods. Our proposed methodologies are exemplified through an example, where we are interested in classifying patients into the normal or schizophrenic groups, based on shapes created by MRI (Magnetic Resonance Image) of their brains. The methods provide us with a new way of diagnosis of this medical condition while controlling the error of misclassification. This is joint work with Athanasios Micheas of the University of Missouri, Columbia.

Mechanistic Systems Biology Modeling Applied to the Pre-Clinical Cardiac Safety Assessment of a Pharmaceutical Compound: From Channels to Cells to Tissue

This presentation will focus on an integrative, mechanistic systems modeling approach to cardiac electrophysiology. Via an integrated suite of models from channel to cellular to ultimately, tissue levels, we used specific compound data from limited pre-clinical cardiac electrophysiological studies, such as channel assay as well as one action potential assay, to: (i) estimate missing compound data at the channel level through the application of reverse-engineering techniques; (ii) integrate measured and estimated channel values into action potentials at the cellular level; and (iii) further integrate such cellular responses to predict transmural ventricular responses, which in effect, represent ECG-like features at the tissue level, such as QT prolongation and transmural dispersion of repolarization.

The combination of experimental data and computer-based predictions of compound-induced changes at every level of cardiac biology organization (channel, cell, tissue) provides valuable, quantifiable information to aid in the pre-clinical cardiac safety assessment of new compounds. Joint work with G. Helmlinger, D. Bottino (Novartis Pharmaceuticals, USA), B. Dumotier, M. Traebert (Novartis Pharmaceuticals, CH), S. Lett (The BioAnalytics Group LLC, USA), C. Penland (Predix Pharmaceuticals, USA), and A. Stamps (Dept. of Chemical Engineering, University of South Carolina).

Vector Soliton Collision Dynamics in Nonlinear Optical Fibers

We consider the interactions of two identical, orthogonally polarized vector solitons in a nonlinear optical fiber with two polarization directions, described by a coupled pair of nonlinear Schrödinger equations. We study a low-dimensional model system of Hamiltonian ordinary differential equations (ODEs) derived by Ueda and Kath and also studied by Tan and Yang. We derive a further simplified model, which has similar dynamics but is more amenable to analysis. Sufficiently fast solitons move past each other without much interaction, but below a critical velocity, the solitons may be captured. In certain bands of initial conditions, the solitons are initially captured, but separate after passing each other twice, a phenomenon known as the two-bounce or two-pass resonance. We derive an analytic formula for the critical velocity. Using matched asymptotic expansions for separatrix crossing, we determine the location of these resonance windows. Numerical simulations of the ODE models show they compare quite well with our asymptotic theory. This is joint work with Roy Goodman (NJIT).
Shelby Haberman

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Identifiability of Parameters in Item Response Models with Unconstrained Ability Distributions

If a parametric model for the ability distribution is not assumed, then the customary two-parameter and three-parameter logistic models for item response analysis present identifiability problems not encountered with the Rasch model. These problems impose substantial restrictions on possible models for ability distributions. Attempts to circumvent these problems by use of latent-class versions of two-parameter and three-parameter logistic models are strongly limited by problems of near singularity of the information matrix, even for a modest number of latent classes. Thus efforts to use ability distributions that are not normal must be made with great caution.

W. Jackson Hall

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Secondary Inference after a Sequential Clinical Trial

Consider the following prototype situation: A two-arm randomized, staggered entry, clinical trial, designed to test hypotheses about a treatment effect, has just been completed, utilizing a planned sequential stopping rule. The primary analysis may have been a survival analysis, with treatment arm as the sole risk factor, or one based on the difference between mean responses after a prescribed observation period. No doubt, the trial statistician knew how to take the stopping rule into account in carrying out primary inferences, both hypothesis testing and estimation. But now secondary questions are raised: (i) Do the data provide evidence of a main effect for gender? (ii) Do the data provide evidence of a treatment-by-gender interaction? (iii) How big are any such effects?

Standard analyses that ignore the stopping rule are biased. We review a very simple example to clarify the issues.

