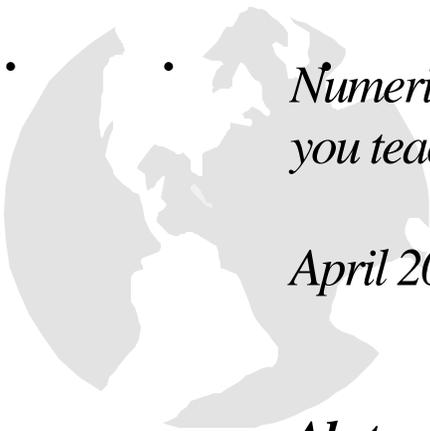




Pavel Bochev (SNL)
Rich Lehoucq (SNL)
Max Gunzburger (FSU)
Amnon (A. J.) Meir (AU)

CSRI Workshop



Numerical PDEs in the 21st century: can you teach new tricks to an old dog?

April 20-22, 2006, Albuquerque, NM

Abstracts



Sandia National Laboratories



Timothy Barth, NASA Ames Research Center

Error Representation for Time Dependent Calculations

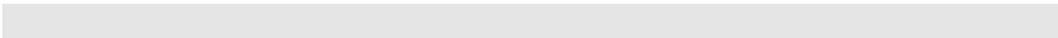
For better or worse, our physical world is constantly evolving in time. Many important physical phenomena depend fundamentally on time either deterministically or through dynamical system behavior. These leads to a multitude of open problems associated with identifying, quantifying, and controlling numerical errors in complex time dependent numerical simulations. For example, in turbulent flow simulations it is well known that the control of pointwise solution errors quickly becomes an insurmountable task as the flow Reynolds number increases but the control of errors occurring in statistics and space-time averaged quantities may still be tractable.

In this presentation, we pursue the representation of numerical solution errors in space-time using standard duality techniques as succinctly described in [1,2]. For quantities of interest that are mathematically described as functionals, these techniques provide the precise relationship between numerical solution errors and weighted combinations of computable element residuals. The goal of this presentation is not to give some precise recounting of this theory, but rather to show the magnitude and structure of terms arising in this error representation formula for "real life" time dependent compressible Navier-Stokes flow problems.

To the novice observer, the magnitude and structure of these error representation terms may not always follow the intuition of the observer. A common mischaracterization of the error representation theory described above is that the residual weights appearing in the error representation formula are directly related to the solution, ϕ of a linearized dual (adjoint) problem. In fact, for Galerkin FE methods the weights actually only depend on $\phi - \pi_h \phi$ where π_h is any projection into the primal numerical approximation space. Consequently, when ϕ exhibits sufficient regularity, the error estimation weights do not depend essentially on ϕ but rather the *derivatives* of ϕ . This has rather profound implications in the representation of solution errors that can sometimes lead one's intuition astray.

The presentation of numerical results will hopefully accentuate the challenges and difficulties in space-time error representation as well as stimulate fruitful discussions addressing the feasibility of genuine error control for time dependent problems.

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[2] R. Becker and R. Rannacher, "An Optimal Control Approach to A-Posteriori Error Estimation in Finite Element Methods, Acta Numerica, 2001.



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Susanne Brenner

Fast Solvers for C^0 Interior Penalty Methods

C^0 interior penalty methods are discontinuous Galerkin methods for fourth order elliptic boundary value problems that have many advantages. In this talk we will first give a brief introduction to C^0 interior penalty methods and then discuss multigrid and domain decomposition methods for solving the resulting systems. We will present convergence results for the V-cycle, W-cycle and F-cycle multigrid algorithms, and also condition number estimates for two-level additive Schwarz preconditioners. Numerical results will also be reported.



John Burns, Virginia Tech

Approximation and numerical methods for design and optimization of PDE systems

The problem of constructing numerical schemes for optimization based design and control of infinite dimensional systems leads to technical and practical issues that are not present if one is interested only in simulation. This observation is often stated in the form:

*An approximation scheme “good for simulation” **may** not be suitable for design, control or optimization.*

Although numerous researchers have noted this point over the past three decades, the interpretation of this statement varies widely from area to area. The basic idea as stated above is rather vague, it is often ignored and sometimes (in certain special cases) it is not valid. However, if this issue is ignored when one develops an approximation scheme for control design and optimization, then the resulting numerical algorithm may not converge to the optimal design and hence fail to produce accurate and useful results. In addition, even if the approximation scheme converges, the resulting finite dimensional problem may be ill conditioned and difficult to solve.

