CP1

FDEM: A New Method with Error Estimate for the Numerical Simulation of Industrial Problems

The Finite Difference Element Method (FDEM) is an efficiently parallelized black-box solver for the numerical solution of nonlinear systems of PDEs in 2-D and 3-D like they appear for numerical simulations of technical problems. Unprecedented for such a general black-box is the computation of an error estimate. We present the simulation of industrial problems to demonstrate the possible fields of application. We offer a service for the solution of PDEs in cooperations with industrial and academic partners.

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CP1

Analytic Solution of An Axial Dispersion Model Involving Retardation Coefficient for the Packed Bed of Porous Particles

An axial dispersion model involving axial dispersion and retardation coefficients is presented. Model is solved analytically using Laplace transforms for large range of Peclet number and retardation coefficient. Two limiting cases, Perfect mixing and Perfect displacement are considered. To check the applicability, model is applied on a lab scale pilot plant. Data of mixture of Indian wood and non wood pulp fibers has been used. Analytic results obtained from model are compared with experimental results.

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CP1

Sensitivity Issues Concerning Inverse Heat Tranfer Analysis of Welds

Data adopted for inverse heat-transfer analysis of welds includes solidification cross-sections, thermocouple measurements and microstructural changes. We discuss here the sensitivity of temperature histories, obtained by inverse analysis, with respect to shape characteristics of longitudinal solidification cross-sections, which are strongly correlated with convective heat transfer, but are difficult to determine experimentally. Accordingly, we consider the sensitivity of temperature histories with respect to assumptions concerning the shapes of longitudinal solidification cross-sections.

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CP1

Cramer-Rao Bounds for Chemical Species Separation in Magnetic Resonance Imaging

Separation of chemical species (e.g. water and fat) in MRI in the presence of imperfections in the magnetic field is a nonlinear inverse problem. Optimization of the image acquisition based on the Cramer-Rao bound leads to a new optimal acquisition which shows improvements in the clinical images. The maximum likelihood estimator achieves the Cramer-Rao bound in Monte Carlo simulations and experimentally. This project is conducted by an interdisciplinary team from radiology, engineering and mathematics.

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CP1

Teaching and Learning Computational Science and Engineering

I would like to discuss (together with the audience!) how we can go forward with computational science and engineering. Getting students involved has to be the key – they will develop ideas for projects (and better use of software). It is a fascinating and creative subject that combines applied mathematics with scientific computing. One question is how to present both of those essential parts. My goal is that each lecture discusses a model problem and a code to solve it. This MIT course is popular with engineering students and their departments, who want exposure to ideas and also to software (especially MATLAB). The main sections of the course are Applied Linear Algebra, Differential Equations, Finite Differences and Finite Elements, Fourier Methods, Analytical Methods, Large Sparse Systems, and Optimization. The need to move beyond the older courses in engineering mathematics, and connect directly to computing, is widely recognized. A pure software course misses the foundations for understanding new problems. The combination of analysis with computational science and engineering is powerful.

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CP2

Iterative Methods for the Approximation of Solutions to Variational Inequalities

In general, a variational inequality is a problem that is usually defined as follows. Let F be a vector valued function on $K \subseteq R^n$, for K convex. Then we seek $x^* \subseteq R^n$ with the property that[1]

$$\langle F(x^*), (x - x^*)\rangle \geq 0 \; \forall x \in K$$

Such inequalities (which I specify using the notation V_F^K for the specific Variational Inequality) are important within operations research, mechanics, optimisation and game theory. In particular, Variational Inequality Problems may find applications in those areas of mathematics and other mathematical sciences that concern themselves with optimisation. Historically, Variational Inequalities were traditionally associated with the study of Partial Differential Equations. Moreover, it is well known that each variational inequality can be considered as being associated with an Optimisation problem as follows. If we seek to minimise $f(x)$ subject to the constraint that $x \in K$, then it is possible to associate this with the Variational Inequality problem $V_{(\nabla f)}^K$. It is worth noting that there are a whole plethora of methods that can be used in order to go about solving variational problems, some of which include an application of techniques such as the Finite Element Method to finding approximations to such Variational Inequalities. In this paper, I shall consider an abstract framework that may be used in order to generate the solution to variational inequalities in Hilbert spaces via the application of an iterative procedure. On particular set of techniques that I shall consider include multiplicative Schwartz methods as have previously been applied to the simple case of elliptic linear problems (see GeometryRelatedConvergenceResults:1990, ComplementarityModels:1990 and SensitivityAnalysis:1990). I shall also consider whether the iterative procedure outlined can be applied to Banach spaces in general. In my conclusion, I summarise the techniques of this paper via a considered convergence analysis of such techniques.

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CP2

Parallel, Effective, and Robust Preconditioning Based on Incomplete Factorization

We present practical enhancements to significantly improve the robustness and effectiveness of threshold-based incomplete Cholesky factorization as a preconditioning technique for symmetric positive-definite and mildly indefinite (i.e., with few negative eigenvalues relative to the rank) sparse systems of linear equations. Experimental data on a suite of industrial problems for memory and CPU-time consumption and parallel scalability is presented and compared with that for various preconditioners in well-known packages such as PETSc, Trilinos, Hypre, and pARMS, etc.

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[1]A geometric interpretation of the variational inequalities problem is that we seek x^* with the property that $F(x^*)$ shall be 'orthogonal' to the feasible region of $K \subseteq R^n$. Where, of course, I make free use of the notion of 'orthogonal', in this case - a more accurate and intuitive description is that $F(x^*)$ contains an orthogonal component not within $K \subseteq R^n$. This aids the general interpretation of Variational Inequality Problems and their applications within several fields of Mathematics.

CP2

Geometrical Frame-Work for Modeling Non-Linear Flows in Porous Media, and Its Applications in Engineering.

The current study is focused on the discovery of a new relationship between flows in porous media and geometric surfaces with modified scaled metrics. Using fundamental geometric methods, we have proved the existence of a nonlinear scaling operator which relates constant mean curvature surfaces and pressure distribution graphs constrained by the Darcy-Forchheimer law. The hereby obtained properties of fast flows and their geometric interpretation can be used as analytical tools to evaluate basic technological parameters in reservoir engineering.

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CP2

Multi-Scale Analysis of Coherent Structures in Turbulent Dynamics

Viscoelasticity modifies turbulence leading to such effects as drag reduction. In this work we examine the role of large-scale coherent structures in turbulence and drag reduction [K. D. Housiadas, A. N. Beris, and R. A. Handler. Phys.Fluids, 17:035106, 2005]. We project Direct Numerical Simulations (DNS) results onto the corresponding Karhunen-Loeve (K-L) modes, the variations and correlations of which are then studied to explore the possibility of low-order models of viscoelastic turbulence.

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CP2

Analytic Solution of Two-Dimensional Transient Heat Conduction Problem for Axisymmetric Cylinder

To the convective heat transfer in the cylindrical coordinate system, it was no solution that the boundary condition was both non-homogeneous, such as the steam temperatures of the cylinder inside and outside were different. A method was presented to solve the problem in this paper. An equivalent coefficient of convective heat transfer (ECCHT) was defined. Using the ECCHT, the non-homogeneous boundaries were transformed to homogeneous boundaries, and the equation of heat conduction could be solved. At the

same boundary condition, it was carried through that calculation by the ECCHT method and simulation by ANSYS. The results of calculation and simulation are consistent, and the opposite errors attenuate less than 5% quickly.