We then describe the sequential primary inference problem as a stopping problem for a Brownian motion that approximates the score process for the trial on an information time scale. The secondary inference may then be based on the conditional distribution of another stopped Brownian motion (efficient score) given the primary process with modified stopping boundaries. The formal solution is summarized.

We exemplify with an analysis of a 2-strata clinical trial of implanted cardioverter defibrillators--the problem that stimulated the research.

John Harris

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Coupled Elastic Waveguide Modes

The talk begins by describing an example of elastic-waveguide mode coupling at low frequencies: the curvature of an elastic ring couples the longitudinal and flexural propagating modes. Then a more complicated problem containing coupling is analyzed in detail; this is the main subject of the talk: A layer of homogeneous, isotropic, elastic material overlies a faster substrate. At the interface, a long inclusion, whose shear wavespeed is less than that of the layer and whose thickness varies, is introduced. It is imagined that the lowest surface-wave mode of the structure is incident to the growing inclusion. Numerical calculations show that the growth of the slow inclusion draws this lowest mode into an interval where it couples to the second mode, thus exciting it. This process is repeated when the second mode is drawn into...
an interval where it couples to the third. Outside of these localized intervals, the modes propagate independently of one another (that is, adiabatically). The problem is formulated and solved within a framework of coupled local modes. An indication of a future asymptotic analysis of the wave fields in the coupling interval closes the talk.

JAN HESTHAVEN
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Solving the Time-Domain Maxwell’s Equations with Uncertainties

While the modeling of EM processes for known geometries and materials has advanced dramatically over the last decade, these advances are often lost when comparing with actual measurements. This can, to a large extent, be attributed to insufficient knowledge of the geometries, materials, dynamics, illumination, etc. of the actual experiment. To achieve a better agreement, one must include this uncertainty into the computational models.

In the past, statistical methods, e.g., Monte-Carlo-type methods, have been the dominant tool for such studies. However, this approach is expensive due to the slow convergence in the number of samples, and it is not feasible to use such techniques for large scale problems with uncertainty, in particular, when higher order statistical moments are needed.

In this talk, we introduce the use of homogeneous chaos expansions for the direct modeling of uncertainty in EM processes, modeled by the linear time-domain Maxwell’s equations. This approach, which is probabilistic rather than statistical in nature, effectively transforms the stochastic problem into a sequence of deterministic equations, which we subsequently solve efficiently using a high-order accurate discontinuous Galerkin method.

We consider examples involving uncertainties in illumination/source, material properties, and geometric shapes to show the potential for obtaining results 50-100 times faster than computed to similar accuracy using Monte Carlo methods.

Joint work with Laura Lurati (Division of Applied Mathematics, Brown University) and Cedric Chauviere (Laboratoire de Mathematiques Appliquees, Universite Blaise Pascal, 63177 Aubiere Cedex, France).

PHILIP HOLMES
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A Central Pattern Generator for Insect Locomotion

We model a central pattern generator (CPG) for insect locomotion. We reduce ion-channel, Hodgkin-Huxley (HH)-type models of bursting neurons to single-variable phase oscillators and assemble a circuit of six representative interneurons that each feed a fast and a slow motoneuron. Our phase description retains sufficient detail to allow investigation and prediction of biophysical parameter changes, and it encompasses stepping frequency, duty cycle, and motoneuron output variations observed in cockroaches. The model’s modular form allows dynamical analyses of individual components and the addition of other components, so we expect it to be more generally useful.

The methods involve computation of phase response curves, averaging, and elementary ideas from symmetric networks.