Most numerical schemes for approximating systems governed by partial differential equations (PDEs) developed during the past fifty years has focused on methods that provided convergent and efficient simulations. In recent years, considerable work has been devoted to the problem of constructing numerical and computational methods specifically for design, control and optimization of PDE systems. The applications of these methods are immense in number and include aerodynamic design, flow control, superconductivity, nano-technology, inflatable space structures, control of epidemics, cancer and other biological systems. For example, Gunzburger and co-workers have produced outstanding results in the broad areas of flow control, aerodynamic design and optimization of PDE systems. These results and other recent developments have produced a better understanding of some key theoretical and computational issues that impact this field.

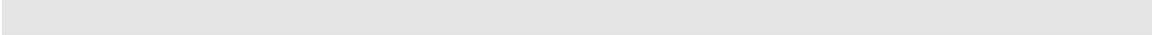
Although it is obvious that one must introduce approximations into the design process at some point in the analysis, it is not always clear at what point approximations should be introduced. Often this issue is stated in terms of “approximate then-design” or “design-then-approximate” approaches. When “approximate-then-design” methods are used, the numerical scheme must produce a finite dimensional design-optimization problem with a (sub)optimal solution. The point here is that in order to develop approximation schemes for design, control and optimization of infinite dimensional PDE systems, one must first ensure that certain design properties are preserved under the approximation. Once this issue is resolved, it is important to consider the problem of numerically solving the finite dimensional problem. In particular, it is possible to construct several numerical schemes that lead

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to finite dimensional design problems with suboptimal solutions, but the resulting finite dimensional problems may differ dramatically in conditioning and computational complexity.

Clearly it is impossible to address all potential issues so we focus on a few of these points and indicate how they impact the construction of practical numerical methods for design and control. In particular, we use the LQR control problem to illustrate the ideas and to clearly identify additional requirements that need to be placed on an approximation scheme to ensure convergence of the optimal designs. Moreover, these requirements also play a role in determining mesh independence of the Kleinman-Newton algorithm. In particular, dual convergence and preservation of exponential stability (POES) play central roles in both convergence and mesh independence.

In this presentation we focus on these issues and suggest areas where the numerical PDE community can have a big impact in optimization based design and control. We give a brief review of what is known about approximation schemes for the infinite dimensional LQR control problem and present new results that relate mesh independence to dual convergence and the preservation of control system properties under approximation. Finally, we provide applications and numerical examples to illustrate these ideas.





Suncica Canic, University of Houston

Fluid-Structure Interaction in Blood Flow

We will focus on a fluid-structure interaction problem arising in modeling blood flow through compliant (elastic/viscoelastic) arteries. The model is based on the viscous incompressible Navier-Stokes equations modeling blood flow in medium-to-large arteries, coupled with the elastic/viscoelastic Koiter shell equations modeling the dynamics of arterial walls. The resulting problem is of hyperbolic-parabolic type coupling wave propagation in arterial walls with the flow of a viscoelastic incompressible (Newtonian) fluid. Due to the hyperbolic nature of arterial wave propagation and due to the fact that the density of arterial walls is close to the density of the fluid, this fluid-structure interaction problem suffers from various difficulties associated with the lack of smoothing in the iteration procedures typically employed in the theoretical and numerical solution methods. To understand the main underlying difficulties, and to provide a model that can be efficiently solved numerically using one-dimensional methods, we derived a two-dimensional ("almost" one-dimensional) effective model obtained from the three-dimensional, axially symmetric problem by using homogenization theory for porous media flows. The resulting, effective model, is of Biot-type with memory. It captures the main features of blood flow in elastic/viscoelastic arteries. A comparison between the numerical simulations of the effective equations and the experimental measurements performed at the Texas Heart Institute in Houston showed excellent agreement. In particular, the viscoelastic arterial wall model captured well the hysteresis behavior of human and canine arteries. We will discuss the existence of a solution to the effective free-boundary problem and the difficult challenges and new insights that it brings towards the understanding of the fluid-structure interaction in blood flow. Collaborators include: A. Mikelic (University of Lyon 1, FR), J. Tambaca, University of Zagreb, Croatia, G. Guidoboni, UH, Dr. Z Krajcer, Texas Heart Institute, Dr. C. Hartley, Baylor College of Medicine, and Dr. D. Rosenstrauch, Texas Heart Institute.