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CP3

Elliptic Grid Generator with Adaptive Control Functions

A new formulation to generate two-dimensional boundary conforming structured grids is developed. The new algorithm is designed to regulate and homogenize the jacobian at the grid points. As a consequence, two main grid properties are inherited. First, the capacity to conform boundaries with severe singularities without self-overlapping of the mesh points. Second, the ability to bound the cell-size within certain limits. The new method will drive the size of the cells closer to the average cell-size over the entire domain. In contrast with other elliptic grid generators, the control functions are held as dependent variables. They are automatically adjusted through the homogenization of the jacobian to match the geometry described by the physical boundaries of the domain. The new algorithm is successfully tested over a variety of multiply connected domains. Numerical experiments show that the smoothness and the cell-size uniformity improve the stability of explicit time-dependent simulations, and result in accurate numerical solutions in vibration and scattering problems at low computational cost.

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CP3

Automatic Conversion of Conceptual Geometry to Cfd Geometry for Aircraft Design

Conceptual aircraft design is usually based on simple analysis codes. Its objective is to provide an overall system performance of the developed concept, while preliminary aircraft design uses high-fidelity analysis tools such as computational fluid dynamics (CFD) analysis codes or finite element structural analysis codes. In some applications, such as low-boom supersonic concept development, it is important to be able to explore a variety of drastically different configurations while using CFD analysis to check whether a given configuration can be tailored to have a low-boom ground signature. It poses an extremely challenging problem of integrating CFD analysis in conceptual design. This presentation will discuss a computer code, called iPatch, for automatic conversion of conceptual geometry to CFD geometry.

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CP3

Computational Topology for the Film Industry

How did mathematical modeling of engineering tolerances lead to applications in animation? In short, the answer is the power of appropriate mathematical abstraction. The history, science and application of this process will be presented.

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CP3

Modeling-Based Minimization of time-to-uniformity in Microwave Heating Systems

A fundamental problem of microwave thermal processing of materials is the intrinsic non-uniformity of the resulting internal heating pattern. The paper outlines a general technique for solving this problem by using comprehensive numerical modeling to determine the optimal process guaranteeing uniformity. The model relies on an iterative 3D FDTD solution of the coupled (electromagnetic wave propagation and heat diffusion) boundary value problem. The algorithm is implemented as a collection of MATLAB scripts producing a description of the optimal microwave heating process along with the final 3D temperature field. The functionality of the proposed optimization is illustrated by several computational experiments.

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CP4

Blood Pressure and Blood Flow Variation During Hyperventilation

Short-term cardio-respiratory responses to ventilation changes require complex autonomic and autoregulatory interactions. We present a model that attempts to predict dynamic changes in beat-to-beat arterial blood pressure, middle cerebral artery blood flow, and expiratory carbon dioxide during voluntary hyperventilation, accounting for such interactions. An inverse least-squares problem formulated to identify model parameters specific to an individual patient time series validates the model by minimizing the error between the model and data.

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CP4

Dynamic Analysis of Drug-Induced Ventricular Repolarization Effects in Ambulatory Patients

Drug-induced QT-interval prolongation has become a major economic and health issue in the pharmaceutical industry. Little has been done to link analytically the QT-interval prolongation and the risk of torsades de pointes, a potentially fatal arrhythmia. This presentation introduces a dynamic approach to modeling the changes in QT-intervals from a 24-hour electrocardiograph in ambulatory patients. The similarities and differences between the model behavior and the physiology literature are compared. Results from selected cases are reviewed.

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CP4

Modeling Glioblastoma Treatments

Glioblastoma is a type of malignant brain tumor which accounts for 30 percent of all brain tumors in adults. Current treatments of glioblastoma include surgery, radiation and chemotherapy. In this talk, we develop mathematical models to analyze the efficacy of these treatments. Numerical simulation is performed to study the long term behavior of the tumor growth under different therapies. We compare our results with clinical measurements. We also discuss some challenges, as well as possible improvements, of these tumor treatments.

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CP4

Self-Organization of Spiral and Scroll Waves in 2D and 3D Excitable Media

We review our previous results for the spontaneous formation of stable multi-armed spirals in 2D excitable media and share new findings for the spontaneous formation of persisting multi-armed scroll waves in 3D excitable media, represented by a variety of alternative models. Such higher-frequency multi-armed structures are an amazing example of excitable media capacity to advanced self-organization. These findings were made possible by Linux cluster supercomputing and may be relevant to cardiac defibrillation research.

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CP4

Mathemtical Problems in Electrostatic Mediated Molecular Diffusion

Diffusion is one of the most fundamental mechanisms of molecular transport in living cells. Electrostatics plays an extremely important role in mediating the diffusion involved in cell signaling. Poisson-Nernst-Planck (PNP) equations are usually employed to describe the electrostatic mediated diffusion. In this talk I will present a number of critical mathematical problems in the modeling and the numerical solution of PNP equations, and discuss the biological implications of these mathematical treatments.

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CP5

Biologically Inspired Hybrid Algorithms for the Solution of Nonlinear Systems of Equations

Although the difficulties associated to the solution of nonlinear systems of equations are amplified as the number of equations increases, there are not uncommon nonlinear systems of difficult solution by traditional numerical techniques with ten or less equations. In this work, a different, biologically-inspired hybrid approach is used to solve nonlinear systems. The parallelization of the proposed hybrid algorithms on computer clusters is also investigated. The experimental results obtained show the effectiveness of this approach.

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CP5

Limiting Availability of a One-Unit System Backed by a Spare under Repair Or Preventive Maintenance

We consider a one-unit system under continuous monitoring, aided by an identical spare unit and serviced by a facility that performs repair on a failed unit or preventive maintenance on a recalled unit making it as good as new. We find the distribution of the system up time and down time when lifetime, recall time and service times have arbitrary probability density functions. Hence, we obtain the limiting availability of the system.

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CP5

Efficient Transient Noise Analysis in Circuit Simulation

We discuss adaptive linear multi-step methods for the numerical integration of stochastic differential-algebraic equations(SDAEs), and study their mean-square convergence. SDAEs arise as a model for electrical network equations that are influenced by additional sources of Gaussian white noise. For small noise we present a strategy for controlling time and chance discretization. It is based on estimating the mean-square local errors by calculating the optimal number of computed paths and results in a solution path tree.

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CP5
The Statistical Mechanics of the Learning Curve

A foundational theory of the learning curve is proposed based on information theory and statistical mechanics. The motivation for this theory is the since statistical mechanics is the primary model for learning rates in the artificial intelligence context, it is appropriate for a general theory of learning. This theory is found to match the form of actual data better than the previous models.

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MS1
Clinical Utility of QEEG in Neuropsychiatric Disorders

The clinical utility of EEG has been greatly enhanced by the use of quantitative methods which describe abnormal brain function as statistical deviations from age expected normal vales. Using such an approach to describe electrophysiological heterogeneity within clinically homogeneous diagnostic groups has led to improvements in diagnosis, treatment outcome and prediction of evolution of disorders. Application of source localization algorithms allows the study of the underlying pathophysiology of the subtypes identified from the scalp recorded data.

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MS1
Modeling Cortical Rhythms in Schizophrenia

Schizophrenia symptoms may indicate impairment constructing neural cell assemblies during sensory processing, for which the gamma and beta frequency bands (15-70Hz) are believed relevant. Experimental examination of auditory entrainment indicates control subjects favor 40Hz response to 20Hz and 40Hz stimuli while schizophrenic subjects favor a 20 Hz response. We have simulated auditory entrainment based on evidence of altered inhibition. Study of a one-parameter family of discontinuous discrete maps indicates schizophrenic network 20Hz response is robust.

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MS1
EEG for Biomarkers

Cortical responses to drugs acting on the nervous system can be non-invasively recorded from electrodes on the scalp as electroencephalographic (EEG) data. EEG evidence of sleep, wake, cognitive engagement and anesthetic dissociation is remarkably similar across mammalian species. We will discuss our efforts to develop EEG biomarkers and to build a high-throughput, automated EEG feature extraction and statistical analysis program for use in translational (pre-clinical to clinical) drug discovery.