Joint work with Raffaele Ghigliazza.
**FRANK HOPPENSTEADT**

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**Dynamics of Coalitions in Aggregates and Networks of Oscillators**

Consider a large array of harmonic oscillators whose center frequencies are arranged in increasing order, \( w_1 < w_2 < w_3 < \ldots < w_N \). These oscillators need not be arranged in any order in the three dimensional space where they reside; this addressing is in terms only of their center frequencies. We first consider an aggregate where the center frequencies are perturbed by a common external signal:

\[
d^2x_j/dt^2 + (w_j^2 + p(t)) x_j = 0,
\]

\[ j=1,2,3,\ldots,N. \] Here the common parametric forcing is \( p(t) = \varepsilon \cos \mu t \), which has frequency \( \mu \) and amplitude \( \varepsilon \) (note that \( \mu \) and \( \varepsilon \) do not depend on \( j \)). Such equations are well-studied, and it is known how to determine the number and identity of oscillators that are entrained at a common frequency. We refer to such a group of synchronized oscillators as being a *coalition*. There is no physical connection between these oscillators, but if the center frequencies are sufficiently dense between \( w_i \) and \( w_j \), the diagram of response frequencies across the array for a given value of \( \mu \) resembles a staircase having treads located at rational number multiples of \( \mu \). The treads describe coalitions. Moreover, as \( \mu \) is changed, the staircase changes. Thus, the coalitions move through the population of oscillators, as determined by relationships between \( \mu \) and the center frequencies. There is a rich structure of coalitions of various sizes (i.e., the lengths of treads) that is indexed by \( (\varepsilon, \mu) \) in this simple network. We use observations about the linear system to reveal coalitions in aggregates of nonlinear oscillators of the form

\[
d^2x_j/dt^2 + \alpha dx_j/dt + (w_j^2 + p(t)) \cos x_j = 0
\]

Such equations are well studied in physics, engineering, and mathematical neuroscience. We demonstrate how, within a coalition, information can be carried in the timing of oscillations (i.e., in phase deviations). Finally, we consider networks where

\[
p(t) = \varepsilon \cos \mu t + C_j(\sin x(t))
\]

where \( C_j(\sin x(t)) \) describes connections to site \( j \) from all other oscillators. We use known methodologies from mathematical neuroscience to construct connections \( C \) that embed desired patterns of phase deviations, and we show that these patterns can be made to appear or disappear by changing the single parameter \( \mu \). Supported in part by MARCO grant 2003-NT-1107.

**ANETTE (PEKO) HOSOI**

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**From Sliding Paper to Crawling Snails: Novel Applications of Thin Films**

Liquid thin films have long been studied in the context of industrial, biological, and geophysical applications from spin coating in microcircuit fabrication to the liquid lining in the lung. In general, typical length-scales in these systems are set by surface tension. However, when the film is bounded by a flexible membrane, elasticity takes on the role of surface tension. We discuss some of the consequences of substituting elastic effects for surface tension in the context of several commonly observed phenomena, such as sliding paper and floppy drives, and in more exotic applications such as microfluidic switches and robotic snails.
ASHWANI K. KAPILA

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Detonations in Heterogeneous Explosives: Model and Computational Results

A heterogeneous explosive is morphologically complex. Upon application of an igniting stimulus, the microstructure responds heterogeneously in two salient ways. First, the mechanical response is nonuniform in terms of local deformation and the associated deposition of energy. Second, the mechanical nonuniformity gives rise to thermal, and hence kinetic nonuniformity, so that ignition occurs at certain preferential sites, or hot spots, where the local temperature is significantly higher than the bulk temperature. In due course, the hot spots grow and merge, and reaction spreads from the hot spots to the bulk. As a rule, the scale of the device employing the explosive is substantially larger (of the order of tens of centimeters) than the micro scales (of the order of tens of microns) at which energy is released. Thus, predicting macro-scale device behavior by direct computation at the micro scale would be prohibitively expensive. One gets around this difficulty by posing continuum models that contain approximate submodels for the micro-scale input. Either implicitly or explicitly, these approximations represent an average behavior, in effect homogenizing the fine-scale description if such a description were available. This talk will describe one such model, its predictions, and its strengths and weaknesses.