M. Gregory Forest, UNC at Chapel Hill

Nano-rod composite films: flows and effective properties

There is a technological interest in composite films with nano-rod and nano-platelet inclusions at small volume fractions. Unlike fiber processes, shear-dominated film flow in confined spaces does not yet yield robust, predictable, controllable nano-composite film properties; indeed, there are almost no property characterizations. We present benchmark numerical predictions of complex orientational distributions of the rod ensemble. We start with assumed homogeneity in space, with the flow imposed as simple linear flow, then move to 1-d and 2-d spatial morphology with solvers of the coupled Smoluchowski equation for the rod ensemble and Navier-Stokes equations for the flow feedback. We then map those results onto effective property tensors of the nano-composite film, based on homogenized volume averaging. Next, we study percolation and cluster statistics of the flow-processed rod ensembles; percolation occurs at remarkably low volume fractions due to high aspect ratio of the inclusions. These results call into question all property characterization methods that ignore contacts and percolating paths of the inclusions. Time permitting, we raise the challenge of controlling properties. This is joint work with Xiaoyu Zheng¹, Qi Wang² and Ruhai Zhou³.

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Matthias Heinkenschloss, Rice University

SQP algorithms with inexact linear system solvers for the solution of PDE constrained optimization problems

Sequential quadratic programming (SQP) algorithms are the state-of-the-art for the solution of large-scale nonlinear programming problems. These methods have also been used for the solution of several PDE constrained optimization problems. However, for these problems, the rigorous application of SQP algorithms poses several challenges. One set of challenges arises from the need to solve the large-scale linear systems that arise inside SQP algorithms and which involve linearized PDEs iteratively. In this case, one has to design implementable stopping criteria that ensure convergence of the SQP method while avoiding "over-solving" of the linear systems, one has to devise new ways of rigorously handling negative curvature, and one has to design effective preconditioners for the solution of so-called KKT systems. I will describe our approach to overcome these challenges, outline our SQP algorithm with inexact linear system solvers that is backed by rigorous convergence theory, and illustrate its performance on several PDE constrained optimization problems.



Thomas J.R. Hughes, ICES UT Austin

Designing the PDE Algorithms of the Future: An Example of the Role of Optimization in Variational Multiscale Analysis

This talk is based on joint work with Giancarlo Sangalli. Optimization has played a significant role in at least one area of algorithm development, specifically, the integration of constitutive equations for inelastic materials. It is fair to say that ideas of convex optimization completely revolutionized this application during the last two decades and are now almost universally employed. But this application involves ODEs. In this talk we introduce ideas of optimization to constrain the fine-scale field in the variational multiscale analysis of PDEs. This approach enables us to derive an explicit formula for the fine-scale Green's function, a fundamental but heretofore elusive object in variational multiscale analysis. The formula is expressed in terms of the classical Green's function and a projector, derived from the optimality criterion, that uniquely defines the decomposition of the solution into coarse and fine scales. The theory is presented in an abstract operator format and subsequently specialized for the advection-diffusion equation. It is shown that different projectors lead to fine-scale Green's functions with very different properties. For example, in the advection-dominated case, the projector induced by the H^1 -seminorm yields a fine-scale Green's function that is highly attenuated and localized. These are very desirable properties in a multiscale method, and ones that are not shared by the L^2 -projector. By design, the coarse-scale solution attains optimality in the norm associated with the projector. This property, combined with a localized fine-scale Green's function, indicates the realizability of effective methods with local character for dominantly hyperbolic problems. The approach leads to a new class of stabilized methods, and the relationship between H^1 -optimality and SUPG is elucidated. It is suggested that appropriate optimality criteria may provide a rational pathway for deriving new and more effective algorithms for PDEs and may eventually replace ad hoc constructs currently in use.

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T.J.R. Hughes, G.R. Feijoo, L. Mazzei, and J.B. Quincy, "The variational multiscale method - a paradigm for computational mechanics," *Computer Methods in Applied Mechanics and Engineering*, 166 (1998), 3-24.

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J.C. Simo and T.J.R. Hughes, *Computational Inelasticity*, Springer, New York, 1998.