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MS2
Title not available at time of publication.

Abstract not available at time of publication.

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MS2
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MS2
Modeling HCV Antivirals

Hepatitis C affects between 4 and 5 million people in the United States with nearly 75% suffering chronic infection. Further, current estimates indicate 170 million people are infected, worldwide, with the Hepatitis C virus (HCV). Pegylated interferon and ribavirin combination therapy is currently the standard of care for treatment of HCV but is considered less than optimal. For example, sustained virologic response (SVR) for genotype 1 virus is observed in pivotal clinical trials for only 54% of treated patients. SVR is defined as undetectable HCV RNA in plasma on the order of 6 months after cessation of treatment. This combination therapy is also associated with a high incidence of significant side effects suffered over a treatment interval of at least six months. Identification of better treatment alternatives is the goal of a vigorous antiviral program at Merck. In this talk we describe mathematical models explaining HCV infection and response to treatment. The model equations and resultant simulations were chiefly derived from the literature. Simulations have already provided support for the antiviral drug development program at Merck. Mathematical modeling gives evidence of target engagement and drug efficacy. Using accumulated simulation experience gained from basic research, preclinical data, and the literature, design optimizations for early clinical studies may be proposed. As internal modeling expertise is enhanced by experience gained in early development, this mathematical knowledgebase may help optimize costly phase III trials by guiding key decisions such as dose selection and length of dosing.

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MS3
Parametric Study on the Effect of Weld Misalignment on the Local Buckling Response of Pipelines

The demand for oil and natural gas resources has seen continuous growth. Pipelines are vital elements used for the transportation of oil and gas from field to consumption regions or exporting ports. Therefore, it is essential to understand the reliability and the integrity of these pipelines. The mechanical behavior of shell structures, like pipelines, is imperfection sensitive. The presence of initial geometric or material imperfections can significantly reduce the pipeline load and deformation capacity. This paper deals with initial geometric misalignment imperfections that may be present due to the girth welding process when connecting pipeline segments. This investigation was conducted using finite element methods to assess the effects of internal pressure, axial force, misalignment amplitude, and misalignment orientation on the local buckling response of pipelines. Through this parametric analysis, the moment-curvature response and variation in section geometry with increasing curvature was examined. Simplified design curves for peak moment and its corresponding limit strain were constructed as functions of internal pressure, axial force, and misalignment amplitude and orientation. This sensitivity study concludes that misalignment imperfection considerably affects the pipeline load and strain capacity.

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MS3
Establishing a Successful Internship Network

Mr. Baird was hired from industry to join MITACS in the summer of 2005. The internship program in Atlantic Canada the region which was to become Mr. Bairds responsibility was launched in April 2005. In this presentation, Mr. Baird will discuss how he approached the tasks of building an awareness of the MITACS internship program within the universities and industry in the region, and how these two disparate groups were brought together to engage in collaborative, applied research. Examples of early successes will be discussed, as well as the feedback from students, professors, and industry partners. Successes in the retention of Highly Qualified Personnel (HQP), both regionally and nationally, will be presented. Mr. Baird will also touch on the new directions which the program has taken in the last 12 months, and future opportunities.

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MS3
Industry perspective of internship program - title and speaker information not available at time of publication

Abstract not available at time of publication.

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MS4
Re-gridding Techniques for Non-Cartesian MRI

The MRI community has shown that a great variety of benefits can be obtained when collecting data along non-Cartesian trajectories, such as decreased scan time and reduced sensitivity to motion and displacement. The fast Fourier transform (FFT) is used to reconstruct MRI data from Cartesian grids. Regridding from non-Cartesian to Cartesian coordinates in k-space and the subsequent FFT has been somewhat successful in reconstructing images, however, the numerical analysis of these methods is not completely understood. This talk discusses advances in non-Cartesian FFTs in a mathematical framework and proposes new methods that would enhance convergence to the underlying "true" solution.

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MS4

Off-Resonance Correction in Spiral MRI

Spiral scanning is a rapid MRI method that collects data along interleaved spiral trajectories in k-space. Off-resonance effects lead to image blurring in spiral scanning, if not corrected for during image reconstruction. If the off-resonance varies slowly enough, conjugate phase reconstruction can correct for these effects, although it requires significant computation. A number of fast approximations have been developed, including frequency segmentation and polynomial approximations. For more rapid frequency variations, modeling approaches show promise.

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MS4

NonCartesian Sampling in MRI; Rationale, Challenges, and Examples

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MS5

Meshless Discrete Galerkin Methods for Polymer Chemistry

Abstract not available at time of publication.

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MS5

Efficient Simulation of Polymerization Processes with several Property Indices

The talk will demonstrate how to construct models and associated simulation tools that allow to seamlessly integrate algorithms for simulating nano-properties into professional software for modelling polymerization processes. The key idea is to device a stochastic/deterministic hybrid model along the lines of a stochastic generalization of the quadrature method of moments: moments of architecture indices computed via Monte-Carlo simulations are to be coupled into otherwise deterministic differential equations, e.g., for size distribution.

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MS5

Nested Stochastic Simulation Algorithm for Chemical Kinetic Systems

Abstract not available at time of publication.

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MS5

Emulsion Polymerization as an Example for Sophisticated Product Design on a Nano-scale

The mathematical description of *emulsion polymerization* - a process aiming at specialized polymer materials - is particularly interesting, since a careful modeling requires a combination of different approaches and scales (polymers as chains *within* particles). This leads to a mixture of high-dimensional systems of ordinary and partial differential equations linked to thermodynamics and chemical kinetics. For the simulation of such processes within a realistic time scale, several modelling steps and sophisticated numerical methods have to be applied. The talk provides an overview on actual developments.

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MS6

Industrial Mathematics Clinics at the Claremont Colleges

The 3-year CGU-Boeing Mathematics-Industry Projects are supported by an NSF grant (PI: Ali Nadim). This year, the team (Michael Franklin (team leader), Garret Hechel, Eric Johnson, Prof. Weiqing Gu (faculty adviser), Prof. Ali Nadim (consultant), Dr. Thomas Grandine (Boeing liaison)) is investigating the use of weighted extended B-splines (WEB-splines) as a basis for the finite element method. Traditionally the finite element method involves creating a mesh grid to discretize the domain of the problem which adheres closely to the boundary. This is a very time consuming and memory intensive step in the process. WEB-splines alleviate the need to create a mesh grid, and rely upon a uniform grid across the domain. This fact, in addition to the approximation properties of B-splines make the method highly desirable alternative to more traditional finite elements.

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MS6

The Challenges of Starting a PSM Program in Industrial Mathematics

The PSM program in Industrial Mathematics at the University of Northern Iowa was officially approved by the Iowa Board of Regents in March of 2006. This followed more than two years of planning and development, which included support provided by the Sloan Foundation and administered by the Council of Graduate Schools. Initial program offerings were made in Fall 2006, with the first full cohort of students to begin in Fall 2007. The talk will focus on successes and failures, dos and don'ts, the role of the external advisory board, the importance of finding appropriate industry contacts, ways in which resources have been found in support of the program, and so on.

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MS6

Graduate Student Mathematical Modeling Camp and the MPI Workshop

Rensselaer's GSMM Camp is a week-long meeting held annually in June. At the Camp, graduate students work together in teams, with the guidance of a faculty mentor, on highly interdisciplinary problems inspired by industrial applications. The graduate student who attend the Camp also attend the MPI Workshop held at a participating university during the following week. There, the graduate student teams are joined by faculty, postdocs and visiting scientists all working together on problems brought by representatives from industry. The combined program promotes a broad range of problem-solving and scientific communication skills, and provides the graduate students with a valuable educational and career-enhancing experience outside of the traditional academic setting. The talk will focus on the organization and challenges of the program, and will highlight further opportunities for academic-industry collaborations.