THOMAS B. KEPLER

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Inducible Reorganization of the Immune System

The vertebrate immune system consists of a great diversity of motile cells whose activities become coordinated during infection. This orchestration is mediated by signaling molecules either secreted (cytokines) or engaged by direct cell-cell contact. Pathogenic microorganisms (and other stimuli) induce internal changes in the responding immune cells which, in turn, lead to spatial reorganization of these cells in a process arguably akin to a phase transition.

The models we are developing to explore these phenomena represent the cells of the immune system as individual "agents" with non-trivial internal states. The motion of these agents in a three-dimensional continuum is described by a continuous-time stochastic process, as are their internal dynamics. Soluble factors, such as cytokines, are represented as fields obeying reaction-diffusion equations on the continuum. Both the internal states of the agents and their motions are responsive to the state of the cytokine fields, which, in turn, are influenced by the agents, which act as time-dependent sources and sinks. I will present these models and illustrate them with examples of the inflammation-mediated spatial reorganization of the immune system.
In order to establish the stability of an equilibrium solution $U$ of an infinite-dimensional dynamical system $\dot{U} = X(U)$, one is interested in the spectrum of the linear operator $L[U]$ obtained by linearizing the dynamical system around $U$. We use a spectrally accurate method for the computation of such spectra. In essence, the method is due to Hill, who used it in the study of the equation that now bears his name. The method is particularly well suited to the case of periodic $U$, but is not restricted to it. By incorporating the fundamentals of Floquet theory, an almost uniform approximation to the entire spectrum is obtained, as opposed to an approximation of a few selected elements. The numerical component of the method is limited to (i) choosing the size of the matrices to be used, and (ii) an eigenvalue solver, such as the QR algorithm. Compared to often-used finite-difference approaches, the method is orders of magnitude faster for comparable accuracy.

Most biophysical models of the nonlinear spatially-extended dynamics of intracellular calcium assume that one can neglect stochastic fluctuations. Recent experiments have, however, directly implicated noise due to the opening and closing of finite numbers of channels in a variety of dynamical behaviors. This talk focuses on some of the mathematical issues which arise when one adds fluctuations to non-equilibrium pattern-forming systems.

Viewed on a hydrodynamic scale, flames in experiments are often thin so that they may be described as gasdynamic discontinuities separating the dense, cold fresh mixture from the light, hot burned products. The original model of a flame as a gasdynamic discontinuity was due to Darrieus and to Landau. In addition to the fluid dynamical equations, the model consists of a flame speed relation describing the evolution of the discontinuity surface, and jump conditions across the surface which relate the fluid variables on the two sides of the surface. The Darrieus-Landau model predicts, in contrast to observations, that a uniformly propagating planar flame is absolutely unstable and that the strength of the instability grows with increasing perturbation wave number so that there is no high wave number cutoff of the instability. The model was modified by Markstein to exhibit a high wave number cutoff if a phenomenological constant in the model has an appropriate sign. Both models are postulated, rather than derived from first principles, and both ignore the flame structure, which depends on chemical kinetics and transport processes within the flame. At present, there are two models which have been derived, rather than postulated, and which are valid in two nonoverlapping regions of parameter space. Sivashinsky derived a generalization of the Darrieus-Landau model which is valid for Lewis numbers (ratio of thermal diffusivity to mass diffusivity of the deficient reaction component) bounded away from unity. Matalon and Matkowsky derived a model valid for Lewis numbers close to unity. Each model has its own advantages and disadvantages. Under appropriate conditions, the Matalon-Matkowsky model exhibits a high wave number cutoff of the Darrieus-Landau instability. However, since the Lewis numbers considered lie too close to unity, the Matalon-Matkowsky model does not capture the pulsating instability. The Sivashinsky model does capture the pulsating insta-
bility, but does not exhibit the high wave number cutoff of this instability. Here, we derive a model consisting of a new flame speed relation and new jump conditions, which is valid for arbitrary Lewis numbers. It captures both monotonic and pulsating instabilities, and exhibits a high wave number cutoff for each. The flame speed relation includes the effect of short wave lengths, not previously considered, which leads to stabilizing transverse surface diffusion terms.