Angela Kunoth, University of Bonn, Germany

Speed Windsurfing: Modeling and Numerics

Many windsurfers want to achieve enough speed for planing, a certain state of gliding over the water surface which depends, in addition to a strong enough wind, on the size of the board and its fin and of the size of the sail. We assume that the surfer has an optimal technique to reach the maximal speed and that his/her weight uniquely determines the strength with which he/she is able to hold the sail by means of the boom with hands and/or a harness. Moreover, any experienced windsurfer knows which board to pick to balance between sufficient stability and speed. The current world record of 48.7 kn (90.2 km/h) was achieved on April 10, 2005, in the 'French Trench' near St. Maries de la Mer (France) where a certain natural tunnel generates very high wind speeds and which is too narrow for the sea to produce any waves, with a board of size 220 cm (64 ltr) with a 28 cm fin and a 10 m² sail; the weight of the surfer was 117 kg [2]. My talk is concerned with modeling the movement of the windsurfer and determining over a finite number of given sails of prescribed shape the optimal sail by which he can reach maximal velocity. Naively, one thinks that the maximal speed occurs by picking the sail with largest area of attack for the wind that, however, opposes the requirement that the surfer needs to be able to still hold the sail. Too large a sail for his weight will force him to fall into the water. In that situation, picking too large a sail may present an additional problem: in case of a sea level too deep for him to stand, he would have to use a water start which is very energy-consuming and, already after a few unsuccessful attempts, a dangerous enterprise, in particular, in case of offshore wind with high wind speed and large waves, which, in turn, often do not allow for a beginner-type basic start. Summarizing, it is of vital importance for the practical surfer to pick the sail of the right size that allows him both for planning and, simultaneously, is safe enough for him to use even in case of offshore wind. Thus, we consider the following problem: Given a finite number of sails of different sizes with prescribed shapes, given the speed of the wind, the weight of a surfer, the size and shape of a surfboard and a corresponding fin; determine the sail and the direction such that the windsurfer achieves maximal speed. Here not only want to solve this problem with sufficient accuracy – in view of this particular application, we wish to provide the solution by developing a program which runs on a common laptop computer at a beach station in an amount of time which is less than five minutes, an estimated time that an experienced surfer needs to switch the sail twice. We develop a simple model for describing the movement of the windsurfer for maximizing the speed in terms of a nonlinear ODE. I would like to present a number of numerical results from [1] and would like to conclude with some remarks on the validation of our model compared with the world record data and on improving the simple model.

References

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- [2] The Professional Windsurfers Association:
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Rich Lehoucq, Sandia National Laboratories

On stabilized finite element methods for the Stokes problem in the small time-step limit

Recent studies indicate that consistently stabilized methods for unsteady incompressible flows, obtained by a method of lines approach, may experience difficulty when the time step is small relative to the spatial grid size. Using as a model problem the unsteady Stokes equations, we show that the semi-discrete pressure operator associated with such methods is not uniformly coercive. We prove that for sufficiently large (relative to the square of the spatial grid size) time steps, implicit time discretizations contribute terms that stabilize this operator. However, we also prove that if the time step is sufficiently small, then the fully discrete problem necessarily leads to unstable pressure approximations. The semi-discrete pressure operator studied in the paper also arises in pressure projection methods, thereby making our results potentially useful in other settings. This is joint work with Pavel Bochev and Max Gunzburger.

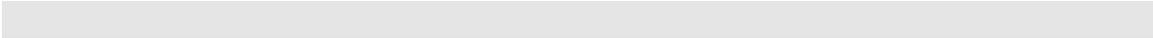


Tom Manteuffel, University of Colorado, Boulder

Optimizing solution strategies for systems of PDEs

In any computation, the bottom line should be accuracy per computational cost. In this talk a Nested Iteration-Newton-FOSLS-AMG method is presented that yields approximate solutions to nonlinear systems of PDEs with any desired accuracy in several dozen work units. A work unit is the amount of computation required to evaluate the nonlinear equation on the finest grid. We consider incompressible Navier/Stokes, geometrically nonlinear elasticity, and coupled fluid/structure problems as test problems.

In addition, a local adaptive mesh strategy will be presented that attempts to optimize efficiency. In this context, efficiency is defined to be accuracy per computational cost, or, equivalently, work times error. This approach starts on a coarse mesh and chooses refinement based on a FOSLS a posteriori error measure to optimize efficiency. After several levels of refinement, the error is nearly equi-distributed across elements. Subsequent refinements are essentially global, which minimizes load balancing on the finest grids.