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MS6

Professional Science Master's (PSM) Program in Industrial Mathematics at MSU

The PSM degrees provide graduates with an opportunity of rewarding career paths. The goal of our industrial mathematics program is to produce generalized problem solvers of versatility, capable of moving within an organization. One core course requires students to spend the spring semester working on real-world problems proposed by local industries. We have a history of 50 successfully completed projects and case studies will be given to highlight MSU's PSM program in industrial mathematics.

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MS7

A Graphical Analysis of fMRI Predicts Global Functional Architecture of Neocortex

We demonstrate that the topological structure of functional brain networks can be represented statistically by a simple physical model based on a spin system; moreover, the model parameters are determined by both local and global properties of the networks. We also show that the topology has a dramatic impact on the dynamics of the networks, as it significantly reduces the number of feedback loops and increases the stability of the corresponding dynamical systems.

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MS7

Multi-scale Models of Neocortical Self-organization Predict Tissue Structure from Information Theoretic Objectives

Primate primary visual cortex is a topographic map of sparse-coding receptive fields. Here we present a model of neocortex that implements a neural multigrid and approximates an infomax optimization in a locally connected network to generate receptive fields and topographic maps comparable to those found in neocortex. Our implementation exploits the neural multigrid to estimate covariance between outputs that are not connected, and controls learning automatically based on formal relationships between evolved modes of the infomax solution.

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MS7

Cytoarchitectural Models of Neocortex Predict Mechanisms of Microcircuit Development

Simulating the structure of neural tissue requires composing at minimum 10,000 models of anatomical structures known as neurons within a confined geometrical space. We present a method for simulating the growth of neuronal processes within these structural models. Our method avoids physical overlap between neural processes while preserving neural structures taken from real tissue. We show that neural development can be simulated and neural circuits analyzed using simulation techniques from molecular dynamics.

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MS7

Parallel Decompositions of Hodgkin-Huxley Permit Rapid Execution of Complex Circuit Simulations Using Multi-threaded, Multi-processor Systems

We present a method for decomposing and distributing large-scale, Hodgkin-Huxley type neuronal computations across large numbers of processors. Using an implementation of the classic Hodgkin-Huxley model extended to large numbers of interacting neurons, we show the feasibility of this approach, including scaling, and discuss its use in multi-threaded environments containing large numbers of processors with multiple cores. Our results demonstrate that fine-grained distribution of neuronal computations is a feasible approach to large-scale, Hodgkin-Huxley type calculations.

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MS8

Multiscale Models of Tumors

The multiscale model includes gene mutations, densities of cell populations, and the running time of cells in each phase of the cell cycle. The model is formulated as a free boundary problem for a coupled system of PDEs: many hyperbolic equations and several diffusion equations. We shall also present simplified models where much more can be said about the shape of the tumor and the development of instabilities.

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MS8

Mathematical Modeling of Neointimal Hyperplasia in Hemodialysis Patients

Hemodialysis vascular access complications due to progressive intimal hyperplasia (IH) remains the most common cause of morbidity/hospitalization among dialysis patients worldwide. Mathematical modeling is used to understand the influence of oxidative stress and turbulent flow on the IH formation, to predict vascular access failure, and more important, to explore innovative therapies for IH target various growth factors that facilitate migration/proliferation of various cellular phenotypes involved, delaying/preventing IH formation.

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MS8

A Hybrid Model of Tumor Spheroid Growth

Multicellular tumor spheroids are made of three layers with different mechanical properties, i.e. proliferating outer layer, quiescent middle zone, and necrotic zone. Helmlinger et al (1997)'s experiment showed that tumor growth can be regulated by stress and that mechanical properties of the outer gel, such as stiffness, can inhibit tumor growth in vitro. Using the cell-based model on the proliferating zone, continuum model on other regions, and reaction-diffusion model for nutrients on whole domain, I investigate the stress effect on tumor growth.

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MS8

A Mathematical Model on the Role of Oxygen in Dermal Wound Angiogenesis

Angiogenesis is the formation of blood vessels from existing blood vessels. Oxygen plays a central role in the angiogenesis of dermal wound healing. Experimentally, small deviations of oxygen tension from the normoxic state aid in the angiogenic response of the wound. I will present a mathematical model, which describes the role of oxygen in angiogenesis for a dermal, excisional wound. Computational simulations of our model illustrating experimentally-derived angiogenic responses of the wound will be presented.

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MS9

Application of Math-Based Analytical Methods in Vehicle Crashworthiness Design

Automotive vehicle design from a crashworthiness and occupant crash protection perspective is an important part of the overall vehicle product development cycle. Federal Motor Vehicle Safety Administration (FMVSS) regulations are extensive and cover many aspects of vehicle crash safety: crash characteristics, vehicle systems and sub-systems, environment, injury assessment tools and injury risk. The product development phase is very time consuming, resource intensive and costly. As a result, math-based analytical tools are rigorously used early in the process to minimize expensive physical testing and validation efforts. The computer-aided-engineering tools (CAE) are based on fundamental principles of structural and material mechanics, impact biomechanics and injury risk assessment; vehicle interior restraint system design and optimization typically make use of stochastic methods to identify a robust design space. From a mathematics standpoint, for linear static finite element analysis, stiffness matrices are determined and solved for unknowns; for large deformation, non-linear dynamic finite element analysis, the problem is formulated using the Lagrangian and the equations of motion are solved using numerical integration methods such as Central Difference Method; explicit time integration is the preferred calculation methodology for the Central Difference Method. In the multi-body dynamics analysis utilized for crash test dummy modeling, the equations of motion (Newton-Euler) are generated and the subsequent system of coupled non-linear second order differential equations are solved using numerical methods such as: modified Euler method with a fixed or variable time step, Runge-Kutta method with a fixed or variable time step, Runge-Kutta Merson method with a variable time step. The injury criteria are developed using experimental data and statistical approaches such as logistic regression to develop the injury risk model to tie experimental data to mechanical responses (loads, accelerations) from the anthropomorphic test devices.

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MS9

Advances in Computational Stochastic Mechanics and Reliability Prediction for Ground Vehicles

The presentation will discuss an innovative vehicle reliability approach for military vehicles that employs the most recent advances in engineering and numerical analysis software using high-performance computing. The proposed reliability approach uses a fast stochastic physics-based model simulation, including finite element and progressive damage models that is integrated with refined stochastic response approximation techniques based on high-order stochastic field models. Bayesian framework is applied for handling modeling uncertainties, lack of data and stochastic model updating based on new evidence from test data or field observations. The proposed reliability approach includes the key multi-physics, including interactions between damage mechanisms, such low-cycle-fatigue-high-cycle fatigue and corrosion-fatigue interactions that can affect significantly predicted failure risks. Multi-scale aspects are integrated from the overall vehicle system behavior, to subsystem and component behavior, and down to very local material fracture mechanics behavior. The proposed vehicle reliability approach bases on a fast HPC stochastic finite element analysis technology that uses parallel graph-partitioning and parallel algebraic multi-grid gradient combined with gradient conjugate solvers. The effects of modeling uncertainties, due to finite element modeling and limited number of analysis runs will be discussed.

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MS9

Full Vehicle Reliability with Stochastics

The "holy grail" of current efforts to predict and optimize ground vehicle designs for reliability is the consideration of full vehicle systems with all subsystems and components, in all physical regimes which lead to failure, and with lots of sources of uncertainty being considered. Work done by a team lead out of the Army is making great strides toward this goal, by using the massively parallel capabilities of modern High Performance Computing (HPC) systems. Many significant area of mathematics are involved with this effort.

