Johann Radon Institute
for Computational and Applied Mathematics
Austrian Academy of Sciences

Workshop
Control of Complex Fluids

October 10–13, 2005

Schedule of Talks

	Monday	**Tuesday**	**Wednesday**	**Thursday**
9:45–10:00	**Opening**			
10:00–11:00	M. Behr	A. Meir	O. Ghattas	T. Bewley
11:00–11:15	**Coffee Break**			
11:15–12:15	M. Berggren	R. Griesse	M. Heinkenschloss	V. Heuveline
12:15–13:30	**Lunch Break**			
13:30–14:30	G. Haller	N. Zabaras	V. Schulz	
14:30–14:45	**Coffee Break**			
14:45–15:45	B. Vexler	M. Braack	N. Gauger	

		17:15 (HF 9901) J. Bramble	17:00 (HS 9) R. Bulirsch	
			18:30 (Kepler's) **Conference Dinner**	

During the week of the workshop, additional talks will be offered by

- James Bramble: Analysis of a finite PML approximation for the three dimensional time-harmonic maxwell and acoustic scattering problems
- Roland Bulirsch: Keplers Spuren in unseren Tagen

List of Abstracts

Marek Behr

Complex Fluids and Biomedical Device Design

Modeling and computational analysis play an increasingly-important role in bioengineering, particularly in the design of ventricular assist devices. Numerical simulation of flow in blood pumps has the potential to shorten the design cycle and give the designers important insights into causes of blood damage and suboptimal performance.

A set of modeling techniques will be presented which are based on stabilized space-time finite element formulation of the Navier-Stokes equations, with a shear-slip mesh update used to accommodate the movement of the impeller with respect to a non-axisymmetric housing. The computed global flow characteristics (performance curves) are compared with experimentally-measured data.

This application presents a ripe target for shape optimization and optimal control. In order to assess the influence of the fluid constitutive model on the outcome of shape optimization tasks, a comparison of model problem computations based on the Navier-Stokes equations on one hand, and on a more accurate shear-thinning modified Cross model on the other, will be presented.

More complex description of blood behavior takes into account viscoelastic phenomena, in particular via an Oldroyd-B constitutive model. Recent developments in stabilized methods of GLS-type for simulation of Oldroyd-B flows using low-order extra-stress interpolations will be outlined.

Finally, in order to obtain quantitative hemolysis prediction, cumulative tensor-based measures of strain experienced by individual blood cells are being developed and correlated with available blood damage data. In the first approximation, red blood cells under shear are modeled as deforming droplets, and their deformation is tracked along pathlines of the computed flow field.

Martin Berggren

A Unified Discrete-Continuous Sensitivity Analysis Method for Shape Optimization

A crucial step when attacking shape optimization problems using gradient-based methods is the sensitivity analysis, that is, the computation of gradients of objective functions or constraints with respect to the design variables. Completely different strategies are often used for the sensitivity analysis of the original system of PDE:s compared to the analysis of the discretized equations. It can even be hard to see any resemblance at all between the "continuous" and "discrete" case. One major difference and complication is the presence of a deforming mesh in the discrete case.

In this talk, I will present an approach that unifies the "continuous" and "discrete" sensitivity analysis by a systematic use of so-called material derivatives. For equations given in variational form, the derivation proceeds in a general case and produces a variational expression for the gradient that holds both for the original and discretized equation. Under regularity assumptions on the state and adjoint states that are made explicit using this approach, the variational gradient expression reduces to the boundary expression that is well known for the "continuous" case. In essence, the relation between the "continuous" and "discrete" gradient expressions are the same as the relation between a strong and weak solution of an elliptic partial differntial equation. This unified approach should make it easier to perform error estimates of the discrete gradient expression and to analyze the effects of different kinds of mesh deformations.

Thomas Bewley

to be announced

Malte Braack

On Primal-Dual Consistent Finite Element Stabilization Methods for Optimal Control Problems in Fluids

In optimal control problems an adjoint problem has to be solved numerically. This dual problem has to be discretized in a stable way. Hence, there are two possibilities:

(i) Building the adjoint out of the discretized stabilized primal problem

(ii) Building the adjoint out of the continuous primal problem and then stabilize it.

These two possibilities are not equal in general. Possibility (ii) has the drawback, that the adjoint problem is in general not consistent with the optimization problem, because the gradient is perturbed. In contrast, possibility (i) is consistent, but not necessarily stable.