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John Shadid, Sandia National Laboratories

Efficient Fully-coupled Solution of Transport/Reaction Systems with Newton-Krylov Methods*

The need to simulate fluid flow systems with thermal energy and mass species transport, along with non-equilibrium chemical reaction is common in advanced technology applications. These systems are strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a very large range of length and time scales. These characteristics make the scalable, robust, accurate, and efficient computational solution of these systems extremely challenging.

This presentation will overview a number of the important solution methods that our research group has applied in the computational simulation of transport/reaction systems. These include, fully-implicit time integration, direct-to-steady-state solution methods, continuation, bifurcation, and optimization techniques. The resulting large sparse linear systems that are generated by these methods are solved by the application of parallel preconditioned Krylov methods employing additive Schwarz domain decomposition (DD) and multi-level preconditioners. The multi-level preconditioners include geometric and algebraic methods along with approximate block factorization preconditioners.

To demonstrate the capability of these methods I will present simulation results for representative low heat release and high heat release transport / reaction simulations. In this context I will discuss robustness, efficiency, and the parallel and algorithmic scaling of solution methods.

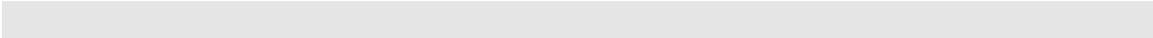
*This work was partially funded by the Department of Energy's Mathematical, Information and Computational Sciences Division, and was carried out at Sandia National Laboratories operated for the U.S. Department of Energy under contract no. DE-ACO4-94AL85000



Mikhail Shashkov, Los Alamos National Laboratory

Mimetic Finite Difference Methods for Partial Differential Equations and Discrete Vector and Tensor Analysis

In past 15 years we have developed new high-quality, mimetic finite-difference methods based on discrete analog of vector and tensor analysis (DVTA). The basis of DVTA is the design of discrete operators that preserve certain essential properties of, and relationships between, the corresponding analytic operators. The DVTA is the basis for new techniques for large-scale numerical simulations approximating the solution of partial differential equations (PDEs). The new methods provide a significant extension of the well known and useful finite volume methods and are designed to more faithfully represent important properties of physical processes and the continuum mathematical models of such processes. Algorithms based on these techniques are used for modeling high-speed flows, porous media flows, diffusion processes, and electromagnetic problems. In this presentation we will describe DVTA and demonstrate how it can be used to construct high-quality finite-difference methods for PDEs.





Ralph C. Smith, NC State University

Model Development, Numerical Approximation and Control Design for High Performance Nonlinear Smart Material Systems

High performance transducers utilizing piezoceramic, electrostrictive, magnetostrictive or shape memory elements offer novel control capabilities in applications ranging from flow control to precision placement for nanoconstruction. To achieve the full potential of these materials, however, models, numerical methods and control designs that accommodate the constitutive nonlinearities and hysteresis inherent to the compounds must be employed. Furthermore, it is advantageous to consider material characterization, model development, numerical approximation, and control design in concert to fully exploit the novel sensor and actuator capabilities of these materials in coupled systems.

In this presentation, the speaker will discuss recent advances in the development of model-based control strategies for high performance smart material systems. The presentation will focus on the development of unified nonlinear hysteresis models, nonlinear distributed system models, inverse compensators, reduced-order approximation techniques, and nonlinear control strategies for high precision or high drive regimes. Significant attention will be focused on the discussion of numerical techniques and control designs that facilitate real-time implementation of smart material actuators and sensors operating in highly nonlinear regimes. Examples will be drawn from problems arising in structural acoustics, high-speed milling, deformable mirror design, artificial muscle development, tendon design to minimize earthquake damage, and atomic force microscopy.



Tim Trucano, Sandia National Laboratories

Key Principles and Objectives of V&V: A Sandia ASC Perspective

In this talk I will review the key principles and objectives of computational science verification and validation (V&V) from the perspective of the Sandia ASC (NNSA Advanced Simulation and Computing) V&V program. I will quickly summarize core concepts associated with V&V. Then, I will highlight some technical themes that are specific to verification, that is a rigorous numerical accuracy assessment, and to validation, that is rigorous physical accuracy assessment. For example, a critical technical theme in verification, at least for numerical partial differential equation solutions, is convergence. A critical technical theme for validation is uncertainty quantification. I will suggest how the technical themes come together in the arena of computational credibility for consequential application of computational science, especially in the relationship to complex decision-making. My main goal for this talk is to emphasize the degree to which V&V is an important and ongoing challenge for computational science.

A keynote presentation that will take place during the conference dinner on Friday, April 21, 2006.