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MS9

HMMWV Modeling for High Fidelity Dynamics Analysis

A co-simulation approach is proposed to address the increasing multidisciplinary character of ground vehicle virtual prototyping. Unlike current insular approaches in which subsystems are treated in isolation, the virtual prototyping process proposed relies on (a) accurate modeling of subsystems (encapsulation), and (b) seamless co-simulation of these subsystems drawing on established commercial simulation packages (integration). The presentation reports on the system level analysis of an US Army HMMWV that follows the proposed co-simulation paradigm. The vehicle model is represented in ADAMS/Car; the powertrain is modeled in PSAT; the tire is modeled in FTire; finally, the driver and road models rely on ADAMS support.

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MS10

High-Performance Quantum Cascade Laser Modelling and Design

Quantum cascade (QC) lasers are compact high power mid infrared light sources that can be custom tailored for specific wavelengths. High temperature performance of these devices, however, is degraded by thermal effects that reduce gain and limit the maximum output power. In this talk we will present experimental results and a self-consistent thermal-optical-quantum model of QC lasers that can be used to understand and design high-performance QC lasers.

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MS10

Computational Aspects of the Design of Mid-infrared Quantum Cascade Lasers

Active region of Quantum Cascade Lasers (QCL) contains many periods, each period in turn consisting of up to 30 semiconductor layers. Thus the eigenvalue problem is computationally intensive. Usually the issue is circumvented by truncating the problem to a few periods. In this talk I will explain why truncating leads to large errors in determining the position of excited levels and explore strategies that give a good precision while reducing the computational intensity.

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MS10
Modelocking in Quantum Cascade Lasers

Work to date on modelocking in quantum cascade lasers will be reviewed. Both active and passive modelocking will be covered.

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MS10
Computational Modeling of Quartz-Enhanced Photoacoustic Spectroscopy (qepas) Sensors

We will describe a computational model of the QEPAS sensor currently being developed by the Laser Science Group at Rice University. This sensor will offer optical and chemical sensing capabilities for environmental monitoring, homeland security and medical diagnostics. Our goal is to understand the sensitivity of the sensor to the modulation frequency of the laser. Pressure waves generated from conversion of laser heat are modeled via the acoustic wave equation.

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MS11
Adaptive Approximations of Curves and Surfaces

Let c denote a non-self-intersecting C^3 curve that is an image of $[0,1]$ and is embedded in $\Re^3$. For visualization in chemistry and biology, it is desirable to select a finite open cover of c that supports efficient approximation algorithms. A method for defining a particular open cover that is locally adaptive to curvature is presented. The notion of discrepancy will be discussed for generalizing to surface patches.

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MS11
A Knot Computation Using Newton's Method

Typical methods for spline curve approximation, via subdivision or piecewise-linear interpolation, are critical for display and analysis of such curves. It is desirable to know if such approximations are topologically equivalent to the curve they are approximating. Examples will first be given to show that, without any pre-determined constraints, these curve approximations can easily lead to incorrect topology in terms of a measure useful in contemporary knot theory. Discussions of a tractable algorithm using Newton's method for computing such constraints and how this method can be integrated into an industrial environment will be provided, along with animations of the algorithm in action.

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MS11
Simulation Topology – An Overview

The intuitively pleasing mathematics of knot theory will be used to motivate discussions of simulations for the life sciences. This will lead to importance of the emergence of computational topology for fundamentally new algorithmic paradigms in both scientific and engineering simulations. An open challenge within the high performance computing industry is to achieve performance and accuracy appropriate for computer-assisted open-heart surgery.

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MS11
Low Discrepancy Sets for Efficient Computation on Manifolds

We will discuss the application of low discrepancy point sets to such problems as efficiently obtaining linear approximations and covers of low-dimensional manifolds. The principal novelty is replacement of uniform sampling methods with methods depending on low-discrepancy sets and exploration of the relationship between discrepancy and curvature. This generalizes recent work on adaptive approximation of smooth curves.

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MS12
Powder Modeling Challenges From a Pharmaceutical Industry Perspective

Powders are an integral part of various processes in multiple industries. Compared to fluids, gases and solids, granular materials are the least understood, exhibit a wide array of behaviors and are harder to model primarily due to the huge computational requirements. Powder modeling is an exciting, promising and challenging field for computational research. This talk will give a brief overview of the main powder modeling techniques. We will then focus on the challenges from a pharmaceutical industry perspective: multi-scale nature, polydispersity, numerical accuracy, parameter estimation and the differences in physical properties of each drug substance.

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MS12

Controlling Particle Mixing and Segregation: Exploiting Cohesion and Flow Modulation

Segregation or unmixing of particles is a common occurrence whenever the particles have a distribution of properties. Recently, we have used computer simulations (DEM-based), to devise ways to control segregation. Specifically, we have determined that cohesion, both due to van der Waals forces and liquid bridges, can be used either to cause or prevent segregation. Also, by introducing carefully chosen flow perturbations it is possible to eliminate segregation in a much more general way (spanning both free-flowing and cohesive systems). Advances using both of these techniques will be discussed.

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MS12

Powder Flow: Scale Coupling and History Effects

Two central problem pose substantial challenges to the development of effective modeling approaches for flow processes involving cohesive powders (i.e., the great majority of relevant systems). A major problem is that there are multiple scales that cannot be easily decoupled: the particle scale, the "lump" scale determined by the interplay of interparticle forces and shear rates, and the scales imposed by system geometry. Inmost relevant systems, these scales are too close to each other to allow effective decoupling, thus limiting the application of continuum models. A second major issue hindering the modeling of such systems is that adhesive forces provide strong quenching of local microstructures, resulting in wide distributions of local densities and local yield strengths. As a result, flow behavior is strongly dependent on strain histories, that, different than classic non-newtonian fluids, do not relax espontaneously. Besides being fascinating mind teasers, these intrinsic characteristics of cohesive powders have important practical consequences: very limited capabilities for modeling, difficulties in understanding factors of scale, and lack of predictability of powder flow processes both in industry and in nature.

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MS12

Computational Studies of Jamming in Model Powders

We investigate the jamming transition in model frictionless powders with short-range attractive interactions by performing extensive discrete element simulations. In contrast to model granular systems with purely repulsive interactions, we find that these systems can possess three distinct regimes of mechanical response—completely floppy, partially rigid, and completely rigid behavior—separated by two critical phase transitions. We characterize the structural and mechanical properties of these model powders and compare our results to those found previously for percolation and rigidity percolation transitions in colloidal gels and other weakly attractive systems.

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MS13

Toward 4D PET Image Reconstruction

Positron emission tomography (PET) provides quantitative dynamic images of radiotracer concentration. Combined with tracer kinetic modeling, parametric images of physiological parameters can be obtained. Conventionally, this analysis is performed as separate steps of image reconstruction followed by kinetic analysis. The more theoretically ideal approach is 4-D reconstruction, i.e., direct creation of parametric images of kinetic parameters from PET data. The presentation will discuss the likely advantages and the computational challenges of 4D PET reconstruction.

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MS13

Ultra Fast Fully 3D PET Reconstruction

In high resolution PET scanners, obtaining one set of reconstructed images requires many hours of image reconstruction. To remedy this reconstruction problem, we developed a new algorithm based on the symmetry and SIMD projection-backprojection (SSP) in 3D PET reconstruction. Image reconstruction time is reduced from 5 hours to 4 minutes by using SSP. The details of the technique will be discussed and an example of the application to the HRRT will be presented.

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MS13

Group Discussion

Group discussion.

All Participants
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MS13

Opportunities and Challenges for Improved HRRT PET Reconstruction Quality and Performance us-

ing the Blue Gene/L Supercomputer

HRRT PET scanners have nearly 120,000 crystals and 4.5 billion potential lines of response. This dramatic increase in information over traditional PET scanners produces both higher resolution images and tremendous computational burdens. The Blue Gene/L supercomputer provides both opportunities and challenges for addressing these burdens and improving reconstruction quality and performance. A Blue Gene/L refactorization of a reconstruction algorithm and an approach for accommodating subject movement are detailed. Improved reconstruction and performance results are presented.