This is exactly the situation for the classical residual based stabilization techniques in finite elements, e.g., PSPG [2] and SUPG [3]. Nevertheless, they are widely used for the Navier-Stokes equations.

However, a symmetric stabilization cures this problem, because the possibilities (i) and (ii) become equal. In this talk, we address this topic and present a symmetric stabilization, see [1], especially suitable for optimization problems in fluids.

References:

[1] M. Braack and E. Burman, "Local projection stabilization for the Oseen problem and its interpretation as a variational multiscale method," *SIAM J. Numer. Anal.*, to appear 2005.

[2] T. Hughes, L. Franca, and M. Balestra. A new finite element formulation for computational fluid dynamics: V. circumvent the Babuska-Brezzi condition: A stable Petrov-Galerkin formulation for the Stokes problem accommodating equal order interpolation. *Comput. Methods Appl. Mech. Engrg.*, 59:89–99, 1986.

[3] C. Johnson. *Numerical Solution of Partial Differential Equations by the Finite Element Method.* Cambridge University Press, Cambridge, UK, 1987.

Nicolas Gauger

Aerodynamic Shape Pptimization Using Continuous and Discrete Adjoint Flow Solvers

The detailed aerodynamic design distinguishes itself by being both dependant on a large number of design variables as well as the complex numerical modelling of the flow. One should use the compressible Reynolds-averaged Navier-Stokes Equations as control equations in conjunction with adequate models for transition and turbulence. As the resulting CFD computation time for complex geometries with high Reynolds numbers is very high, deterministic optimization strategies that use so-called adjoint methods for computing the sensitivities are needed. That is why the DLR in Braunschweig has been developing and testing continuous and discrete adjoint flow solvers. Furthermore, the development of an even more efficient one-shot or piggy-back method based on adjoint flow solvers has begun recently in cooperation with the University of Trier and the Humbold University Berlin. The talk illustrates the development of the different adjoint solvers, their extension to multi-disciplinary design and the necessary modifications for use in aerodynamic one-shot optimizations.

Omar Ghattas

Towards Real-Time Identification and Prediction of Airborne Contaminant Transport

We are interested in the localization of airborne contaminant releases in regional atmospheric transport models from sparse observations, in time scales short enough for predictions to be useful for hazard assessment, mitigation, and evacuation procedures. In particular, our goal is rapid reconstruction — via solution of an inverse problem — of the unknown initial concentration of the airborne contaminant in a scalar convection-diffusion transport model, from limited-time spatially-discrete measurements of the contaminant concentration, and from a velocity field as predicted, for example, by a mesoscopic weather model. We employ special-purpose parallel multigrid algorithms that exploit the spectral structure of the inverse operator. Experiments on problems of localizing airborne contaminant release from sparse observations in a regional atmospheric transport model demonstrate that 17-million-parameter inversion can be effected at a cost of just 18 forward simulations with high parallel efficiency. On 1024 Alphaserver EV68 processors, the turnaround time is just 29 minutes. Moreover, inverse problems with 135 million parameters — corresponding to 139 billion total space-time unknowns — are solved in less than 5 hours on the same number of processors. These results suggest that ultra-high resolution data-driven inversion can be carried out sufficiently rapidly for simulation-based "real-time" hazard assessment. We conclude with a discussion of challenges for airborne contaminant identification, including uncertainty quantification and propagation, integration with complex weather models and urban region models, and sensor steering.

This work is joint with Volkan Akcelik (CMU); George Biros (Penn); Andrei Draganescu, Judy Hill, and Bart van Bloemen Waanders (Sandia); and Karen Willcox (MIT).

Roland Griesse

Modeling and Optimal Control in Instationary Magnetohydrodynamics

Magnetohydrodynamics, or MHD, deals with the mutual interaction of electrically conducting fluids and magnetic fields. The nature of the coupling between fluid motion and the electromagnetic quantities arises from the following three phenomena:

1. The relative movements of a conducting fluid and a magnetic field induce an electromotive force (Faraday's law) to the effect that an electric current develops in the fluid.
2. This current in turn induces a magnetic field (Ampère's law).
3. The magnetic field interacts with the current in the fluid and exerts a Lorentz force in the fluid.

It is the third feature in the nature of MHD which renders it so phenomenally attractive for exploitation especially in metallurgical processes. The Lorentz force offers a unique possibility of generating a volume force in the fluid and hence to control its motion in a contactless fashion and without any mechanical interference.