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Self-Organized Patterns in Bacterial Colonies

It is observed by Budrene and Berg [1], [2] that chemotactic bacteria form regularized but complex patterns. They emphasized that such patterns are generated in a self-organized way due to the balance among substrate consumption, cell proliferation, excretion of attractant, and chemotactic motility. My talk is to understand theoretically how these four elements can possibly generate such patterns by using a mesoscopic continuous model.


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New Nonlinear Water Wave Models over Highly Variable Topographies

Recently, we formulated a weakly nonlinear, weakly dispersive terrain-following Boussinesq system (SIAP 2003) in order to study solitary waves over highly variable (random) topographies. The modeling allows for multiply-valued topography profiles. The reduced model is obtained through the standard power series expansion for the velocity potential along the free surface. In this talk, we will give a brief overview of this earlier study and present a new, fully dispersive, Boussinesq system (Phys.Rev.Lett., 2004) that generalizes the terrain-following system mentioned above. The full linear (hyperbolic tangent) dispersion relation is entirely retained by constructing a Dirichlet-to-Neumann (DtN) map along the top boundary of the highly corrugated strip representing the channel. Moreover, an efficient FFT-based method naturally arises from the DtN boundary integral formulation.

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Regularizations of Vortex Sheet Motion

The vortex sheet is a mathematical model for a shear layer in which the layer is approximated by a surface. Generally, vortex sheets develop singularities in finite time. To approximate the fluid past this time, the motion is regularized, and the sheet is defined as the limit of zero regularization. However, very little is known about this limit, not even whether it is unique or depends on the regularization. I will discuss several regularization mechanisms, including physical ones such as fluid viscosity, and purely numerical ones such as the vortex blob and the Euler-alpha methods. I will show results for a model problem and discuss some of the unanswered questions of interest.
ANDREW NORRIS
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Crack Front Waves using Matched Asymptotic Expansions

A steadily propagating crack with a straight edge is not stable under perturbation. This surprising result was found ten years ago, but is still not fully understood despite many studies using analytical, computational, and experimental techniques. The problem is exacerbated by the difficulty involved in the analysis of even the simplest case of mode I crack propagation. This talk provides a simple and physically appealing method for analyzing the crack front stability based on matched asymptotics. The inner region of the crack with the wavy edge is considered separately from the outer problem of the steadily propagating straight crack. By matching the solutions, the stability criterion is found. The simplicity of this method allows us to consider more complicated crack scenarios, including a crack on a bimaterial interface, and a crack with a cohesive zone. The talk will emphasize the power of using matched asymptotics to analyze stability of propagating material fronts, of which the crack is but one example.

HILLARY OCKENDON
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Turbulent Flow in Long Thin Channels

Turbulent compressible flow in long thin channels arises in many practical situations from a train in a long tunnel to a pressure transducer to the effect of a rock fall in a mine. This talk will describe the Fanno model for such flows and show how it can be applied in some of these examples.

JOHAN PAULSSON
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Suppressing Fluctuations in Living Cells

Life in single cells is dictated by chance: Reactions that involve small numbers of molecules generate spontaneous fluctuations that enslave all dependent processes. Such noise can be suppressed by negative feedback control where a molecule directly or indirectly represses its own synthesis. I will use a reinterpretation of the Fluctuation-Dissipation Theorem to demonstrate generic trade-offs where suppressing one type of fluctuations automatically amplifies other types. Strongly nonlinear strategies for breaking the trade-offs will also be discussed.

JOHN PEARSON
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Equivalence and Identification of Markov Models for Ion Channel Kinetics

Deducing plausible reaction schemes from single channel current traces is time consuming and difficult. The goal is to find the simplest possible scheme, but there are many ways to connect even a small number of states (more than 2.5 million schemes with four open and four closed states). Many of those schemes make identical predictions, and even an exhaustive search over model space does not address the problem of how to represent the many equivalent schemes that may result.

We have found a canonical form that can express all reaction schemes for binary channels. This form has the minimal