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MS13
Introduction

Introduction.

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MS14
Semi-Automated Doppler Toolbox for Integrated Hemodynamic Analysis

The utility of an automated Doppler analysis system is significant in both clinical and research settings. Elimination of subjective bias through automation yields greater precision and accuracy than standard methods in obtaining the recorded Doppler velocity. Here we describe a semi-automated method to extract Doppler peak velocity waveforms and calculate pertinent clinical and experimental hemodynamic biomarkers. When integrated with ECG, respiration and pressure data, this toolbox gives a detailed picture of both cardiac and vascular responses to medical interventions.

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MS14
Models and Devices for Diagnostic and Therapeutic Applications to Hypertension

Identification of mechanisms and markers for hypertension etiology and effective treatment often require use of mathematical models. Linear and nonlinear models-derived pulse transmission and arterio-ventricular wall parameters from pulsatile pressure and flow are used to analyze isolated systolic hypertension, hypertension, and that compounded with aortic valve stenosis. Results show various hypertensions differ, depending on extent of parametric alterations. Therapeutic anti-hypertensive drugs are more effective when aimed at reverting such parametric changes towards normal levels.

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MS14
Modeling Cerebral Blood Flow Regulation During Postural Change from Sitting to Standing

When standing up, blood is pooled in the legs due to the effect of gravity resulting in a drop in systemic arterial pressure and widening of the blood flow velocity. To restore blood pressure and blood flow velocity a number of regulatory mechanisms are activated. The most important mechanisms are autonomic reflexes mediated by the sympathetic nervous system and cerebral autoregulation mediated by changes in concentrations of oxygen and carbon dioxide. The response to standing is an increase in nervous activity, which results in increased heart rate and cardiac contractility, vasoconstriction of the systemic arterioles, and changes in unstressed volume and venous compliance. The response by the cerebral autoregulation is to dilate arterioles in the cerebral vascular bed. In this work we present a mathematical model predicting these regulaotry mechanisms and show how this model can be validated against experimental blood pressure and flow data.

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MS14
Mathematical Models of Flow in Elastic Tubes

Three-dimensional computer models have been developed to simulate fluid flow though an elastic tube. The models are based on the immersed boundary method, which is designed to handle a flexible elastic boundary immersed in fluid. In one model, the tube simulation involves a fiber-wound elastic tube subjected to an upstream pressure, a downstream pressure, and an external pressure. Such models may be applied to cardio-pulmonary studies.

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MS15

Analysis of Chemical-Mechanical Polishing via Elastohydrodynamic Lubrication (Araca)

Chemical-mechanical polishing is a process used to make the surfaces of silicon wafers used in microprocessors sufficiently smooth and level. A material pad is rubbed against the wafer's surface in the presence of a liquid slurry containing fine abrasive particles. The asperities on the pad flatten under the applied load, and the particles aid in smoothing the wafer's surface. We present a mathematical model for the wet contact problem and look at the heat transfer processes taking place.

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MS15

Enhanced Leak Detection (Veeder-Root/Gilbarto)

Regulations require that gasoline delivery systems be tested for leaks after installation using conditions as close to operational as possible. Since any leak is almost invisible relative to environmental noise, this poses significant challenges in devising an effective test strategy. This problem was addressed at the MPI 2005 workshop at WPI by academic researchers collaborating with representatives from Veeder-Root. Ideas included procedures to drive the signal-to-noise ratio higher, forcing the lines at high frequency, and flushing tracer gases or sending an acoustic wave through the insulating space.

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MS15

Backward Diffusion Methods for Digital Halftoning (IBM)

We examine using discrete backward diffusion to produce digital halftones. We formulate our method by considering the Human Visual System norm and approximating the inverse of the blurring operator. The noise introduced by the discrete approximation to backwards diffusion forces the intensity away from uniform values, so that rounding each pixel to black or white can produce a pleasing halftone. We also investigate several possible mobility functions for use in a nonlinear backward diffusion equation for higher quality results.

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MS15

Stability of the Oil-Air Boundary in Fluid Dynamic Bearings of Hard Disk Drives (HitachiGST)

We study the dynamics of the oil-air interface (OAI) (also called meniscus) of the fluid dynamic bearings of hard disk drives in two different contexts. The first investigates when the OAI is located among bearing grooves. We derive a simple analytical expression for the evolution of the OAI of an herringbone-type journal bearing with the assumption that the interfacial shear layer is passive. Numerical experiments in which we include surface tension as a regularization parameter show that large interfacial deflections are possible under operating conditions. The second considers the region local to the interfacial region in the absense of grooves. A linear stability analysis in this shear layer is investigated in the planar limit. We find that for zero Reynolds number no instability exists, but sufficiently large flows result in a linear instability and rotational flow in the fluid near the interfacial region.

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MS17

CRT Response or Nonresponse: Insights Gained from Computational Modelling

Currently, Patients with NYHA class III or IV heart failure with an EF ¡35% and QRS¿120 ms are indicated for CRT. These requirements, originally believed to provide the substrate for response to the therapy, have resulted in a 70% response rate. We are employing a modeling approach

to investigate what factors are responsible for 30% nonresponse. We are focusing on hard (objective) endpoints to define response compared with clinically used soft (subjective) endpoints. The hard endpoint variables include end-systolic volume and tissue synchrony. Factors that impact these variables include 1) the electro-mechanical basis for CRT, 2) impact of myocardial scar and scar location on CRT and 3) impact of lead position on CRT response rate. We have taken a computational approach to this issue and have identified significant differences in global and regional function as infarct size, location and pacing site are altered. Our goal is to develop patient specific models that allow the physician to improve their chances of creating a CRT response.

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MS17

Successes and Challenges Ahead in Multiscale Cardiac Models for Industry

Cardiac modeling has evolved greatly in the last 45 years to improve the level of sophistication and accuracy of mathematical models. Models now include electrophysiology, calcium and other cellular signaling, muscle mechanics, and detailed anatomy. Important challenges yet remain for models to reach their full potential in guiding therapeutic interventions. For example, important heterogeneity exists at subcellular, cell and tissue levels. The speakers will focus on past and future efforts to improve models to meet these challenges in idustry.

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MS17

Mathematical Challenges in Modeling PreClinical Drug Effects

Drug-induced cardiac electrophysiology liability poses a concern for the pharmaceutical industry as several drug withdrawals have occurred in the last decade. By affecting the ion channels, drugs may alter the myocyte action potentials, which, in turn, affect the electrical activity of the heart. This talk will discuss the computational challenges of reconstructing the drug mechanisms as an inverse problem by using an example of a real compound.

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MS17

Challenges in Capturing Spatial Heterogeneity in Heart Models

Abstract not available at time of publication.