The talk addresses modeling issues of the instationary MHD problem with thermal coupling, and the formulation, analyis and numerical solution of associated optimal control problems.

George Haller

Nonlinear Dynamics and Control of Aerodynamic Separation

Flow separation (the detachment of fluid from a no-slip boundary) is a major cause of performance loss in engineering devices, including diffusers, airfoils and jet engines. In a landmark 1904 paper on boundary layers, L. Prandtl derived a criterion for flow separation in steady two-dimensional incompressible flows. Despite widespread effort, no generally applicable extension of this result has emerged for unsteady flows or even three-dimensional steady flows.

In this talk, I describe an analytic criterion that predicts the location of flow separation in two-dimensional unsteady fluid flows. I show numerical and experimental results confirming the above criterion, as well as applications of the new separation criterion to flow control. I also describe recent three-dimensional extensions.

Matthias Heinkenschloss

Domain Decomposition Methods For Flow Control

Domain Decomposition Methods (DDMs) are routinely used for the parallel solution of systems of partial differential equations (PDEs) and, more recently, they have been successfully applied to PDE constrained optimization problems. In the latter context, DDMs introduce the parallelism at the optimization level, but also offer opportunities for storage management and subdomain model reduction. In this talk we discuss DDMs for optimal flow control and demonstrate how some existing optimization approaches can be reinterpreted in the DD context.

Vincent Heuveline

to be announced

Amnon Meir

Advances in MHD Flow Simulation

MHD (magnetohydrodynamic) flows are of importance in connection with many engineering applications, specifically in metallurgy and materials processing. In the viscous incompressible regime these complex flows are governed by the Navier-Stokes equations (in the fluid region) and Maxwell's equations (in all of space), coupled via Ohm's law and the Lorentz force. Using the Biot-Savart law, we are able to reduce the problem to a system of integro-differential equations in the fluid region, derive a mixed variational formulation and treat flows with non-ideal boundary conditions.

In this talk I will give a brief introduction to viscous incompressible magnetohydrodynamics, highlight some novel applications, and describe some new results for the finite-element simulation of MHD flows. I will also hint to how externally applied magnetic fields, electric currents and fields, or variations in the boundary's electrical properties can be used to stir, to dampen the motion of, and to control the motion of, the fluid.

Volker Schulz

New One-Shot Approaches for Aerodynamic Optimization

Aerodynamic flow simulation is an integral part in current design of parts of commercial aircrafts. The next step, computer aided optimization, is so far limited by the fact that the use of standard optimization tools raises the computational effort by orders of magnitudes. In this paper, we suggest new one-shot approach as a potential remedy. Special emphasis is laid on recent 3D results and results with additional aerodynamic constraints.

Boris Vexler

Optimal Vortex Reduction for Instationary Flows

We consider the problem of an appropriate choice of a cost functional for vortex reduction for unsteady flows described by the Navier-Stokes equations. This choice is directly related to a physically correct definition of a vortex. Therefore, we discuss different possibilities for the cost functional and analyze the resulting optimal control problem. Moreover, we present an efficient numerical realization of this concept based on space time finite element discretization and demonstrate its behavior on some numerical experiments.

Nicolas Zabaras

Mathematical and Computational Aspects of the Control of Solidification and Crystal Growth Processes

Solidification and crystal growth processes involve the interaction of a variety of physical phenomena at different length scales. Due to the required large scale, high resolution simulations for solidification modeling, solidification control provides a number of mathematical and computational challenges.

We will review our recent work on the control of solidification processes of various materials (particularly semiconductors) using an externally imposed magnetic field. The ability to achieve a homogeneous distribution of the solute and a flat freezing interface are usually the main objectives in the control of such solidification processes. The control of the fluid flow in the melt has been shown to have a direct impact on the above two objectives. We focus on the design of a tailored magnetic field (both spatially and temporally varying) that controls the fluid flow in the melt. The design problem is posed as an infinite-dimensional optimization problem. The solution to this problem is achieved through the solution of direct, sensitivity and adjoint partial differential equations. The computational parallel framework needed to address such problems will be discussed.

In addition, we will address a number of mathematical challenges required for: (i) multi-scale solidification control e.g. control of dendritic morphology using macro design variables (e.g. combination of optimal furnace conditions and optimal external magnetic field), (ii) real time control of solidification processes (model reduction for multi-physics multi-scale processes, role of uncertainty, etc.) and (iii) control of protein crystallization processes.