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MS18

Patient-Specific Radioiodine Dosage for Graves Disease Using a Computational Model of the Thyroid

Graves' disease, the most common cause of hyperthyroidism, is an autoimmune disorder where the body's immune system excessively stimulates the thyroid gland. The thyroid secretes thyroid hormones which play an important role in the body's metabolism. Graves' patients can suffer serious side effects such as rapid heart rate, nervousness, and heat sensitivity. It is estimated that 2% of women, 8 times the rate of men, will be affected by this disease in their lifetimes. Radioiodine therapy is now the most common treatment protocol of the disease. Traditionally, two different approaches are used: (1) administration of a fixed 131I activity (usually 555 MBq), and (2) administration of a 131I activity whose calculation is based on a fixed thyroid absorbed dose (100-400 Gy is the value reported in literature, without agreement between the researchers). The traditional approaches for computing the required 131I therapeutic dose are the so-called (empirical) Marinelli-Quimby formula and the more recent and probably more used MIRD system. Both require knowledge of the thyroid uptake and the biological half-life of iodine within the thyroid. A great percentage of patients (up to 90%, depending on the thyroid absorbed dose and on the 131I kinetics) treated using one of these two approaches become hypothyroid within a year. Numerous variations of the protocol have been suggested based on different levels of fixed activity or absorbed dose, however, comments that "...it seems impossible to modify [radioiodine therapy] of Graves' disease in such a way as to achieve both early control of hyperthyroidism and low incidence of hypothyroidism" (Reinhardt MJ, Brink I, Joe AY, Von Mallek D, Ezziddin S, Palmedo H, Krause TM, Radioiodine therapy in Graves' disease based on tissue-absorbed dose calculations: effect of pre-treatment thyroid volume on clinical outcome., Eur J Nucl Med Mol Imaging. 2002 29(9):1118-24.). It should come as a surprise that many practitioners aim at a single, large dose to reach hypothyrodism. In this paper we consider a different approach. We propose a new protocol whose goal is to achieve a euthyroid state based on minimal number of measurements required to parameterize the computational model to fit the patient's overall iodine metabolism dynamics and cell death. We describe the rationale behind this approach and present results based on clinical data and simulations.

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MS18

Reconciling the Continuous and Discrete Models of Circadian Oscillator Entrainment

Most organisms contain a functional, light-entrainable oscillator that: (i) produces a persistent rhythm (of near 24-hour period) in constant conditions (such as complete darkness), and (ii) entrains to the environment's light-dark cycle. When entrained, the organism's oscillator phase-locks to the transitions of dawn and dusk, helping to synchronize its processes and activities with the environment. Pioneering circadian scientists Jurgen Aschoff and Colin Pittendrigh each hypothesized models for circadian oscillator entrainment. Aschoff proposed that light intensity continuously modifies oscillator velocity to set phase, while Pittendrigh maintained that discrete transitions of dawn and dusk act to reset the clock. These two hypotheses became known as the continuous and discrete models of entrainment. Aschoff's rule, which allows that constant light intensity speeds-up or slows-down an organism's oscillator, is the mantra of the continuous model, while the phase response curve (PRC) is the symbol of the discrete model. A PRC describes the phase shift an oscillator undergoes when subjected to short light pulses at given phases, and it successfully predicts entrainment to pulsatile entraining stimuli. In this research we reconcile these two different views by introducing a differential equation model of a circadian oscillator that contains elements of both continuous and discrete entrainment. Namely, the model allows light intensity to directly affect oscillator velocity while directly incorporating a PRC. The differential equation's response adheres to Aschoff's rule and its entrainment to pulsatile stimuli is dictated by the PRC. Most interestingly, the model explains how a circadian oscillator entrains to arbitrary light stimuli. The key to reconciliation is to model light pulses using impulse functions. This helps reveal the role of the PRC in an entrainable oscillator, and also allows continuous and pulsatile entraining stimuli to be considered in the same analysis framework. A conclusion of this work is that a continuous model is sufficient to explain entrainment of a circadian oscillator to general zeitgebers. However, the role of Pittendrigh's discrete model remains vital; light pulses probe a circadian oscillator's fundamental behavior, they reveal its PRC, which in turn, plays a central (but not sole) role in entrainment.

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MS18

Dissipative Model for the Regulation of Blood Coagulation: Steady-state Principles

Blood coagulation represents a unique system, in that it is always ready to react to a break in the vascular endothelium so that it can form a clot, while at the same time it avoids spontaneous thrombus formation. A model designed to describe the behavior of coagulation system should address these two points. The coagulation system consists of multiple catalytic steps and includes both negative and positive feedback. If one assumes that the coagulation factors are in constant supply then one need incorporate only the activated factors. Our model simplifies the multiple steps by dealing with the major activated factors that act at the beginning, the middle and the end of the process. In the extrinsic pathway, activated factor VII, indicated as f VIIa, combines with tissue factor, from a disruption of the endothelial layer of the vessels or circulating on small particulate bodies. The tissue factor f VIIa complex catalyzes the activation of factor X to f Xa. Factor Xa then catalyzed the conversion of prothrombin to thrombin (f IIa). Thrombin has multiple activities, its most prominent being the catalytic conversion of fibrinogen to fibrin, which would either form a clot or a thrombus. High concentrations result in significant clot or thrombus formation. At low concentrations of thrombin, not necessarily zero, fibrin monomers are removed faster than it can polymerize into a fibrin clot or thrombus. Other catalytic or cofactor reactions occur around these major features, but in the simplified model we will ignore them. In addition to its catalysis of fibrin formation, thrombin catalyzes the conversion of factor VII to f VIIa. Factor Xa also converts factor VII to VIIa. The activated factor VIIa must be complexed with tissue factor. These two components represent the positive feedbacks in the system. Both factors Xa and thrombin are removed from the system by passive means dependent on their own concentration through contact with anti-thrombin III. Factor Xa complexes with TFPI which then removes VIIa from the system. This step entails a nonlinear negative feedback. Our model consists of a system of three differential equations. The first represents the formation of factor VIIa, the second, of factor Xa and the third of thrombin. One can simplify the calculation by scaling the system so that each constant coefficient is equal to one. Given such simplification, two singularity points occur, one at the origin, and the other when each of the three variables equals 2. One can apply the Hartman-Groban theorem to linearize set of equations and examine the local behavior around each singularity. Near the origin, the three eigenvalues are equal to 0.325 and -1.66 + 0.56i and -1.66-0.56i. Thus, the system is hyperbolic and represents a saddle point. Near the non-zero singularity, the eigenvalues are -0.46, -1.77 + 1.115i and -1.77 1.115i. Thus, this point is also hyperbolic, but represents a sink. These results imply that a very low concentration of activated factors, the system is driven away from the origin to activate more factors. Thus, the system would always be ready to respond to a stimulus. At higher concentrations, the system would be attracted to second singularity, thus the system would never run away on its own. At this second singularity, it could be presumed that any fibrin formed as the result of the presence of thrombin, would be removed faster than it could polymerize.

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MS18

A Computational Model of Acute Response of PTH to Changes in Plasma Ionized Calcium in Hu-

mans

Regulation of calcium ion concentration in blood within a narrow range is crucial for maintaining normal physiology and metabolism in the human body. This is achieved by an intricate system of positive and negative feedback pathways involving calcium, parathyroid hormone (PTH), vitamin D, and phosphate. Low blood calcium stimulates PTH secretion. PTH in turn stimulates bone calcium resorption and active renal reabsorption of calcium. PTH also indirectly stimulates conversion of vitamin D into its metabolically active form, 1,25-dihydroxyvitamin D3, by upregulating the production of renal alpha hydoxylase. 1,25-dihydroxyvitamin D3 upregulates active intestinal calcium absorption and active renal calcium reabsorption. 1,25-dihydroxyvitamin D3 downregulates PTH formation in the parathyroid cells and production of renal alpha hydroxylase enzyme, resulting in downregulation of its own production. Phosphate in high concentrations stimulates PTH secretion but PTH upregulates phosphate clearance through the kidney. Vitamin D upregulates calcium trapping for bone remodeling and intermittent rise in PTH helps in net positive bone formation. This feedback system runs at two time scales: a slow (days to weeks) scale involving calcium fluxes between blood and bone, and a fast (minutes to hours) scale involving all other processes. In this presentation we describe the construction of a detailed computational model of blood calcium homeostasis focusing on the fast time scale aspect by assuming zero net calcium flux between bone and blood. We have used recent molecular-level discoveries and clinical observations to define the overall feedback structure and to parameterize the model. Simulation results using the computational model match well with clinical observations during rapid calcium fluctuations. The aim of the ongoing research is to develop a high-fidelity computational model that describes all the major events in human blood calcium homeostasis and that can be used to predict calcium and PTH levels under different physiological conditions. The model could offer new insights into this complex homeostatic system, suggest hypotheses for focused clinical studies, and ultimately lead to improved protocols. The model can potentially be parameterized based on an individual patient's clinical measurements so that treatment protocols can be adapted to make it patient specific as opposed to be being based on population statistics. Finally, we plan to integrate this model with available bone growth models.

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MS19

Agent-Based Modeling of Carcinogenesis and Therapeutic Resistance

Carcinogenesis and the emergence of therapeutic resistance are processes of natural selection and evolution at the cellular level. Mutations in tumors that provide a reproductive or survival advantage to the cell drive expansions of the mutant cell population in the tumor. This is the basis of both how we get cancer and why it has been so hard to cure. We use agent-based computational models, in which each individual cell (and mutation) is explicitly represented in the data structures, to simulate the evolution of cells in tumors. We have used these models to develop new ideas for cancer prevention and therapeutic strategies that should be less vulnerable to selection for resistant cells than are traditional therapies.

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MS19

Title not available at time of publication.

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MS19

Multiscale Brain Tumor Modeling

This multi-resolution agent-based brain tumor model is designed to investigate how changes on the molecular level can impacting microscopic behavior as well as multicellular patterns. This project is part of CViT.org (http://www.cvit.org ¡http://www.cvit.org/¿).

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MS20

Optimization of the Sierpinski Carpet Fractal Antenna

The Sierpinski Carpet fractal antenna is studied in terms of optimality. A 3D full-wave FDTD model of the structure is developed and used in conjunction with a neural network optimization procedure. An original engineering design based on the idea of a broken fractal geometry is suggested. The modified fractal antennas are shown to have the capability of being optimized, in terms of its input impedence, in a narrow frequency band.

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MS20
Modeling of Torque for Screw Insertion Process

A self-tapping screw is a high-strength one-piece fastener that is driven into preformed holes. We analyze and improve a mathematical model of the self-tapping screw insertion process so that it can be used in manufacturing processes at the BOSE Corporation. We build a Graphical User Interface in MATLAB which allows users to enter fundamental data and produces the corresponding torque curve. The accuracy and robustness of the model is tested by comparing predictions to empirical data collected at BOSE.

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MS20
Vapor Leak Detection for an Underground Storage Tank

This project models the pressure inside the vapor space of a UST. The model takes into account dispensing activities, vapor recovery, evaporation and leaks in the system. Using mass balance, a system of ordinary differential equations is obtained. The equations are solved numerically and two of the variables in the equations are optimized to find the leak rate. Results are tested against data from Veeder-Root Company

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MS20
Modeling Glioblastoma Multiforme

Glioblastoma multiforme (GBM), a highly lethal brain cancer, accounts for over 30 percent of brain tumors in adult patients. Patients typically survive only 12-18 months after diagnosis. Our model describes the dynamics of GBM via a system of partial differential equations for tumor cells, nutrients, toxins, and mechanical resistance of brain matter. Using a 2D conservative Alternating Direction Implicit scheme, we numerically approximate the solution to our model and implement it in C for simulation on a parallel computer.

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MS21
Pharmacovigilance: A View from the Pharmaceutical Industry

Pharmacovigilance is unique in the variety of clinical morbidities under surveillance: adverse drug reactions can have virtually any clinical presentation and range from common to extremely rare phenomena in treated and untreated populations. Traditionally, manual case reviews and quantitative heuristics have been used to screen pharmacovigilance data bases for important safety phenomena. Various quantitative tools can assist in this task, and the use of some of these will be discussed from an industry perspective.

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MS21
Drug Safety Surveillance - Beyond 2X2 Tables

Standard statistical methods for monitoring the safety of marketed drugs focus on large numbers of low-dimensional analyses. In this talk I will argue that high dimensional analyses represent a more satisfactory alternative and are now within computational reach. I will present some sample results from VAERS.

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MS21
A Survey of Current Pharmacovigilance Data Mining Methods

In last several years, data mining methods has received considerable attention as a tool for pharmacovigilance (PV). There has been increasing promotion and use of statistical data mining algorithms (DMAs) in safety surveillance and signal detection processes. The majority of contemporary DMAs are variants of disproportionality analysis based upon 2 x 2 contingency tables. This session provides an overview of various DMAs currently used in PV and the underlying principles, potential benefits and limitations.

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MS21

Measuring the Impact of Non-ideal Data Sources on Pharmacovigilance Analysis

Spontaneous reporting databases like AERS are large, incomplete, and highly heterogeneous, greatly complicating their analysis. This talk illustrates these points with examples and considers some of the consequences, especially the impact of non-obvious incompleteness (e.g., disguised missing data) and heterogeneity (e.g., foreign vs. domestic reports, lawyers vs. consumers vs. physicians, etc.) on analysis results. The question of how to meaningfully assess these effects is considered, and some recently developed assessment tools are described and demonstrated.

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PP0

A Drug-Drug Interaction Parameter Estimation Problem

A two drug interaction is usually predicted by individual drug pharmacokinetic. An innovative drug-drug interaction method based on a three-level hierarchical Bayesian meta-analysis model is developed that includes a Monte Carlo Markov chain pharmacokinetic parameter estimation procedure. Underlying the parameter estimation procedure is a fast integration method of the stiff pharmacokinetic equations. We report the results of the fast integration method and comparisons with standard stiff solvers.

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PP0

Reconstructing Surfaces with Envelopes: A Study Between Theory and Practice

Reconstruction of surfaces with boundary from point data remains a challenge. Recent theoretical advances by the authors define envelopes as surfaces without boundary to approximate those with boundary in order to guarantee ambient isotopic reconstructions. Though practical implementations are still emerging, applications will be relevant for life science simulations such as prosthetic modeling. We present progress toward development of an algorithm that robustly implements this new theorem.

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Implementing the Projected Polyhedron Algorithm for Nurbs Curves Intersections

Computing curve intersections is necessary in a wide variety of applications in Life sciences from protein folding to robotic path planning of medical instruments. The projected polyhedron algorithm is an elegant method for computing roots of polynomials in power basis form; however, the most common curve representation in computer graphics are NURBS. We discuss the care that must be taken to adapt and maintain the efficiency of this algorithm when computing intersections of NURBS curves.

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Adaptive Approximations of Curves

Let c be a C^3 space curve. We determine a family of cylinder which cover the curve and locally approximate the curve. We find as the error tolerance ϵ tends to 0 the number of cylinders approaches $O(\sqrt{\frac{K}{\epsilon}})$ where $K = \int ||c''(t)||dt$. We will also discuss the convergence rates of this limit.

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PP0

Optimizing the Computation of the Gsvd to Improve Performance of Lda Classification

Linear discriminant analysis coupled with the generalized singular value decomposition (LDA/GSVD) performs well in text classification and face recognition, and LDA/GSVD should also perform admirably when classifying medical images. Using the GSVD we are able to overcome the small sample size problem–high dimensional data, low number of observations. Computing the GSVD requires computing various matrix decompositions. This poster exams the optimization of a basic building block of the GSVD using newer hardware.

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PP0

Validation of Semi-Automated Doppler Ultrasound Image Processing to Compute Hemodynamic Biomarkers

Doppler ultrasound imaging of blood flow in rodents supports drug discovery programs. Through laborious manual tracing of the images, hemodynamic parameters such as peak velocity, velocity-time integral, and pulse transit time are extracted. Algorithms are developed to automate this processing and minimize human intervention. Here we compare the automated output with manual measurements using Bland-Altman analysis and other statistical methods, assess precision and accuracy.

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